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Foreword

It gives us great pleasure to welcome all participants to the 23rd IFIP TC7 Conference on System Modeling and Optimization. We hope that it will provide a platform for interchanging ideas, research results and experiences for an international community, actively interested in modeling and optimization.

The conference has been organized by two institutions: the 7th Technical Committee "System Modeling and Optimization" of the International Federation for Information Processing, and by the AGH University of Science and Technology in Cracow.

We are indebted to the organizers of invited sessions, and to the members of the Program Committee who refereed regular contributions. We would like to acknowledge the initiative and guidance of Irena Lasiecka and Kazimierz Malanowski.

The success of the conference is largely dependent on the support from the AGH University of Science and Technology, the Faculty of Electrical Engineering, Automatics, Computer Science and Electronics, and the Chair of Automatics.

An event such as this would not be possible but for the professional help of many persons. We owe sincere thanks to them all, and in particular to Anna Sury whose help in all organizational matters was invaluable.

We wish you a nice stay in Cracow and fruitful proceedings.

Wojciech Mitkowski Adam Korytowski Maciej Szymkat

Cracow, July 2007

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PERFORMANCE-BASED DESIGN AS A DECISION STRATEGY FOR RISK REDUCTION

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Keywords: Performance-based design; seismic risk; aeolian (wind) risk; composite steel-concrete constructions; pedestrian comfort.

1. INTRODUCTION

It is now generally accepted that several types of "risks" can be recognized for built facilities and environments: they are not limited to collapses and heavy damages but involve comfort and way of life (cf. e.g. Augusti *et al.*, 2003).
The most rational way of tackling such risks and their reduction is Performance-based Design PBD (or, better, Performance-based Engineering).
This lecture will present and discuss briefly the general approach to PBD, and illustrate some examples of application.

2. PERFORMANCE BASED DESIGN: GENERALITIES

By definition, "Performance-Based Design" (PBD) requires the satisfaction of the relevant performance requirements with a sufficiently high probability throughout the lifetime of an engineering system.
Indeed, design is always addressed to fulfil one or more performance objectives, but while up to a few years ago this aim was pursued on the basis of engineering experience and practice, PBD is a design philosophy specifically constructed in order to reach rationally and with a given reliability the chosen objectives.
In this context, the "risk" is usually expressed in terms of the mean annual frequencies of exceeding relevant limit states (LS). These mean annual frequencies can be calculated by combining the site-specific hazard (in turn, measured by the mean annual frequency that the "action" exceeds a given intensity level) with information on the "exposure" (i.e. the probability that the action finds facilities to damage) and the "fragility" of the facility (the conditional probability of exceeding a limit state for a given intensity of the action).
Such "complete" approach to risk evaluation (and consequent reduction) is however very complicated: on the one side the possible combined effects of several actions (earthquakes, wind, voluntary and/or accidental human actions...) should be considered, with an enormous increase of statistics and mathematics; on the other side a number of non-technical questions rise, including comparisons and choices between incommensurable quantities such as casualties, economic losses, quality of life...
These questions will be hinted in the lecture, but the main part will follow the most usual "technical" approach, i.e. focus on one facility subject to a specific action, and calculate its risk neglecting the question of "exposure"; two examples, dealing with to two different types of actions, will be presented.

3. PERFORMANCE BASED DESIGN: APPLICATIONS

Under the above limitations the risk of a structure, identified with the mean annual frequency $\lambda(LS)$ of exceeding a specified limit state, can be assessed by a convolution of two variables: the damage measure *(DM)*, an appropriate measure of the structural damage; and intensity measure

(IM), representing the characteristics of the action at the site, and is usually expressed by a measure of the ground motion intensity.
The total probability theorem allows to evaluate $\lambda(LS)$ by the double integral, Eq.(1):

$$\lambda(LS) = \iint G[LS \mid DM] \cdot dG[DM \mid IM] \cdot d\lambda(IM)$$

where: $G[LS|DM]$ is the conditional probability of exceeding the *LS* given *DM* (describing the failure or loss); $G[DM|IM]$ is the conditional probability of exceeding *DM* given *IM* (derived by structural analysis, and describing the demand prediction for a given *IM*); $\lambda(IM)$, also known as the hazard curve, is the mean annual frequency of occurrence of the action with an intensity higher than *IM* at the specific site (given by the hazard analysis).
The choice of *IM* in Eq.(1) must be based on the requirements of sufficiency, efficiency, and hazard computability (Giovenale *et al.*, 2003).
A sufficient *IM* yields *DM* conditionally independent, given *IM*, on other quantities that may affect the action; thus, it (i) permits an unbiased evaluation of $\lambda(LS)$ by Eq.(1), (ii) simplifies the choice of the records to be used in nonlinear dynamic analyses (to take into account the record-to-record variability), (iii) legitimizes the operation of scaling the action input diagrams,, and (iv) allows decoupling hazard and structural analysis.
An *IM* is (relatively) "more efficient" if it results in a "smaller" variability in the structural response for any given intensity. The variability is expressed by the dispersion in *DM* for any given value of *IM*. Since $G[DM|IM]$ in Eq.(1) can be estimated by running nonlinear dynamic analyses, using a "more efficient" *IM* reduce the number of runs that are needed to estimate $\lambda(LS)$ with the same confidence level. The dispersion in the structural response given *IM* will be assumed as a quantitative measure of the efficiency of that *IM*.
Hazard computability of an *IM* is related to the effort required by the assessment of the hazard curve, $\lambda(IM)$.
Anyway, it is evident that sufficiency is an essential property of an *IM*, and non-compliance with it may result in discarding that *IM*. Once the sufficiency of a candidate *IM*'s is established, efficiency and hazard computability are two relative criteria that can be used to favour that candidate *IM* over the others.
This procedure has been followed in great rigour in Augusti & Ciampoli, 2007, to evaluate the seismic risk of composite steel-concrete: particular attention has been devoted to an appropriate choice of the "best" intensity measure among several "candidates". This paper and its results will be illustrated in the lecture and summarized in the final text.
Sibilio and Ciampoli (2007) have tackled another action and another risk: namely, the discomfort of pedestrians on a bridge that oscillates due to wind actions.
The examined footbridge is an actual structure whose aeroelastic characteristics are known. The relevant "limit state" is identified with a threshold value of the wind-induced oscillations, in accord with the ISO 2631 standard, taking into account the suggested user perception and acceptance criteria. The buffeting and vortex shedding effects on the footbridge deck have been investigated through a 3D finite element non linear analysis in time domain, and the reliability has been assessed by two numerical simulation techniques, i.e. Monte Carlo and Subset. Also these results will be illustrated in the lecture and summarized in the final text.

4. CONCLUSIONS

The general discussion and the example presented demonstrate that Performance-Based Engineering (or Performance-Based Design, PBD, as it is more usually called), although still in its infancy, can already be a powerful tool to estimate rationally, and consequently reduce, risk of built facilities.
Much remains to be done in this direction, e.g. to estimate risks of environments under real-world combination of actions. These problems are much too often tackled in an emotional way: a scientific approach and an appropriate modelling can help decision-makers to tackle them in a rational way.

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MATHEMATICAL PROGRAMS WITH EQUILIBRIUM CONSTRAINTS: A REVIEW

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A mathematical program with equilibrium constraints (MPEC) is an optimisation problem that includes variables, which satisfy an optimality or equilibrium condition, typically modelled via a parametric variational inequality or complementarity problem. We will present an overview of the state-of-the art in equilibrium-constrained programming, focussing on local optimisation of MPECs with nonlinear data functions. The talk will cover illustrative applications, optimality conditions, and will give an overview of numerical approaches.

SHAPE TUBE METRIC, GEODESIC EQUATION

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Keywords: Shape metric, geodesic, Euler equation, level set

1. MOVING DOMAIN

The Courant metric in shape analysis (16) is extended here to classes of non smooth subsets in D. The intrinsic tube analysis which is evoked here is developped in (25), (24). The characteristic function of Q is $\zeta \in L^\infty(I \times D)$ verifying $\zeta = \zeta^2$ and $\zeta(t) = \chi_{\Omega_t}$ where the measurable set Ω_t is defined in D up to a zero measure subset. That theory can be extended to boundaries with the approach of (2). In the second part we adopt the eulerian modeling (5; 16; 8; 11) which has been extended to non smooth vector fields in (17; 25; 24; 8)... Making use of the transverse field approach (8; 4; 18) we derive the euler equation for the geodesic-tube which has been presented in several image anlysis conferences ("Shape Space" IMA , march 06, MIA06 Paris, Obergurgl ...) with application developed with L. Blanchard (26). The technic is inspired from (7). Following (17), (23), we consider tubes which are continuous with respect to the the $L^1(D)$ topology and with time integrable perimeter, then we introduce the set of characteristic functions

$$\mathcal{P}_D = \{\ \Omega \subset D,\ \chi_\Omega \in BV(D)\ \}$$

and with

$$\mathcal{H}^c = C^0([0,\,1], L^1(D, \{0,1\})) \cap L^1(\,0,\,1, BV(D)\,)$$

Associated with any subset $\Omega_0 \in \mathcal{P}_D$, the family

$$\mathcal{O}_{\Omega_0} = \{\ \Omega \in \mathcal{P}_D\ s.t.$$

$$\exists \zeta \in \mathcal{H}^c,\ s.t.,\quad \zeta(0) = \chi_{\Omega_0},\ \zeta(1) = \chi_\Omega\quad \}$$

Associated with any two sets $\Omega_i \in \mathcal{O}_{\Omega_0}$, the non empty set of connecting tubes is :

$$T(\Omega_1, \Omega_2) = \{\zeta \in \mathcal{H}^c,\ \zeta(0) = \chi_{\Omega_1},$$

$$\zeta(1) = \chi_{\Omega_2}\ \}$$

The set of jump lines of $\zeta(t) \in BV(D)$ is denoted by Γ_t. we consider the $N+1$ dimensional perimeter

$$P_{I\times D}(Q) = ||\nabla_{t,x}\zeta||_{M^1(I\times D)}$$

$$= \int_0^1 \int_{\Gamma_t} \sqrt{1+v^2}\, d\Gamma_t\ dt\ \le \int_0^1 P_D(\Omega_t)\, dt$$

$$+ \int_0^1 \int_{\Gamma_t} |v(t)|\, d\Gamma_t\, dt\ \ \text{(in smooth case)}$$

Consider also the fact that

$$< \frac{\partial}{\partial t}\zeta,\ g\ >_{\mathcal{M}(I\times D)\times C^0_{comp}(I\times D)}$$

$$= \int_0^1 \int_{\Gamma_t} v\, g\, d\Gamma_t\, dt = \int_0^1 \int_{\Omega_t} div(g\, V\,) dx dt$$

As

$$\int_0^1 \int_{\Gamma_t} |v|\, d\Gamma_t\, dt\ =\ ||\frac{\partial}{\partial t}\zeta||_{M^1(I\times D)},$$

$$P_D(\Omega_t)\ =\ ||\nabla_x \zeta(t)||_{M^1(D,R^N)}$$

Then we have :

$$||\nabla_{t,x}\zeta||_{M^1(I\times D)} \le\ ||\frac{\partial}{\partial t}\zeta||_{M^1(I\times D)}$$

$$+ \int_0^1 ||\nabla_x \zeta(t)||_{M^1(D,R^N)}\ dt \qquad (1)$$

We shall consider the weak closure of such smooth tubes ζ and verify that the estimate 1 still hold true on the closure:

Proposition 1.1 *let ζ_n be a sequence of smooth tubes such that*

$$||\frac{\partial}{\partial t}\zeta_n||_{M^1(I\times D)}$$

$$+ \int_0^1 ||\nabla_x \zeta_n(t)||_{M^1(D,R^N)}\ dt \le M \qquad (2)$$

Then there exists a subsequence (still denoted ζ_n) and ζ such that $\zeta_n \to \zeta$ stongly in $L^1(I \times D)$ (so that $\zeta = \zeta^2$) and we have :

$$||\nabla_{t,x}\zeta||_{M^1(I\times D)} \leq lim\, inf\, ||\frac{\partial}{\partial t}\zeta_n||_{M^1(I\times D)} + \int_0^1 ||\nabla_x \zeta_n(t)||_{M^1(D,R^N)}\, dt \qquad (3)$$

Corollary 1.2 *Let $\zeta \in L^1(I, BV(D)) \cap W^{1,1}(I, M^1(D))$ then $\zeta \in C^0(I, L^1(D))$ and a.e. $t \in I$, $\zeta(t) = \chi_{\Omega_t}$ with $P_D(\Omega_t) < \infty$ and $t \to P_D(\Omega_t)$ is l.s.c.*

The weak closures $\mathcal{H}_p^{c,*}$ and $\mathcal{H}_\theta^{c,*}$ of $\mathcal{H}^k$:

$$\mathcal{H}_p^{c,*} = \{\zeta = \zeta^2 \in \mathcal{H}^c \cap \mathcal{H}^*,\ s.t.$$
$$, \exists \zeta_n \in \mathcal{H}^k,\ \zeta_n \to \zeta \text{ in } L^1(I\times D)\ ,$$
$$\nabla_{t,x}\zeta_n \to \nabla_{t,x}\zeta \text{ (weakly in)}\, M^1(I\times D),$$
$$\text{with } \frac{\partial}{\partial t}(\zeta_n - \zeta) \to 0 \ weakly\ in\ L^P(I, M^1(D))\ \}$$

$$\mathcal{H}_\theta^{c,*} = \{\zeta = \zeta^2 \in \mathcal{H}^c \cap \mathcal{H}^*,\ s.t.$$
$$\exists \zeta_n \in \mathcal{H}^k,\ \zeta_n \to \zeta \text{ in } L^1(I\times D)\ ,$$
$$\nabla_{t,x}\zeta_n \to \nabla_{t,x}\zeta \text{ (weakly in)}\, M^1(I\times D),$$
$$\text{with } a.e.t \in I,\ ||\frac{\partial}{\partial t}\zeta_n(t)||_{M^1(D)} \leq \theta(t)\ \}$$

2. A COMPLETE QUASI-METRIC SPACE

$$\mathcal{H}_p^{c,*} := \{\ \zeta \in \mathcal{H}^c \cap W^{1,1}(I, M^1(D)),\ \frac{\partial}{\partial t}\zeta \in L^p(I, M^1(D))\ \} \qquad (4)$$

when the moving boundary is smooth :

$$||\frac{\partial}{\partial t}\zeta||_{L^1(I,M^1(D,R^N))} = \int_0^1 ||v(t)||_{M^1(\partial\Omega_t)} dt$$

We consider the variationnal problem

$$\mathcal{T}_p^{c,*}(\Omega_1,\Omega_2) = \{\ \zeta \in \bar{\mathcal{T}}(\Omega_1,\Omega_2) \cap \mathcal{H}_p^{c,*}\ \} \quad (5)$$
$$= \{\, \zeta \in \mathcal{H}_p^{c,*}\, s.t.\ \zeta(0) = \chi_{\Omega_1},\ \zeta(1) = \chi_{\Omega_2}\ \}$$
$$j = Inf_{\{\zeta\in\mathcal{T}_p^{c,*}(\Omega_1,\Omega_2)\}}\ \{\ ||\frac{\partial}{\partial t}\zeta||_{L^1(I,M^1(D,R^N))} + ||p||_{L^1(I)}\ \} \qquad (6)$$

Proposition 2.1 *Let $p > 1$, there exists (at least one) tube ζ in $\mathcal{T}_p^{c,*}(\Omega_1,\Omega_2) \subset \mathcal{H}_p^{c,*}$ verifying the minimum in the variational problems 6*

The positive number j cannot be zero, $j > 0$, so that j fails to be a distance on the family $\mathcal{O}^*_{\Omega_0,p}$

$$= \{\Omega\, s.t. \exists\, \zeta \in \mathcal{H}_p^{c,*}, \chi_\Omega = \zeta(1), \zeta(0) = \chi_{\Omega_0}\}$$

Incorporate the perimeter integral as a constraint in the family:

for given $M > 0$ consider $\mathcal{O}^{*,P_M}_{\Omega_0,p}$

$$= \{\ \Omega \in \mathcal{O}^*_{\Omega_0,p}\ s.t.\ \chi_\Omega = \zeta(1),\ \zeta \in \mathcal{T}^{c,*}(\Omega_0,\Omega),\ \int_0^1 ||\nabla\zeta(t)||_{M^1(D)}\, dt \leq M\ \}$$

Notice that for two element $\Omega_i \in \mathcal{O}_p^{*,p_M}$ there exists connecting tubes verifying the perimeter constraint:

Lemma 2.2 *Let $\Omega_i \in \mathcal{O}^*_{\Omega_0,p},\ i = 1, 2$. Then the set $\bar{\mathcal{T}}(\Omega_1,\Omega_2) \cap \mathcal{O}^*_{\Omega_0,p}$ is non empty*

Theorem 2.3 *Let $M > ||\nabla\chi_{\Omega_0}||_{M^1(D,R^N)}$.Let $p = 1$, equipped with $\bar{\delta}$ the family $\mathcal{O}^{*,p_M} \subset \mathcal{P}_D$ is a metric space.*

Let $p > 1$, equipped with $\bar{\delta}$ the family $\mathcal{O}^{*,p_M} \subset \mathcal{P}_D$ is a complete quasi-metric space, in the sense that the triangle inequality is replaced by the following one :

$$\bar{\delta}_p(\Omega_1,\Omega_3) \leq 2^{p-1}\{\ \bar{\delta}_p(\Omega_1,\Omega_2) + \bar{\delta}_p(\Omega_2,\Omega_3)\ \} \qquad (7)$$

In a full paper (27) we discuss the possibility to introduce the *curvature* term p' in the metric .

3. FULLY EULERIAN METRIC SPACE

As soon as the speed vector field V verifies some BV properties ($V \in L^2(I, BV(D)^N)$) (24; 15), there is a unique tube associated to V, then we do have an application $V \to \zeta_V$ and with such regularity on V we can revisit the complete metric d being completely delivered of the non differential perimeter and curature terms that we were obliged to introduce in order to apply the compacity theorems. From the tube analysis we consider several interesting choices for the spacial regularity of the speed vector field (together with its divergence field). Let

$$\mathcal{E}^{1,1} = \{V \in L^1(I\times D, R^N),\ divV \in L^1(D), V.n_D,\ W^{-1.1}(\partial D\ \},$$

and let E be by closed subspace in $BV(D) \cap \mathcal{E}^{1,1}$ such that any element $V \in E$ verifies the

required assumptions. A first example is, when working with prescribed volume for the moving domain,

$$E_0 = \{\ V \in BV(D, R^N) \cap \mathcal{E}^{1,1},$$

$$s.t.\ divV = 0\ a.e.\ (t,x) \in I \times D\ \ \}$$

V be a free divergence vector field with $divV = 0,\ ,\ V \in L^1(I, E_0))$, where $E = BV(D, R^N)$ or any closed subspace (for example $E = \{\, V \in H_0^1(D, R^N),\ s.t.\ \ divV = 0\ \}\ )$. An *obvious* metric is to consider the set

$$\mathcal{V}(\Omega_1, \Omega_2) = \{\, V \in \mathcal{E}^{1,1}\ s.t. V,\ divV\ \in L^p(I, E_0),$$

$$s.t.\ \zeta_0 = \chi_{\Omega_1},\ \zeta(1) = \chi_{\Omega_2}\ \}$$

$$\delta_{E_0}(\Omega_1, \Omega_2) = Inf_{V \in \mathcal{V}(\Omega_1,\Omega_2)} \int_0^1 ||V(t)||_{E_0}\, dt \tag{8}$$

As V is divergence free the previous boundedness assumption on the divergence are verified and to each V a tube ζ_V is associated trough the convection. Then we get the

Proposition 3.1 *Let E be any subspace of $BV(D, R^N) \cap \mathcal{E}^{1,1}$ such that any element V satisfies assumptions of theorem 2,12 of (25), for example $E = E_0$. Then equipped with δ_E the family $\mathcal{O}^E_{\Omega_0}$ is metric space.*

$$p > 1, d_{E_0}(\Omega_1, \Omega_2) = Inf_{V \in \mathcal{V}(\Omega_1,\Omega_2)} \quad ||V||_{L^p(I,E_0)} + ||\frac{\partial}{\partial t} V||_{L^1(I, M^1(D,R^N)} \tag{9}$$

Theorem 3.2 *Let E be any subspace of $BV(D, R^N) \cap \mathcal{E}^{1,1}$, such that any element V whose divergence satisfies assumptions of theorem 2,12 of (25). Then equipped with d_E the family $\mathcal{O}^E_{\Omega_0}$ is a complete quasi- metric space.*

3.1. Geodesic characterizarion via transverse field Z

That metric can be improved as a complete metric by adding the perimeter terms . Then the transverse tube perturbation will applies. In that setting we are concerned with vector fileds $Z(s,t,x) \in R^N$ such that $Z(s,0,x) = Z(s,1,x) = 0$ so that the extrimities of the pertubed tube are preserved. The previous study for the transverse field implies that for given such a vector filed Z, with $div_x Z(s,t,x) = 0$ we get the admissible perturbation of the field V in the following form $V + sW(s,t,x)$ with

$$W(s,t,x) = \frac{\partial}{\partial t} Z(s,t,x)\ + [Z,\, V]$$

more precisely define the Lipschitz-continuous connecting set

$$\mathcal{V}^{1,\infty}(\Omega_1, \Omega_2) = \{\ V \in L^1(I, W^{1,\infty}$$

$$\cap \mathcal{E}^{1,1},\ s.t.\ \ \zeta_V\ \in \bar{\mathcal{T}}(\Omega_1, \Omega_2)\ \ \}$$

And the set of smooth transverse vector fields:

$$\mathcal{Z} = \{\quad Z(t,x) \in C^\infty_{comp}(I \times D, R^N)\quad \}$$

(Notice that such Z verifies $Z(0,.) = Z(1,.) = 0$ on D)

Proposition 3.3 *Let $V \in \mathcal{V}(\Omega_1, \Omega_2)$ and $Z(t,x) \in \mathcal{Z}$. The Transformation $\mathcal{T} = T_s(Z) o T_t(V)$ maps $\Omega_t(V)$ onto $\Omega^s_t := T_s(Z)(\Omega_t(V))$ so that*

$$\forall s,\ \forall Z,\ V^s(t,x) = \frac{\partial}{\partial t} \mathcal{T} o\, \mathcal{T}^{-1}$$

$$= (\frac{\partial}{\partial t} T_s(Z(t)) + DT_s(Z(t)).V(t)\ ) o T_s(Z(t))^{-1}$$

$$\in\ \mathcal{V}^{1,\infty}(\Omega_1, \Omega_2)$$

Lemma 3.4

$$\frac{\partial}{\partial s} V^s(t,x)|_{s=0}\ =\ \frac{\partial}{\partial t} Z(t) + [Z(t),\, V(t)] \tag{10}$$

Corollary 3.5 *Consider a functional $\mathcal{J}(V) = j(\zeta_V)$ and let $\bar{V}$ be a minimizing element of $\mathcal{J}$ on $\mathcal{V}(\Omega_1, \Omega_2)$ then we have*

$$\forall Z \in \mathcal{Z},\ \frac{\partial}{\partial s} \mathcal{J}(\bar{V}^s)_{s=0}$$

$$= J'(\bar{V};\, (\frac{\partial}{\partial s} V^s)_{s=0})$$

$$= \mathcal{J}'(\bar{V};\ \frac{\partial}{\partial t} Z(t) + [Z(t),\, V(t)]\ )\ \geq\ 0 \tag{11}$$

That variational principle extends to vector field $V \in E$ for which the flow mapping $T_t(V)$ is poorly defined. The element $\zeta_V \in \mathcal{H}^c$ is uniquely defined. For any $Z \in \mathcal{Z}$ the perturbed $\zeta^s_V := \zeta_V o T_s(Z)^{-1} \in \bar{\mathcal{T}}(\Omega_1, \Omega_2)$ on the other hand the following result is easily verified

Proposition 3.6 $\zeta_V^s = \zeta_{V^s}$ *with*

$$V^s(t,.) := -DT_s^{-1}(-Z(t)).(V(t) o T_s(Z(t))^{-1})$$

$$-\frac{\partial}{\partial t} T_s(-Z(t)) \ )$$

In other words:

$$\frac{\partial}{\partial t}\zeta + \nabla\zeta.V = 0 \ \textit{implies}$$

$$\frac{\partial}{\partial t}(\zeta o T_s(Z(t))^{-1}) + \nabla(\zeta o T_s(Z(t))^{-1}).V^s = 0$$

It can also be verified that the expression 10 for the derivative of the field still holds true so that the variational principle (11) is valid for any functional $\mathcal{J}$ minimized over the lipschitzian connecting family $\mathcal{V}^{1,\infty}(\Omega_1, \Omega_2)$. And more generally, without assuming V in E we have :

Proposition 3.7 *Let* $(\zeta, V) \in \mathcal{T}^{p,q}(\Omega_1, \Omega_2)$*, then for all* $s > 0$ *and* $Z \in \mathcal{Z}$ *we have :*

$$(\zeta o T_s(Z)^{-1},\ V^s) \ \in \ \mathcal{T}^{p,q}(\Omega_1, \Omega_2)$$

In order to get a differentiable metric we could consider

$$\tilde{d}(\Omega_1, \Omega_2) \ = \ Inf_{V \in \mathcal{V}(\Omega_1, \Omega_2)}$$

$$\int_0^1 \ (\ ||V(t)||_{H_0^1 \cap E_0} \ + \ ||\frac{\partial}{\partial t} V||_{L^2(D)} \ ) \, dt$$

equipped with $\tilde{d}$, $\mathcal{O}_{\Omega_0}$ would be complete metric space but $\tilde{d}$ fails to be a metric because of the triangle axiom The advantage is that now the associated functional is differentiable with repect to V then we can apply the previous variational principle with transverse vector field Z. Let $\bar{V}$ be a minimizer in $\mathcal{V}(\Omega_1, \Omega_2)$ for $\tilde{d}(\Omega_1, \Omega_2)$. Then $\forall Z \in \mathcal{Z}$ we have

$$\int_0^1 \{ \ ||V(t)||^{-1} \ < V(t), Z_t + [Z, V] >$$

$$+ |V'(t)|^{-1} \, ((V'(t) \, (Z_t + Z, V)' \ )) \ \} dt = 0$$

Where $<,>$ is the $H_0^1(D, R^N)$ inner product while $((,))$ is the $L^2(D, R^N)$ one. In order to recover a differentiable complete metric we introduce again the constraint on the perimeter as in the begining and set

$$\delta_{H^1}(\Omega_1, \Omega_2) \ = \ Inf_{V \in \mathcal{V}(\Omega_1, \Omega_2)}$$

$$\int_0^1 \ ||V(t)||_{H_0^1 \cap E_0} \, dt \qquad (12)$$

The optimality condition is :$\forall Z \in \mathcal{Z}$

$$s.t. \ \int_0^1 \int_{\Gamma_t} H(t) \ < Z(t), n_t > \ d\Gamma_t \, dt \ = \ 0,$$

$$\int_0^1 \ ||V(t)||^{-1} \ < V(t), Z_t + [Z, V] \ > \ dt = 0$$

4. QUASI-METRIC BY LEVEL SET FORMULATION FOR APPLICATIONS

Let $p > 1$ and $\Omega_i, \ i = 1, 2$ be two arbitrary mesurable subsets in D. Let

$$K(\Omega_1, \Omega_2) = \{\phi \in L^2(I, H^1(D)) \cap W^{1,1}(I, L^2(D)),$$

$$\frac{\partial}{\partial t}\phi \in L^p(I, L^2(D)),$$

$$\Omega_1 = \{\Phi(0,.) > 0\}, \ \Omega_2 \ = \{ \, \Phi(1,.) > 0 \, \}$$

Notice that $K(\Omega_1, \Omega_2) \subset \ C^0(\bar{I}, L^2(D))$, we set

$$d_{LS,p} = (\Omega_1, \Omega_2) := Inf_{\{\phi \in K(\Omega_1, \Omega_2)\}}$$

$$\int_0^1 (\, \alpha \ ||\phi(t)||^2_{H^1(D)} \ + \ ||\frac{\partial}{\partial t}\phi(t)||^p_{L^2(D)} \ ) \, dt$$

Theorem 4.1 *Let* $1 \ < \ p \ \leq \ 2$*, equipped with* $d_{LS,p}$ *the family of mesurable subsets in* D *is a complete quasi-metric space.*

5. EULER EQUATION FOR GEODESICS

$$\exists c(t), \ P \quad s.t. \ \frac{\partial}{\partial t}(||V(t)||^{p-2} \, V(t))$$

$$+ ||V(t)||^{p-2} \, (\ DV(t).V \ + \ D^*V.V(t) \,)$$

$$= \nabla P + c \ \chi_{\Gamma_t} \, div_{\Gamma_t}(n_t) \ n_t.$$

That is,

$$(p-2)||V||^{p-4}((V, \frac{\partial}{\partial t} V))V$$

$$+ ||V(t)||^{p-2} \, (\frac{\partial}{\partial t} V \ + \ DV(t).V \ + \ D^*V.V(t) \,)$$

$$= c \ \chi_{\Gamma_t} \, div_{\Gamma_t}(n_t) \ n_t, \qquad (13)$$

which can be written as (with the notations $\bar{V} = ||V||^{-1} \, V, \ \Pi = P - 1/2|V|^2$) :

$$div V = 0,$$

$$\frac{\partial}{\partial t} V + (p-2)((\frac{\partial}{\partial t} V, \bar{V})) \, \bar{V}$$

$$= \ DV.V \ = \nabla\Pi + c(t)||V||^{2-p} \ \chi_{\Gamma_t} \, div_{\Gamma_t}(n_t) \ n_t \qquad (14)$$

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Mathematical challenges and fast solution methods in aerodynamic shape optimization

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Keywords: Aerodynamic shape optimization, one-shot optimization, approximate reduced SQP

1. AERODYNAMIC SHAPE OPTIMIZATION

Aerodynamic shape optimization is a rewarding field for numerical analysis, since it poses several challenges due to the complexity of the subproblems involved and because efficient numerical solution methods have a high economical impact. This is particularly evident in the collaborative effort MEGADESIGN (2003-2007, funded by BMWi), whithin which most of the results presented here have been achieved. The focus of our research lies in the generation of fast numerical methods for optimal shapes of parts of the geometry of civil aircrafts. The objective for the optimization is the minimization of aerodynamic drag, because this immediately reduces fuel consumption. The aerodynamic models are represented in the form of complex flow simulators which are provided by our application partner. They involve costly iterative processes. The *main challenge* in aerodynamic shape optimization is to avoid wrapping another optimization loop around the simulation iterations, but rather to perform optimization steps already during iterative process of the forward simulation tool. Thus, this methodolgy is frequently called a "one-shot-optimization" method.

2. A NOVEL ALGORITHMIC TEMPLATE

From an abstract point of view, we consider optimization problems of the form

$$\min f(u,q) \tag{1}$$

$$\text{s.t. } c(u,q)=0 \quad \exists c_u^{-1} \tag{2}$$

where u denotes the aerodynamic flow state variables, to be solved for in the flow equation. The letter q denotes a finite dimensional parameterization of the shape that we investigate. The scalar valued function $f(u,q)$ denotes the objective of the optimization, i.e., here the aerodynamic drag resulting from the shape chosen. With this abstract problem formulation, we observe that the problem under investigation falls into the class *PDE constrained optimization problems*, which are of major interest in several international research programs.

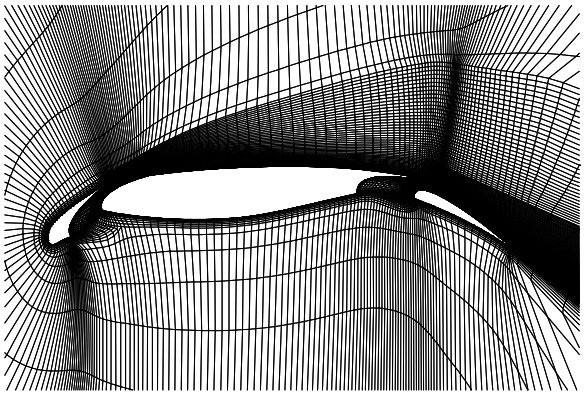

Fig. 1. Three part wing in high lift configuration

By use of the Lagrangian function

$$\mathcal{L}(u,q,\lambda) = f(u,q) - \lambda^* c(u,q)$$

we can formulate our basic one-shot algorithm in the form

$$\begin{aligned} \lambda^{k+1} &= \lambda^k - (A^*)^{-1}\nabla_u \mathcal{L}(u^k,q^k,\lambda^k) \\ q^{k+1} &= q^k - S_A^{-1}\nabla_q \mathcal{L}(u^k,q^k,\lambda^{k+1}) \\ u^{k+1} &= u^k - A^{-1} c(u^k,q^{k+1},\lambda^{k+1}) \end{aligned}$$

where $A \approx \partial c/\partial u$ and S_A is an approximation to what we call the "consistent" reduced Hessian. This algorithm is highly modular but nevertheless iterates simulateously over all variables: state, design and adjoints.

3. MAJOR ISSUES OF THE TALK

The algorithm sketched above can be interpreted as an approximate variant of reduced SQP methods. By use of this interpretation, it is easily generalizable to completely different application areas outside of aerodynamic shape optimization with similar proble characteristics. These characteristics are that one wants to stick to an a-priorily implemented system solver and on the other hand has an adjoint solver at hand. At the core of the numerical analysis of this algorithm lie convergence results. These have been achieved so far for linear-quadratic model problems. We show the essential ideas of these convergence proofs. In addition to the problem formulation (1, 2), one has to treat state constraints modeling the lift requirement for the airplane and also a required pitching moment. Since these are scalar valued constraints, they can be included within the algorithmic framework by adding further adjoint equations, which are solved ”on the fly” as well. Enhancements of the convergence theory justifying this constraint treatment are presented, too. In a practical environment, practical issues of the implementation play a major role for the success of the resulting methods. These issues will be discussed together with several numerical results, e.g., for the three part wing depicted in Figure 1.

The success of the one-shot methods described within the talk has stimulated research towards further aspects: substitution of a fixed shape parameterization by a fine resolution based on the flow grid, incorporation of multigrid ideas in the algorithmic framework, the efficient treatment of uncertainties in the industrial environment, etc. Several of these aspects and recent research results for them will be discussed, as well.

4. CONCLUSIONS

A major part of the talk will be devoted to summarizing the research results presented in the publications (Gherman et al., 2005; Gherman, 2007; Hazra et al., 2004, 2006; Ito et al., 2006; Kroll et.al, 2004; Schulz, 1998, 2004) and so far unpublished results based on them.

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HALF A CENTURY OF DISCRETE MATHEMATICS: A PROGRESS REPORT

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Keywords: Discrete mathematics, optimization, integer programming, operations research

Discrete Mathematics was born when the first concepts of mathematics were invented. The modern meaning of the term *Discrete Mathematics* began to take shape in the fifties of the 20th century and has evolved over the last decades. Today it includes (roughly): classical combinatorics, graph theory, combinatorial optimization, integer programming, matroid theory, coding theory, and even some branches of geometry, algebra, and number theory. Discrete Mathematics overlaps significantly with Theoretical Computer Science, in particular in the theory of algorithms.

Driven by the explosive growth of computing power and by numerous applications, Discrete Mathematics has experienced tremendous progress in the last 50 years - both in theory and in its use in practice. There is no way to cover all the areas and all success stories. I will focus on a few highlights (of my choice) and will try to show the advances that have been achieved along these examples.

Success in theory is typically marked by the proof of important theorems. The max flow-min cut theorem, the characterization of totally unimodular matrices, the matroid intersection theorem, the 4-color theorem, and the perfect graph theorem are five of many examples of a rich harvest of this kind that I will mention.

Progress is often fueled by new notions and theories providing suitable tools and concepts for the understanding of unexplained phenomena. Prime examples here are the concept of NP- and other types of completeness, general complexity theory, and the theory of random graphs, all developed in the last 50 years.

Our daily life is full of (usually unnoticed) contacts with Discrete Mathematics. Whether we produce a car, ride a city bus, fly in an airplane, find a route with a car navigation system, order a book, use a phone, or withdraw money from an ATM, Discrete Mathematics is involved in some fundamental and often important way. I will present some breakthroughs in the algorithmic solution technology focusing on large-scale real-world examples of this kind.

THEORY AND APPLICATIONS OF OPTIMAL BANG-BANG AND SINGULAR CONTROL PROBLEMS

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Keywords: bang–bang control, singular control, optimization of switching times, sufficient conditions, sensitivity analysis, van der Pol oscillator, control of lasers, Goddard problem, fedbatch fermentation

1. OPTIMAL CONTROL PROBLEMS WITH CONTROL APPEARING LINEARLY

We study optimal control problems of the following form: determine a piecewise continuous (measurable) control $u : [0, t_f] \to I\!R^m$ and a state trajectory $x : [0, t_f] \to I\!R^n$ that minimize the cost functional of Mayer type,

$$J(x, u, t_f) := g(x(t_f), t_f),$$

subject to the dynamics, boundary conditions and control-state constraints

$$\begin{aligned} &\dot{x}(t) = f(x(t), u(t), t), \quad 0 \le t \le t_f\,, \\ &\varphi(x(0), x(t_f)) = 0, \\ &C(x(t), u(t)) \le 0, \quad 0 \le t \le t_f\,. \end{aligned}$$

The augmented Hamiltonian is given by

$$H(x, u, \lambda, t) = \lambda f(x, u, t) + \mu C(x, u),$$

where $\lambda \in I\!R^n$ denotes the adjoint variable and μ is the multiplier for the control-state constraint. For this control problem, second–order sufficient conditions, sensitivity analysis and real–time control techniques have been extensively studied in the literature under the assumption that the *strict Legendre condition* $H_{uu}[t] \ge cI_m\,,\ c > 0$, holds; c.f., e.g., Dontchev, Hager [3], Malanowski, Maurer [7], Büskens, Maurer [2], Maurer, Augustin [9].

The situation is different for optimal control problems where all control components appear linearly. In this case, the strict Legendre conditions is violated. The dynamics then has the form

$$\dot{x}(t) = f_1(x(t), t) + f_2(x(t))u(t),$$

where $f_1(x, t)$ is a n–vector and $f_2(x, t)$ is a $n \times m$–matrix, and the control constraints are assumed to be simple box constraints

$$u_{i,\min} \le u_i(t) \le u_{i,\max}\,, \quad i = 1, ..., m.$$

The *switching function* is defined by

$$\begin{aligned} &\sigma(x, \lambda, t) = \lambda f_2(x, t), \\ &\sigma[t] = \sigma(x(t)), \lambda(t)), t) = (\sigma_1[t], ..., \sigma_m[t]). \end{aligned}$$

Then the optimal control which minimizes the Hamiltonian is characterized by

$$u_i(t) = \left\{ \begin{array}{lll} u_{i,\min}, & \text{if} & \sigma_i[t] > 0 \\ u_{i,\max}, & \text{if} & \sigma_i[t] < 0 \\ \text{singular}, & \text{if} & \sigma_i[t] = 0 \end{array} \right\}$$

for $i = 1, ..., m$. If the switching function $\sigma_i[t]$ has only isolated zeros in $[0, t_f]$, then $u_i(t)$ is called a *bang–bang* control component.

2. BANG–BANG CONTROL

Assume that every component $u_i(t)$ of the optimal control is bang–bang and that there are only finitely many switching times which are ordered as $0 < t_1 < ... < t_k < ... < t_s < t_f$. Such a bang-bang control can be computed by solving an *induced optimization problem*, where the switching times t_k, $(k = 1, ..., s)$ are taken as optimization variables. It has been shown in Agrachev, Stefani, Zezza [1] and Osmolovskii, Maurer [11–13] that second order sufficient conditions (SSC) hold for the *bang-bang control problem* provided that SSC hold for the induced optimization problem and, moreover, the switching function satisfies the so–called strict bang–bang property. A related type of sufficient condition has been derived in Ledzewicz, Schättler [6].

An interesting byproduct of the optimization approach is the fact that the well–known sensitivity results for finite–dimensional optimization problems apply to bang–bang control problems, since the strict bang–bang property is stable with respect to perturbations. Numerical time–scaling techniques for verifying SSC and computing parametric sensitivity derivatives have been developed in Maurer et al. [9]. In this talk, we present two practical examples illustrating the numerical techniques and the sufficiency test: time–optimal control of a van der Pol oscillator [11] and control of a semiconductor laser [4].

3. SINGULAR CONTROL

For singular control problems, sufficient otpimality conditions have been obtained only in special cases, e.g., for *totally* singular controls. Here, we concentrate on the case where the singular control can be obtained in *feedback form* $u = u_{\rm sing}(x,t)$. This property holds in many practical examples. To compute a control that is a combination of bang–bang and singular arcs, we solve an induced optimization problem, where switching times of bang–bang arcs and junction times with singular arcs are optimized simultaneously. This numerical approach is illustrated on three examples: (a) van der Pol oscillator [14] (b) Goddard problem [8,14], (c) fedbatch fermentation problem [5,14].

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Efficient Nonlinear Programming Algorithms for Chemical Process Control and Operations

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Keywords: dynamic optimization, nonlinear model predictive control (NMPC), moving horizon estimation (MHE), real-time optimization

Nonlinear programming (NLP) has been a key enabling tool for model-based decision-making in the chemical industry for over 50 years. Optimization is frequently applied in numerous areas of chemical engineering including the development of process models from experimental data, design of process flowsheets and equipment, planning and scheduling of chemical process operations, and the analysis of chemical processes under uncertainty and adverse conditions. These *off-line* tasks frequently require the solution of NLPs formulated with detailed, laregscale process models.

More recently, these tasks are complemented by *time-critical, on-line* optimization problems for challenging process applications. Here NLPs formulated with differential-algebraic equation (DAE) process models are solved to enforce desirable process behavior. The use of nonlinear dynamic models has key advantages; it captures process behavior well over a wide range of conditions, can be fitted to process data over time and leads to models that are compatible with off-line optimization models. However, the challenge remains whether underlying optimization models can be solved sufficiently quickly with on-line DAE process models.

Figure 1 depicts the interplay of tasks for online optimization. Here the plant has manipulated variables and disturbances as inputs, with the former determined by the Control block. In addition, output measurements from the plant are used by the Estimator block to infer the state of the process model as well as unmeasured disturbances. Challenging process applications often require actions for the Control and Estimator blocks to be determined by solving dynamic optimization problems over moving time horizons.

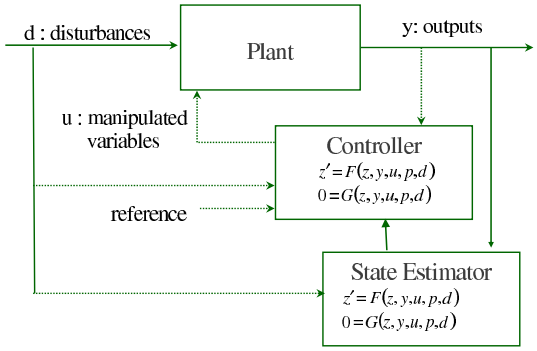

Fig. 1. Block Diagram of Model-Based Control Structures

As process measurements are updated in the process every few minutes or even every few seconds, both the control and estimation problems need to be solved quickly.

Nonlinear model predictive control (NMPC) and Moving Horizon Estimation (MHE) are well-developed NLP formulations to deal with the control and estimation tasks in Figure 1. Here we present the formulations of these dynamic optimization problems based on a simultaneous collocation (or direct transcription) approach. This approach is especially useful as it can deal with unstable systems and exploits sparsity and structure of DAE process models. On the other hand, the discretization of all state and manipulated variables over time leads to large NLPs and requires the application of large scale NLP solvers. For this task we discuss a recently developed barrier, full space NLP solver called IPOPT (4). In particular, this approach solves the KKT system with a Newton-based barrier method that uses a filter line search for global convergence. The algorithm has been embodied into an open source, object oriented code that compares well with competing NLP approaches. Moreover, we

discuss an extension of this code to deal with exploitation of the structure of process models. In addition, we discuss recent implementations of NLP sensitivity analysis arising from the formulation of parametric NLPs. Based on well-known properties of barrier methods (3), the sensitivity of the optimal solution can be computed with only a simple back-solve of a pre-factorized KKT matrix

We show that these IPOPT features are especially important for time-critical, on-line calculations. Moreover, they can address the challenge of process models increasing in size and complexity while still requiring requires frequent on-line updating for the plant. As a result, fast solution of these NLP subproblems, shown in (2), may not be sufficient to avoid computational delays (with resulting loss of performance) in the control loop. Instead, we apply the recently developed concept of *real-time iteration* (1) and discuss its adaptation to barrier algorithms that exploit properties of NLP sensitivity. Here both the NMPC and MHE subproblems can be solved in background between sampling times. Based on these solutions of these parametric NLPs, new process measurements can be used to update the NLP solution; *this update is the only on-line calculation.*

We discuss the adaptation of both MHE and NMPC problems to real-time iteration (5; 6). Here on-line calculations are effected through simple backsolves of a pre-factorized KKT system, assisted by a Schur complement factorization of augmented systems that characterize the perturbed NLP solution. This approach leads to tremendous reductions in on-line optimization calculations and will be demonstrated on a real-world example.

Finally, a number of areas are discussed for future work. These deal with the extension of this approach to larger, integrated subsystems and the treatment hybrid systems that include NLPs formulated with complementarity constraints. In addition we will expand the scope of on-line dynamic models so that they are more tightly integrated with economic and planning decisions made off-line.

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APPLICATIONS OF EVOLUTIONARY OPTIMIZATION IN STRUCTURAL ENGINEERING

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Keywords: Aesthetic Design, Bridge Maintenance, Earthquake Disaster, Genetic Algorithm, Immune Algorithm, Optimization, Restoration Scheduling

1. INTRODUCTION

With the recent advanced development of computer technology, it has been widely recognized that optimization can take an important role in accomplishing an economic and efficient process for various engineering problems. It can provide us with useful information for decision-making. From the practical points of view, the optimization should be flexible and intellectual so as to solve real problems with many difficulties such as vague and uncertain objective function and constraints

In this paper, an attempt is made to develop some efficient optimization methods by introducing the concepts of evolutionary computing. Several application examples are presented to demonstrate the applicability of the proposed methods.

2. EVOLUTIONARY COMPUTING

Evolutionary computing has been paid attention as a promising optimization tool in various fields because of its general possibility to reach the optimal solution, simplicity in theory, and easiness of programming. Among many evolutionary computing techniques, Genetic Algorithm (GA), Immune Algorithm (IA), and Particle Swarm Optimization (PSO) have been successfully applied in the field of structural engineering. GA is an evolutionary computing technique, in which candidates of solutions are mapped into GA space by encoding. The following steps are employed to obtain the optimal solutions: a) initialization, b) crossover, c) mutation, d) natural selection and e) reproduction. Individuals, which are solution candidates, are initially generated at random. Then, steps b, c, d, and e are repeatedly implemented until the termination condition is fulfilled. Each individual has a fitness value to the environment. The environment corresponds to the problem space and the fitness value corresponds to the evaluation value of objective function.

Immune Algorithm (IA) is a kind of optimal solution search algorithms and is said to allow the diversity of solutions to be retained and multiple quasi-optimal solutions to be obtained. It is considered that IA is suitable for practical design problems because of these characteristics, which allow two or more different quasi-optimal solutions rather than a single optimal solution to be obtained to a problem

which is difficult to evaluate in a standardized manner. Consequently, an engineer can select an appropriate candidate from them based on their subjective judgement and preferences.

3. OPTIMAL RESTORATION SCHEDULE FOR EARTHQUAKE DISASTER

Nowadays, our life is realized based upon the daily use of various lifeline systems. Those lifeline systems form the complicated network whose functions are mutually interrelated. All the lifeline systems have not been designed to protect all natural hazards. Moreover, the newest design theory can not guarantee the absolute safety due to the economic constraints. Therefore, it is necessary to develop a synthetic disaster prevention program based on the recognition that lifeline systems may unavoidably suffer when big earthquakes occur.

The main purpose of this research is the early restoration of lifeline systems after the earthquake disasters. Here, two issues are focused on, the first of which is such an allocation problem that which groups will restore which disaster places, and the second is such a scheduling problem what order is the best for the restoration. In order to solve the three problems simultaneously, Genetic Algorithm (GA) is applied, because it has been proven to be very powerful in solving combinatorial problems. However, road networks after earthquake disaster have an uncertain environment as the secondary disaster by aftershock. Therefore, the restoring works are not progressing on schedule. In this study, an attempt is made to develop an efficient disaster restoration method by using Improved GA. A numerical example is presented to compare the proposed method and the ordinal method.

4. OPTIMAL MAINTENANCE PLANNING OF BRIDGE STRUCTURES

The purpose of this study is to develop a method of optimal maintenance planning for many bridges based on Life-Cycle Cost (LCC) by introducing the technique of GA.

Recently, maintenance work is becoming more and more important, because the number of structures requiring repair or replacement increases in the coming ten years, in Japan. In order to establish a rational and economical maintenance program, the concept of LCC has gained great attention, which minimizes the total cost of whole lives of structures.

In this paper, an attempt is made to minimize LCC for many concrete bridge structures. The concrete bridges are deteriorating due to the corrosion of reinforcing bars and neutralization of concrete. Then, it is necessary to achieve an optimal maintenance plan that can provide appropriate methods and times of repairing or replacement. However, the optimal maintenance problem is very difficult to solve, because it is one of combinatorial problems with discrete design variables and discontinuous objective functions. Furthermore, the problem may become tougher, when it becomes larger and more complex. In this study, an attempt is made to develop an efficient bridge maintenance method by using Improved GA. A numerical example is presented to compare the proposed method and the ordinal method.

5. AESTHETIC DESIGN OF BRIDGE STRUCTURES

In the design of bridge structures, it is becoming important to consider the aesthetic design factors. In this paper, an attempt is made to develop a decision-support system for the aesthetic design of bridge handrails. The colours, upper components, lower components and columns are employed as design items as well as the configuration of bridge, the colours of other bridge components and the harmony with the surrounding environment. The present system consists of the evaluation system using neural network and the optimization system based upon Immune Algorithm (IA). Several numerical examples are presented to demonstrate the efficiency of the proposed system. Computer Graphics (CG) is used for visual examination of each alternative.

6. CONCLUSIONS

n this study, attempts were made to develop some new searching methods for optimization problems of structural engineering. The optimization problems in real life are very difficult to solve, because they have objective function and constraint condition with vagueness and uncertainty. By comparing the proposed methods with the usual method, it was proven that the proposed methods can reduce the computation time and improve the convergence of searching procedure.

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SEMI-ALGEBRAIC IDEAS IN NONSMOOTH OPTIMIZATION

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Keywords: semi-algebraic, variational analysis, nonsmooth optimization, semismooth, Lojasiewicz inequality, critical point, Sard's theorem, pseudospectra

Modern variational analysis provides a sophisticated unification of convex and smooth optimization theory, achieving striking generality but at the expense of possible pathology. The general theory must handle highly irregular and oscillatory functions and sets, and yet, on the other hand, a rich family of concrete instances involve no such pathology. In particular, from a variety of variational-analytic perspectives, semi-algebraic sets—finite unions of sets defined by finitely many polynomial inequalities—are well behaved.

In joint work with J. Bolte, A. Daniilidis, A. Ioffe, C.H.J. Pang, and M. Shiota, the author illustrates a variety of situations where semi-algebraic techniques resolve variational-analytic challenges. Most of the following examples extend to sets and functions that are "subanalytic" or, more generally, "tame".

We begin with an algorithmic application. Consider a locally Lipschitz function $: \mathbf{R}^n \to \mathbf{R}^n$. Superlinear convergence of nonsmooth Newton methods for the equation $( ) = 0$, depend on "semismoothness" of . Semi-algebraic locally Lipschitz functions are always semismooth (Bolte et al, 2007b).

A more classical example involves the famous Lojasiewicz inequality, which states that, for any critical point of a real-analytic function $: \mathbf{R}^n \to \mathbf{R}$, there is an exponent $\theta \in [0\ 1)$ such that the function

$$\frac{| - ( )|^\theta}{\| \nabla \|}$$

remains bounded around . An analogous inequality holds for semi-algebraic functions (Bolte et al, 2007a), leading to proofs of the finite length of trajectories of the associated subgradient dynamical system

$$- \in - \quad ( )$$

Critical point theory furnishes another example where semi-algebraic assumptions lead to elegantly simple characterizations. Among notions of critical points available for nonsmooth functions, the approach via the "weak slope" has considerable theoretical appeal. Unfortunately, such critical points seem hard to recognize in general. However, for semi-algebraic functions on $\mathbf{R}^2$, a simple topological characterization suffices (Ioffe and Lewis, 2007).

The graph of any semi-algebraic function admits a Whitney stratification. This technique allows us to relate a classical smooth notion, the size of gradients of the function restricted to its various strata, to a fundamental nonsmooth idea, the size of Clarke subgradients (Bolte et al, 2007c).

Stratification provides one route to a nonsmooth Morse-Sard theorem. The classical version asserts that any sufficiently smooth function $: \mathbf{R}^n \to \mathbf{R}$ is constant along any arc of critical points. Analogous nonsmooth versions hold for semi-algebraic (Bolte et al, 2005, 2006). Consequently, such functions can have only finitely many critical values—a nonsmooth variant of the classical theorem of Sard, and a precursor of recent very general set-valued versions of Sard's theorem due to Ioffe. Such results have striking implications for variational analysis: given any semi-algebraic generalized equation (such as a semi-algebraic system of inequalities, for example), small perturbations almost surely render the system "metrically regular". Metric regularity is a central notion both in variational theory and computational practice, guaranteeing that approximate solutions to the system, as measured

by the *a posteriori* error, are close to exact solutions.

We end with a more concrete example. The eigenvalues of a nonsymmetric matrix may be very sensitive to slight perturbations to the matrix, due to eigenvalue coalescence. Furthermore, it is well known that eigenvalues may be misleading as practical modeling tools. For example, the spectral radius of predicts the asymptotic stability of the dynamical system $_{k+1} = \ _k$, but is insensitive to transient peaks. A more predictive modeling tool is the *pseudospectrum*

$$\Lambda_\epsilon(\ ) = \left\{ \in \mathbf{C} : \|(\ - \ )^{-1}\| \geq \frac{1}{-} \right\}$$

for some small constant 0. The pseudospectrum consists of all eigenvalues of small perturbations to . Since the "resolvent norm" $\mapsto \|(\ - \ )^{-1}\|$ is semi-algebraic, it has at most finitely many critical values. Consequently, unlike the spectrum, the set-valued mapping Λ_ϵ is Lipschitz around for all small 0 (Lewis and Pang, 2006).

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VARIATIONAL ANALYSIS IN OPTIMIZATION AND CONTROL

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Variational analysis has been recognized as a rapidly growing and fruitful area in mathematics concerning mainly the study of optimization and equilibrium problems, while also applying perturbation ideas and *variational principles* to a broad class of problems and situations that may be not of a variational nature. It can be viewed as a modern outgrowth of the classical calculus of variations, optimal control theory, and mathematical programming with the focus on *perturbation/approximation* techniques, sensitivity issues, and applications; see (1; 2; 3)

One of the most characteristic features of modern variational analysis is the intrinsic presence of *nonsmoothness*, i.e., the necessity to deal with nondifferentiable functions, sets with nonsmooth boundaries, and set-valued mappings. Nonsmoothness naturally enters not only through initial data of optimization-related problems (particularly those with inequality and geometric constraints) but largely via *variational principles* and other optimization, approximation, and perturbation techniques applied to problems with even smooth data. In fact, many fundamental objects frequently appearing in the framework of variational analysis (e.g., the distance function, value functions in optimization and control problems, maximum and minimum functions, solution maps to perturbed constraint and variational systems, etc.) are inevitably of nonsmooth and/or set-valued structures requiring the development of new forms of analysis that involve *generalized differentiation*.

It is important to emphasize that even the simplest and historically earliest problems of *optimal control* are *intrinsically nonsmooth*, in contrast to the classical calculus of variations. This is mainly due to pointwise constraints on control functions that often take only discrete values as in typical problems of automatic control, a primary motivation for developing optimal control theory. Optimal control has always been a major source of inspiration as well as a fruitful territory for applications of advanced methods of variational analysis and generalized differentiation.

In this talk we discuss some new trends and developments in variational analysis and its applications mostly based on the author's recent 2-volume book (1; 2). Generalized differentiation lies at the heart of variational analysis and its applications. We systematically develop a *geometric dual-space approach* to generalized differentiation theory revolving around the *extremal principle*, which can be viewed as a local *variational* counterpart of the classical convex separation in nonconvex settings. This principle allows us to deal with *nonconvex* derivative-like constructions for sets (normal cones), set-valued mappings (coderivatives), and extended-real-valued functions (subdifferentials). These constructions are defined directly in dual spaces and, being nonconvex-valued, cannot be generated by any derivative-like constructions in primal spaces (like tangent cones and directional derivatives). Nevertheless, our basic nonconvex constructions enjoy *comprehensive/full calculus*, which happens to be significantly better than those available for their primal and/or convex-valued counterparts. The developed generalized differential calculus based on variational principles provides the *key tools* for various applications.

Observe to this end that dual objects (multipliers, adjoint arcs, shadow prices, etc.) have always been at the center of variational theory and applications used, in particular, for formulating the main optimality conditions in the calculus of variations, mathematical programming, optimal

control, and economic modeling. The usage of variations of optimal solutions in primal spaces can be considered just as a convenient tool for deriving necessary optimality conditions. There are no essential restrictions in such a "primal" approach in smooth and convex frameworks, since primal and dual derivative-like constructions are equivalent for these classical settings. It is not the case any more in the framework of modern variational analysis, where even *nonconvex primal space* local approximations (e.g., tangent cones) inevitably yield, *under duality, convex sets* of normals and subgradients. This convexity of dual objects leads to significant restrictions for the theory and applications. Moreover, there are many situations particularly identified in this book, where primal space approximations simply cannot be used for variational analysis, while the employment of dual space constructions provides comprehensive results.

In this talk we pay the main attention to discussions of the basic constructions of generalized differentiation in variational analysis and their applications to problems of *nonsmooth constrained optimization* and *optimal control*. We present complete characterizations of *Lipschitzian stability* and *metric regularity* of constraint and variational systems and their applications to *sensitivity analysis* with respect to perturbations. Then we discuss necessary optimality conditions for some remarkable classes of optimization problems including *nondifferentiable programming* with functional and geometric constraints and rather new while well-recognized classes of mathematical programs and multiobjective optimization problems with the so-called *equilibrium constraints*, which closely relate to problems of *bilevel programming* particularly considered in the talk. Finally, we consider optimal control systems governed by *evolution/differential inclusions* and present new necessary optimality conditions for them in generalized *Euler-Lagrange* and *Hamiltonian* forms. Our approach to optimal control of systems with continuous-time dynamics is based of *discrete approximations*, which provides efficient tools of analysis from both numerical and qualitative viewpoints. It time permits, we discuss particular applications of the results obtained to optimal control systems with continuous-time dynamics described by *ordinary differential*, *functional differential*, and *partial differential equations*.

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Problems of mathematical finance by stochastic control methods

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Keywords: pricing of financial derivatives, portfolio selection, Bellman equation, risk

1. Introduction

The purpose of the talk is to present main ideas of mathematics of finance using the stochastic control methods. There is an interplay between stochastic control and mathematics of finance. From one hand side stochastic control is a powerful tool to study financial problems. On the other hand financial applications have stimulated development in several research subareas of stochastic control in the last two decades.

2. Pricing of financial derivatives

One of the classical problems of mathematics of finance is pricing of financial derivatives. At a given time T called maturity the buyer of a financial instrument collects a gain which a random variable H (called a contingent claim). We would like to evaluate the price of H at the initial time. One can look at this price from the perspective of the seller or the buyer. An acceptable price for the seller is a such price that for the amount he obtains at time 0 he is able (providing he invests it in an optimal way) to get at least the compensation for H, which he is supposed to deliver to the buyer. This investment to hedge H forms a stochastic optimal control problem. We would like to find the smallest initial capital v, which invested in an optimal way gives us at least the value H at time T. Denote by $p_s(H)$ the minimal seller price. The buyer price is the value v such that if he starts with initial capital $-v$ and invests it in an optimal way, then at time T and the value of his portfolio plus his gain H is nonnegative. Such maximal v forms so called the buyer price $p_b(H)$ and is the maximal price acceptable for the buyer. Clearly $p_b(H) \leq p_s(H)$. The interval $[p_b(H), p_s(H)]$ is called an absence of arbitrage interval and any price from this interval is acceptable in the sense that neither seller nor buyer is able to obtain a positive gain without risk at time T (which we call an arbitrage). In a particular situations when $p_b(H) = p_s(H)$ for all bounded H we say that the market is complete which in turn corresponds to the fair price or fair game between the seller and the buyer. If we assume that the market does not allow an arbitrage (which is a standard assumption) then the buyer and seller prices have an interpretation as the minimum or maximum over the set of martingale measures $\mathcal{Q}$ of the expected value of H with respect to martingale measures. The martingale measure is an equivalent measure to the original probability measure under which the asset prices of our market become martingales i.e integrable stochastic processes such that the conditional expectation of their value at time $t+1$ given an information till time t is equal to their value at time t. It should be pointed out that such nice representation of the seller and buyer prices is valid only when we assume that there are no transaction costs on the market. The case of proportional (to the value of transaction) transaction costs has been studied recently by a number of well known mathematicians and still seems to be open in various aspects. In practice we usually pay fixed plus proportional transaction costs which are much harder to analyze. Furthermore frequently we can expect, in the case of larger transaction, to pay smaller proportional transaction costs which makes the transaction costs to be concave. The recent studies on liquidity effects lead even to convex transaction costs. In the last three cases we have only partial results concerning particular models. The general approach seems to be open.

3. Credit risk

The model and considerations in the previous section were based on the assumption that if the

transaction is made at time 0 the contingent claim H is delivered at time T. It may happen however that this delivery is subject to a certain risk called default. When default happens before or at time T then instead of H only its portion called recovery claim is delivered at time T. From mathematical point of view we may consider two cases: the case when default time is a predictable stopping time basing on the available information and the case when it is an unpredictable stopping time with a known intensity. In both cases we have similar questions for defaultable contingent claims: what is the price for such a claim if there are no or there are transaction costs. Consequently the pricing problems formulated in the section 2 can be considered.

4. Term structure models

In the models above we consider investments in assets or in banking account. An extension of the market is to consider investments in bonds. We denote by $B(t,T)$ the price at time t of the zero coupon bond paying one unit at time T. In so called single factor approach the price $B(t,T)$ is equal to the conditional expected value of the exponent of the negative value of the integral from t to T with respect to short term interest rate $r(t)$, which may be a solution to a certain stochastic differential equation. In more recent models following Heath Jarrow Morton methodology $B(t,T)$ is an exponent of the integral from t to T of a two factor function $f(t,s)$ called an instantaneous forward rate, which for fixed s as a function of t is a solution to a stochastic differential equation. One can again consider the problems of pricing of bond market derivatives or any contingent claims using investments on such extended market.

5. Portfolio selection

A vast literature in mathematics of finance is devoted to portfolio selection problems. We are looking for a portfolio maximizing of certain utility function. Any function which is concave and increasing and is a function of our consumption or value of our wealth process may be used to measure our satisfaction (our utility). The problem of utility maximization can be considered both for dynamical models, where growth of asset prices depends on time and we are looking for an investment strategy maximizing utility over certain time horizon, and for static models, where basing on historical data we model one step growth rate and maximize portfolio over one time step. In the case of dynamic models we maximize the utility of our consumption together with the utility of the terminal wealth process. Another problem is to maximize the growth of portfolio which is a logarithmic utility function of the wealth process. Portfolio selection models can be also used to price financial derivatives using e.g. indifference price, the price which guarantee the same expected value of the terminal value of the utility function of the wealth process, with initial capital diminished by the price, plus the contingent claim as in the case when we start with non diminished initial capital and at the terminal time we do not obtain the contingent claim.

6. Risk

One of the major problems of modern applied mathematics is risk modelling. First of all it is not clear what is risk and how to measure it. Historically the first approach to risk was introduced in 1952 by Harry Markowitz, a later Nobel Price winner in economy in 1990. He measured risk as a variance the random portfolio wealth rate of return. The problem was to maximize over one time step (static portfolio selection) the expected portfolio rate of return with variance considered as a measure of risk not exceeding a certain level. In this problem we practically have two cost functionals one measuring the expected portfolio rate of return and another one corresponding to risk measured in a form of the portfolio variance. The same problem can be considered in dynamic setting. Instead of two cost functionals one also can consider so called risk sensitive cost functional, which measures the expected value plus variance with a certain weight called risk factor. An alternative is to maximize the portfolio wealth rate of return with a restriction on the risk introduced by the Value at Risk (VaR), which is a certain quantile restriction on the lower bound of portfolio or other measures of risk e.g. conditional VaR.

Monotone Random Variational Inequalities on Random Sets with Applications to Traffic Networks

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Keywords: Random Variational Inequality, Random Set, Measurability, Mosco Convergence, Monotone Operators, Averaging, Truncation, Traffic Networks, Wardrop Equilibrium

1. INTRODUCTION

In this contribution we report on recent joint work that extends some results in prior work (1) on random variational inequalities (VI) with a bilinear form on a fixed set. The extension is in two directions: We admit the convex set to be random similarly as in (2), (3). Instead of a bilinear form we admit nonlinear forms from monotone operator theory.

These new results allow us to treat a larger class of applications and are in particular used to treat nonlinear traffic networks in presence of random data.

2. THE RANDOM VI

More specifically in a finite dimensional setting, let $(\Omega, \mathcal{A}, \mu)$ be a complete σ-finite measure space. For all $\omega \in \Omega$, let $\mathcal{K}(\omega)$ be a closed, convex and nonempty subset of $\mathbb{R}^k$. Consider a Carathéodory function $F : \Omega \times \mathbb{R}^k \mapsto \mathbb{R}^k$, i.e. for each fixed $x \in \mathbb{R}^k$, $F(\cdot, x)$ is measurable with respect to $\mathcal{A}$, and for every $\omega \in \Omega$, $F(\omega, \cdot)$ is continuous. Furthermore, let $\lambda : \Omega \mapsto \mathbb{R}^k$ be measurable. Throughout we assume that for each $\omega \in \Omega$, $F(\omega, \cdot)$ is a monotone operator on $\mathbb{R}^k$.

With these data we start from the following

Problem in ω-Formulation. For each $\omega \in \Omega$, find $x^*_\omega \in \mathcal{K}(\omega)$ such that

$$\langle F(\omega, x^*_\omega), x - x^*_\omega \rangle \geq \langle \lambda(\omega), x - x^*_\omega \rangle \, , \forall x \in \mathcal{K}(\omega) \, .$$

First we provide a measurability result for the solution map of this problem.

Then we introduce a probability space $(\Omega, \mathcal{A}, P)$ and the reflexive Banach space $L^\alpha(\Omega, P, \mathbb{R}^k)\, \alpha \geq 2$ of random elements V from Ω to $\mathbb{R}^k$ with finite expectation $E^P[V]$, that is, with finite

$$\{E^P[V]\}^\alpha = E^P \|V\|^\alpha = \int_\Omega \|V(\omega)\|^\alpha dP(\omega) \, .$$

We define the convex and closed set K by $V \in K \iff V \in L^\alpha(\Omega, P, \mathbb{R}^k)$ and $V(\omega) \in \mathcal{K}(\omega)$ P-almost sure.

Under an appropriate growth condition the nonlinear map F becomes an Nemytski operator. Thus we arrive at the following

Problem in Integral Formulation Find $U \in K$ such that for all $V \in K$

$$E^P\{\langle F(U), V - U \rangle\} \geq E^P\{\lambda(V - U)\} \, .$$

We discuss the relations between these problem formulations and give existence and uniqueness results.

3. THE SEPARATED CASE

Here we turn to the special case where the nonlinear map F is separated in deterministic parts and some random variables via

$$F(\omega, x) = S(\omega)\, G(x) + H(x)$$

analogously

$$\lambda(\omega, x) = R(\omega)\, b^T x$$

where $F, G : \mathbb{R}^k \mapsto \mathbb{R}^k$ are monotone maps, $b \in \mathbb{R}^k$, and R and S two real valued random variables on Ω. We assume that $S \in L^\infty(\Omega)$ and $R \in L^\alpha(\Omega)$. Further, we consider the random set

$$\mathcal{M}(\omega) := \{x \in \mathbb{R}^k : Cx \leq T(\omega)\}, \; \omega \in \Omega \, .$$

with a matrix $C \in \mathbb{R}^{m\times k}$ and a random m - vector T such that $T \in L^{\alpha}_{m}(\Omega, P)$ In order to get rid of the abstract sample space Ω, we consider the joint distribution $\mathbb{P}$ of the random vector (R, S, T) and work with the special probability space $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mathbb{P})$, where the dimension $d := 2 + m$. Thus we obtain a probabilistic integral formulation of our VI problem.

In this setting we present a discretization technique based on averaging (piecewise constant approximationof the distributions) and truncation, prove a Mosco convergence result for the feasible random set, and establish norm convergence of the approximation procedure for a unique solution.

4. NUMERICAL EXAMPLES AND APPLICATIONS TO TRAFFOC FLOW

First we expand a numerical example from (4) with an 5×5 matrix and the $\arctan$ nonlinearity in the operator F on a simplex-like subset, where the additive parameter becomes an random vector.

Then we study nonlinear traffic flows in congested networks following the Wardrop equilibrium principle. We distinguish between the link and path formulations and discuss the loss of strong monotionicity when passing from the link to the path formulation. We numerically treat small networks, where we admit that the cost vector function and/or the traffic demand are random.

In all these examples we compute the mean values and variances of the solution.

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EXTENSION OF THE AUXILIARY PROBLEM PRINCIPLE USING LOGARITHMIC-QUADRATIC FUNCTIONS

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Keywords: variational inequalities, auxiliary problem principle, logarithmic-quadratic functions

1. INTRODUCTION

The *proximal-point-algorithm* (PPA), originally introduced by Rockafellar (7), and the *auxiliary-problem-principle* (APP), which goes back to Cohen (3) are well-known solution methods for variational inequalities. In the last years, extensions of these methods have been considered e.g. by Kaplan/Tichatschke (5), Eckstein (4), Censor/Iusem/Cenios (2) and Solodov/Svaiter (8). A proximal-auxiliary-problem (PAP) principle, combining the advantages of APP and PPA, was introduced by Kaplan/Tichatschke (6) and a general convergence theory was developed. In an extension of this method they use Bregman distances to achieve an *interior-point-effect*. In our work we replace these Bregman distances by logarithmic-quadratic distance functions which also lead to an interior-point-effect but don't have the disadvantage of requiring paramonotonicity of the operator of the considered variational inequality. As a consequence, the logarithmic-quadratic PAP (LQPAP) can be used for a broader class of variational inequality problems.

2. LQPAP-METHOD

We suppose that the operator of the given variational inequality is splitted into the sum of a maximal monotone, set-valued operator $\mathcal{Q}$ and a single-valued, continuous operator $\mathcal{F}$ and consider the problem

$\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$:

$$\begin{aligned}&\text{find } x^* \in K \text{ and } q^*(x^*) \in \mathcal{Q}(x^*):\\ &\langle \mathcal{F}(x^*) + q^*(x^*), x - x^* \rangle \geq 0 \quad \forall\, x \in K,\end{aligned}$$

where K has to be a polyhedral subset of $\mathbb{R}^n$, given by

$$K = \{x \in \mathbb{R}^n \colon Ax \leq b\}$$

with $A \in \mathbb{R}^{p \times n}$, $\operatorname{rank}(A) = n$, $b \in \mathbb{R}^p$ and $\operatorname{int}(K) \neq \emptyset$.

Our extension of the APP for solving $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ can be subsumed under the following general iterative scheme:

Starting with $x^1 \in \operatorname{int}(K)$, at the $(k+1)$th step we have a current iterate $x^k \in \operatorname{int}(K)$ and calculate x^{k+1} by solving the problem:

(P_δ^k):

$$\begin{aligned}&\text{find } x^{k+1} \in K,\ q^k(x^{k+1}) \in Q^k(x^{k+1}):\\ &\langle \mathcal{F}(x^k) + q^k(x^{k+1}) + \mathcal{L}^k(x^{k+1}) - \mathcal{L}^k(x^k)\\ &\qquad + \chi_k \nabla_I D(x^{k+1}, x^k), x - x^{k+1} \rangle\\ &\qquad \geq -\delta_k \left\| x - x^{k+1} \right\| \quad \forall\, x \in K.\end{aligned}$$

This scheme includes an outer approximation of the operator $\mathcal{Q}$ in each iteration by set-valued operators $\mathcal{Q}^k$ and an inexact solution of the auxiliary problems. The family of monotone and continuous operators $\{\mathcal{L}^k\}$ allows different types of approximations of the operator $\mathcal{F}$. The term $\chi_k \nabla_I D(x^{k+1}, x^k)$ is made up by a positive parameter χ_k and the gradient (with respect to the first vector argument) of a distance function D.

As a special case we get the classical inexact PPA by setting $\mathcal{Q} = \mathcal{F} + \mathcal{Q}$, $\mathcal{F} = \mathbf{0}$, $\mathcal{Q}^k = \mathcal{Q}, \forall k$, $\mathcal{L}^k = \mathbf{0}, \forall k$, and $D(x, y) = \frac{1}{2} \|x - y\|^2$. A general inexact APP-scheme emerges from (P_δ^k) by choosing $\mathcal{F} = \mathcal{F} + \mathcal{Q}$, $\mathcal{Q}^k = \mathbf{0}, \forall k$, and

$$D(x, y) = h(x) - h(y) - \langle \nabla h(y), x - y \rangle \quad (1)$$

with h continuously differentiable and ∇h Lipschitz on K. Then, $\mathcal{L}^k + \chi_k \nabla h$ plays the role of the auxiliary operator. Kaplan/Tichatschke showed in (5), that in scheme (P_δ^k) it is possible to take a distance function like in (1) but with a Bregman-function h, although the gradient map of a Bregman-function is not Lipschitz.

In our PAP-method with logarithmic-quadratic distances, D is declared with the help of the following function which was first introduced by Auslender (1): For $v \in \mathbb{R}^p_{++}$ define

$$d(u,v) := \begin{cases} \sum_{i=1}^p u_i^2 - u_i v_i - v_i^2 \log \frac{u_i}{v_i} & \text{if } u \in \mathbb{R}^p_{++} \\ +\infty & \text{otherwise.} \end{cases}$$

$d(\cdot, v)$ is a proper, lower semi-continuous and convex function, nonnegative and $d(u,v) = 0$ if and only if $u = v$. Further, $\mathrm{dom}(d(\cdot, v)) = \mathbb{R}^p_{++}$. Setting $l(x) := b - Ax$ we get the distance function

$$D(x,y) := d(l(x), l(y)), \tag{2}$$

which is not of Bregman-type, because it can't be constructed like in (1) with a Bregman-function h.

Two properties of D are important: First of all $\nabla_I D(\cdot, x^k)$ is strictly monotone for all $x^k \in \mathrm{int}(K)$. Together with a positive parameter χ_k this ensures that if the auxiliary problems (P^k_δ) are solvable they are uniquely solvable. This regularization effect enables us to deal with ill-posed problems. Second, it holds that the effective domain of $\nabla_I D(\cdot, x^k)$ coincides with $\mathrm{int}(K)$. This leads to an interior-point-effect, which means that the auxiliary problems (P^k_δ) can be treated as unconstrained ones, because all iterates will automatically belong to the interior of the restriction set K.

3. CONVERGENCE ANALYSIS

The assumptions in our convergence theorem are not stronger than those typically made for the PPA with Bregman-functions or the APP.

Apart from the already mentioned properties of the involved operators, we need that $\mathrm{dom}(\mathcal{Q}) \cap K$ is a nonempty and closed set and $\mathrm{ri}(\mathrm{dom}(\mathcal{Q})) \cap \mathrm{int}(K) \neq \emptyset$. Further, the operators $\mathcal{F} - \mathcal{L}^k$ must fulfill a sort of Dunn-property and the family $\{\mathcal{L}^k\}$ a continuity-property which is especially fulfilled if we have the uniformly Lipschitz continuity of the operators $\mathcal{L}^k$. To approximate the operator $\mathcal{Q}$ one can for example choose the ϵ-enlargements $\mathcal{Q}_{\epsilon_k}$ with $\epsilon_k \geq 0, \forall k$ and $\sum_{k=1}^\infty \epsilon_k < +\infty$.

The regularization parameter χ_k can vary from iteration to iteration, but has to be greater than a special positive constant. The error tolerance criterion is simply

$$\sum_{k=0}^{\infty} \left\| e^{k+1} \right\| < +\infty$$

which can easily be implemented.

If $\mathrm{VI}(\mathcal{F}, \mathcal{Q}, K)$ is solvable we can prove convergence of the iterates $\{x^k\}$ generated by the LQPAP-method towards a solution.

4. CONCLUSIONS

We considered a general iteration scheme for solving variational inequalities, which can be viewed as an extension of the auxiliary-problem-principle. As regularization term we use a logarithmic-quadratic function that leads to an interior-point-effect. In contrast to the usage of Bregman distances we don't have to require paramonotonicity of the operator of the variational inequality which opens our algorithm to a wider class of problems.

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Extended Auxiliary Problem Principle using Bregman distances

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Keywords: Variational inequalities, regularization, Bregman functions

1. Introduction

Let $(V, \|\cdot\|)$ be a Hilbert space with the topological dual V' and the duality pairing $\langle\cdot,\cdot\rangle$ between V and V'. The variational inequality **(VI)**

$$find\ u^* \in K\ and\ q^* \in \mathcal{Q}(u^*):$$
$$\langle \mathcal{F}(u^*) + q^*, u - u^*\rangle \geq 0\ \ \forall\ u \in K \quad (1)$$

is considered, assuming that $K \subset V$ is a convex closed set, $\mathcal{Q} : V \to 2^{V'}$ is a maximal monotone operator and $\mathcal{F} : K \to V'$ is a weakly continuous operator with certain monotonicity properties.

In the sequel we denote by $\{K^k\}$ a family of convex closed sets, approximating K, $K^k \subset V$; and by $\{\mathcal{Q}^k\}$ a family of operators, approximating $\mathcal{Q}$. Usually, it is supposed that $\mathcal{Q}^k$ is maximal monotone, or that

$$\mathcal{Q} \subset \mathcal{Q}^k \subset \mathcal{Q}_{\epsilon_k},$$

$\mathcal{Q}_\epsilon$ means the ϵ-enlargement of $\mathcal{Q}$.

In proximal point methods **(PPM)** and the Auxiliary Problem Principle **(APP)**, a regularizing functional h of Bregman type with zone S is used, where

$$S := V, \qquad h : u \mapsto \frac{1}{2}\|u\|^2.$$

In this paper we use a regularizing functional h of Bregman type with zone $S = \mathrm{int}K$ and consider the following general scheme for solving VI (1):

At step $k+1$, having a current iterate u^k ($u^1 \in K \cap S$ is arbitrarily chosen)
the point u^{k+1} is calculated by solving the problem

$$(P_\delta^k)\ find\ u^{k+1} \in K^k \cap \bar{S},\ q^k \in \mathcal{Q}^k(u^{k+1}):$$
$$\langle \mathcal{F}(u^k) + q^k + \mathcal{L}^k(u^{k+1}) - \mathcal{L}^k(u^k)$$
$$+\chi_k(\nabla h(u^{k+1}) - \nabla h(u^k)), u - u^{k+1}\rangle \quad (2)$$
$$\geq -\delta_k\|u - u^{k+1}\|\ \ \forall\ u \in K^k \cap \bar{S}.$$

Here $\{\delta_k\}$ is a non-negative sequence with $\lim_{k\to\infty}\delta_k = 0$, whereas $0 < \chi_k \leq \bar{\chi} < \infty$.
The main advantage consists in the "interior point effect" of this approach, i.e., (P_δ^k) is in fact an unconstrained problem.

2. Set and operator approximation

In the literature, in different regularization methods when approximation of the set K is included, usually it is supposed that $\{K^k\}$ converges to K "sufficiently" fast in the Hausdorff or Mosco sense, for example:

$$dist_H(K^k, K) \leq c\varphi_k, \qquad \sum \frac{\varphi_k}{\chi_k} < \infty.$$

However, this type of assumptions is not very realistic when dealing with VI's in Mathematical Physics. Indeed, constructing $\{K^k\}$, $K^k = K_{h_k}$, by means of the FEM on a sequence of triangulations with parameter $h_k \to 0$, as well as by related FDM, we meet the following typical situation:

(i) for $v \in K$ and $v^k := \arg\min_{z\in K^k}\|v - z\|$ it holds

$$\lim_{k\to\infty}\|v - v^k\| = 0;$$

(ii) for $v \in U^*$ (solution set) it holds

$$\|v - v^k\| \leq c(v)h_k^{\beta_1},\ \beta_1 > 0;$$

(iii) for a bounded sequence $\{w^k\}$, $w^k \in K^k$, the estimate

$$\min_{v\in K}\|v - w^k\| \leq ch_k^{\beta_2},\ \beta_2 > 0$$

is valid (of course, $c = 0$ fits the case $K^k \subset K$, but this inclusion is not guaranteed, in general).

Thus, because of the weak property (i), FEM cannot provide the required Hausdorff or Mosco approximation of K.

Considering (i)-(iii) as conditions, together with

$$\sum \frac{\varphi_k}{\chi_k} < \infty, \tag{3}$$

where $\varphi_k := \max\{h_k^{\beta_1}, h_k^{\beta_2}\}, \qquad \sum \frac{\delta_k}{\chi_k} < \infty$ we deal with quite different requirements on the type of approximation (cf. (3)).

An approximation of $\mathcal{Q}$ by means of smoothing procedures or the use of the ϵ-enlargement concept will be discussed, too (cf. (4)).

3. Bregman-function-based methods

To our knowledge, Bregman functions h with zone $S \neq V$ have not been used in connection with APP.

In different variants of APP the operator ∇h is supposed to be Lipschitz continuous on K or on some set $\hat{K} \supset K$. This excludes the use of Bregman-like functions with zone $S \not\supset K$, and in particular with $S \subset K$.

In fact, Bregman functions with zone $S \subset K$ provide a full "interior point effect", i.e. with a certain precaution the auxiliary problems can be treated as unconstrained ones.
Now, we consider scheme (2), allowing $S \subset K,\ S := intK$. Conditions on h require that

$$S \cap D(\mathcal{Q}) \cap K^k \neq \emptyset, \qquad \bar{S} \cap U^* \neq \emptyset.$$

In order to use our convergence analysis in this case, an approximation of K has to be inserted into the algorithm for solving the subproblems. I.e., the subproblems are considered with $K^k := K$ and within the process of their solution by an appropriate method the approximation of K is realized.

However, in general some additional assumptions on the operator $\mathcal{Q}$ are needed, even for the exact PPM with strongly convex h. If $\mathcal{Q}$ is not symmetric, the paramonotonicity and pseudo-monotonicity (in the sense of Brezis-Lions) of $\mathcal{Q}$ are supposed. In case $V := \mathbb{R}^n$, Solodov/Svaiter (6) have shown that the pseudo-monotonicity requirement can be omitted, but their arguments are finite-dimensional in essence.

The convergence of the extended APP in form (P_δ^k) with Bregman function h is proved under certain assumptions (cf. (5)).

Up to now, zone - or boundary coercive Bregman functions with zone $\mathrm{int}K$ have been created only for linearly constrained sets K or in the case that K is a ball.

The more general case

$$K = \{x \in \mathbb{R}^n : g_i(x) \leq 0, \quad i \in I_1 \cup I_2\},$$

where $I_1 \cup I_2 = I = \{1, ..., m\}$, and

$$\begin{aligned} &g_i\ (i \in I_1)\ \text{ affine functions,}\\ &g_i\ (i \in I_2)\ \text{convex}, C^1\ \text{functions,}\\ &\max\{g_i :\ i \in I_2\}\ \text{is strictly convex on}\ \ K, \end{aligned}$$

$$\exists\ x :\ g_i(x) < 0, \quad \forall\ i \in I,$$

allows us to use a special class of Bregman functions with zone $\mathrm{int}K$ (see (5)):

$$h(x) = \sum_{i=1}^{m} \varphi(g_i(x)) + c\|x\|^2,\ (c > 0). \tag{4}$$

Certain properties and particular realizations of the function φ will be discussed.

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EVOLUTIONARY METHODS IN MULTISCALE MODELING

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Keywords: multiscale modeling, FEM, evolutionary algorithm.

1. INTRODUCTION

The nanomechanics (Bhushan B., 2004) plays important role in todays world. The models of materials behaviour in the atomistic scale allows to understand the micro, meso and macroscopic events. There is also possibility to connect models in different scales which leads to powerful analysis systems. The analysis at the nanoscale level can be performed using molecular dynamics and statics. The nano model is highly nonlinear and modifications of the Newton-Raphson method are used in molecular statics (Kwon Y. W. 2003). The discrete atomic model can be also analysed with use of global optimization methods. The minimum of the total potential energy is connected with the final positions of atoms. The evolutionary methods (Burczynski T., Osyczka A., 2004), (Michalewicz Z., 1992) are well known global optimization algorithms and can be used in such an approach. The combination of the evolutionary algorithm and classical approaches based on the objective function gradient speeds up the computations reducing overall number of objective function evaluations (Burczyński T., Orantek P., 2001). The multiscale computations are performed by combining the hybrid evolutionary approach for nanoscale and the Finite Element Method (Zienkiewicz O. C., Taylor R. L., 2000) for the microscale level. The evolutionary algorithm can be also used as the shape and topology optimization tool for multiscale models.

2. MULTISCALE ANALYSIS WITH USE OF EVOLUTIONARY ALGORITHM

A material system is divided into regions. For the regions were highly nonlinear phenomena occurs a discrete model is used, the rest of the model is discretized using finite elements (Fig. 1).

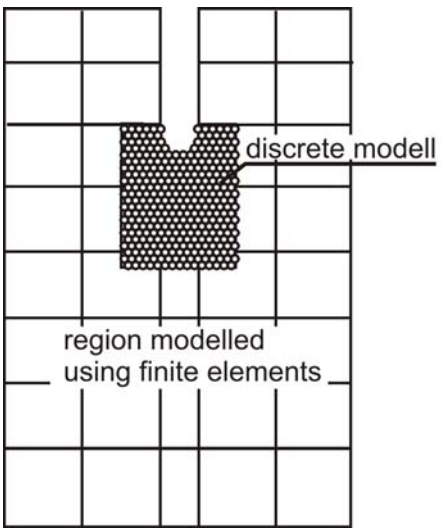

Fig. 1. A two-scale model of the material system

The flowchart of analysis algorithm is presented in Fig. 2. The analysis problem is computed using FEM in the first step. The displacements values on the boundary between the FEM and discrete models are transferred to the nano-model. The evolutionary algorithm is used to find the proper atom positions in discrete model. The resultant forces (the influence from the discrete model on the FEM model) on the boundary between scales are mapped as the forces. The computations of new displacements values are performed using FEM considering forces and previously obtained displacements on the boundary between scales. The algorithm works iteratively until the end computations criterion is fulfilled. The evolutionary computations for the discrete region (Mrozek A., Kuś W., Orantek P., Burczyński T., 2005) are performed by using the fitness function described as the total potential energy of that part of the structure. The chromosomes contain information about atoms positions. The genes values are connected with coordinates of atoms. The number of genes is equal to the number of "free atoms" multiplied by number of degrees of freedom (2 in 2D, 3 in 3D). The term "free atoms" means atoms not constrained. The atoms are constrained on the boundary between scales (the displacements of that atoms are mapped from the finite element model). The real coding is used – the atom coordinates are not coded into binary strings. The ranking selection is used and evolutionary operators such as: the Gaussian and normal mutation and the simple crossover. The gradient mutation (Burczyński T., Orantek P., 2001) is used in hybrid evolutionary algorithm. The gradient mutation are invoked in every iteration of the evolutionary algorithm. The gradient mutation perform few steps toward optimum for the best known solution in the population. The hybrid approach allows to speedup computations, and low number of gradient mutations do not ruin global optimization nature of the evolutionary algorithm.

3. REMARKS

The full paper and presentations during conference will contain more detailed information about used inter atoms potentials, the evolutionary algorithm and the coupling method. The numerical examples of analysis performed with the use of the evolutionary approach and optimization of multiscale structures will be shown.

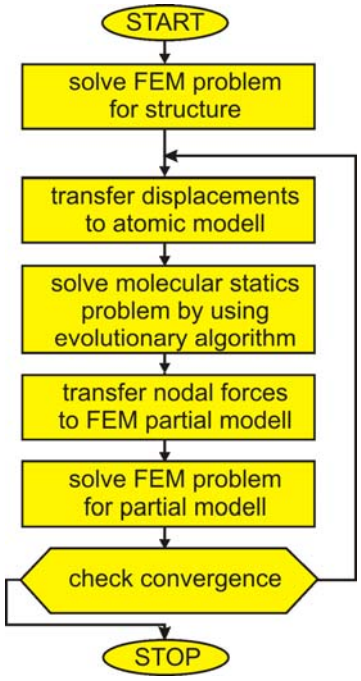

Fig. 2. Flowchart of multiscale analysis

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Identification of the multi scale CAFE model using the inverse method

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1. INTRODUCTION

Accuracy of simulations of materials processing depends on proper description of phenomena occurring during deformation. Rheological models usually treat material as continuum and are unable to describe properly several important phenomena. Therefore, a search for alternative models, which account for non-continuous structure of materials and for the fact, that various phenomena in the materials occur in various scales, is the objective of research. Accounting for the stochastic character of phenomena is an additional challenge. Multiscale models, see eg. (Das, 2002), are one of the solutions capable to overcome mentioned difficulties.

Authors have developed multiscale models based on combination of the Finite Element (FE) method and Cellular Automata (CA). Such model describing development of the strain localization during material processing (Madej et al., 2007) is one of the CAFE method applications. Numerical tests confirmed qualitatively good predictive capability of the model. Problem of quantitative accuracy still remains open.

Application of the inverse analysis methodology (Szeliga et al., 2006) to determine parameters of the developed rheological model is the subject of this work, and is a step towards qualitatively good predictive capabilities of the CAFE model.

2. IDENTIFICATION OF THE CAFE MODEL

Strain localization in deformed material is a result of simultaneous initiation and development of micro and shear bands in the micro and mezo scale, respectively. According to these two scales, in the approach proposed in (Madej et al., 2007), two CA spaces representing the material behavior in the micro scale (micro shear band space - MSB space) and mezoscale (shear band space - SB space) are introduced and attached to the FE code. Both CA spaces are defined by several state variables that describe each cell, as well as by a set of transition rules defined for these spaces. Transition rules, which control changes of states in MSB and SB space, are defined based on experimental knowledge (Korbel, 1998; Cizek 2002). The details describing the assumed cell state and proper transition rules are presented in (Madej et al., 2007).

Information about the occurrence of micro shear and shear bands is exchanged between the CA spaces during each time step, according to the defined mapping operations (Fig.1).

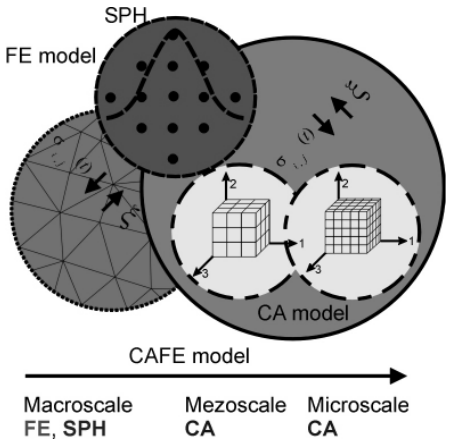

Fig. 1. Scheme of the data flow in the CAFE model.

Financial assistance of MNiI, project 3 T08A 071 26, is acknowledged

Flow of the information between the scales goes in both directions, from macroscale to mezoscale and microscale, as well as from microscale and mezoscale to macroscale. In each time step, information about the stress state is sent from the FE solver to the MSB space, where the development of microshear bands is calculated according to the transition rules. After exchange of information between CA spaces, transition rules for the SB space are introduced, and propagation of the shear bands is modeled. Based on the information supplied by the CA spaces, the flow stress σ_p^{CA} is calculated and is used in the FE program as modified flow curve in the next step. The CAFE model was applied to simulate various tests and industrial processes and good qualitative agreement with the experiment was observe. Evaluation of parameters of the CAFE model by the inverse analysis is performed to obtain better quantitative accuracy.

3. INVERSE ANALYSIS

Particular attention is put on identification of the internal variables that describe each CA cell, such as critical stress $\tau_{\max}^*$ generated by Gauss function (x – expected value σ_{dev} – standard deviation). The slope of the hardening K in the flow stress function $\sigma = K\varepsilon^n$ is the third optimization variable. ε represents effective strain and n is an exponent, which for aluminum is assumed 0.2. Channel test (Fig. 2) is selected as experiment and measurement of the hardness at the cross section of the sample after the test is the experimental data for the inverse analysis. Fig. 2 shows the locations at the cross section where the hardness is measured.

Algorithm was tested first and experimental data were generated by the FE code. Fig. 3 shows distribution of hardness along sample obtained for x = 380 MPa, σ_{dev} = 100 MPa and K = 425 MPa which was considered an experimental results in the objective function defined as:

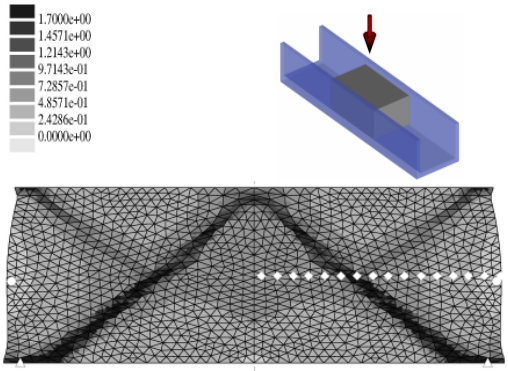

Fig. 2. View of the channel test (top) and cross section of the sample after compression showing distribution of strains and location of points, at which the hardness was measured.

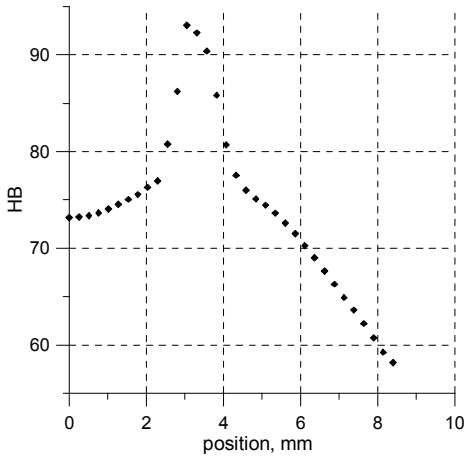

Fig. 3. Harness along the sample, which is used as an input for the inverse analysis.

$$\Phi = \sqrt{\sum_{i=1}^{N} \frac{1}{N} \left(\frac{HB_{\exp}^i - HB_{calc}^i}{HB_{\exp}^i} \right)^2} \qquad (1)$$

where: HB_{exp}, HB_{calc} – measured and predicted hardness, N – number of sampling points.

Optimization yielded the values of the optimization variables (x, σ_{dev}, K), which are close to the assumed.

4. CONCLUSIONS

Method of identification of parameters in the CAFE model is presented in the paper. It is shown that the parameters of the model can be predicted using hardness measurements as input.

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Size-Effects in Metal Forming Processes

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Keywords: Metal Forming, Size-Effects, FEA

1. Introduction

The finite element analysis (FEA) has become a significant tool for planning, analysis and optimization of metal forming processes in industrial manufacturing. Though results obtained by numerical simulations have to be verified experimentally. This leads to high tooling costs for practical trails and results in extra downtimes. For this reason, the experimental investigations are often performed on reduced-scale test models by using the similarity theory. The real process variables are calculated from the computed model values. Up till now, commercial FE-systems for bulk metal forming do not take size-effects into consideration.

2. Experimental Investigations

In a current research work at IFUM, the size effects is determined experimentally. The results will be implemented in commercial FE-softwares by programming user-defined subroutines. First, upsetting and ring compression tests were performed to quantify the size effects for the yield stress σ_f and the friction factor m. Cylinder compression tests are carried out on work pieces of different sizes and temperatures. The specimen sets have a volume ratio of 4:2:1 at a constant diameter to height ratio. The determined yield curves show obvious differences (Fig. 1). Because of the deviations resulting from the inaccuracy of upsetting plates parallelism, it is difficult, up till now, an assured definition of a principle in terms of size effect on the flow stress.

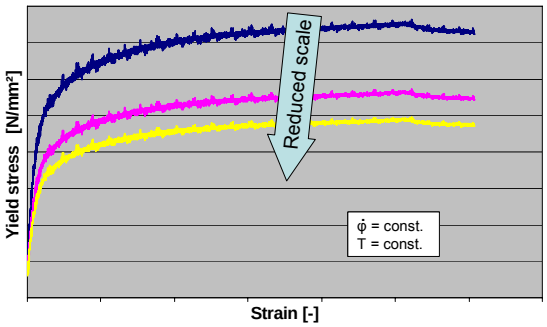

Fig. 1 Array of yield curves (schematic pictorial)

In addition, ring compression tests were performed on different sets of specimens with the same geometric conditions as the upsetting tests. The results of these investigations show that the forming temperature has a significant influence on the friction factor, especially in dry friction conditions, because of adhesion effects. Potential size effects can be superposed. Additional ring compression tests under appropriate lubrication conditions are essential to obtain more precisely predictions concerning the size effects on the friction behavior.
The experimental investigations accomplished so far show significant size effects on the flow stress and the friction factor in bulk metal forming processes. Further upsetting and ring compression tests are necessary for an accurate quantification.

3. Integration of Size-effects in FEA

The next step is to implement the achieved results in the FE-software by programming of user-defined subroutines to generate size dependant yield curves and friction factors. According to mesh size, different flow curves and friction conditions will be called by the FE-Software (Fig. 2).

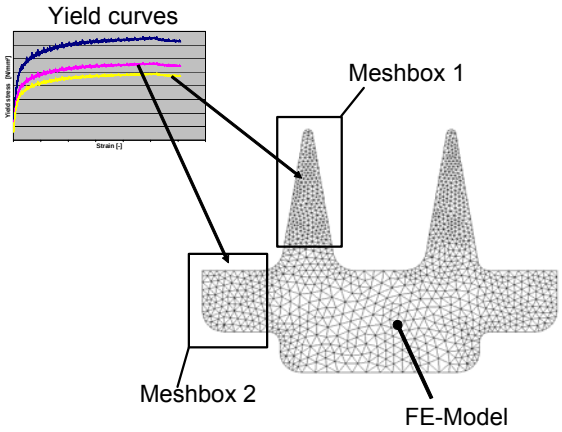

Fig. 2 Implementation of size-effects in the FEA (example)

4. CONCLUSIONS

So far the experimental investigations show significant size-effects on the yield stress and the friction coefficient. Further upsetting and ring compression tests are necessary to determine the results more precisely.
After implement the size-dependent effects in the FEA complex component will be forged to verify the improved simulation.

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GLOBAL OPTIMIZATION OF SHELL STRUCTURES WITH SMALL FEATURES BY USING MULTISCALE APPROACH

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Keywords: multiscale modelling, global optimization, FEM

1. INTRODUCTION

The analysis and optimization of shell structures plays important role in industry. The metallurgical furnace, pressure vessels, housings are modelled as shell surfaces. The important issue in the analysis is sometimes, taking into account small features – holes, holders. The computations without theses small parts give quite good results when a big factor of safety is used. The goal of the paper is to present a global optimization method which allows to use low safety factors due to proper modelling of a structure taking into account small features influence. The multiscale approach is used. The two scales are presented in the paper – one connected with the structure, the other with small features of the structure. The Finite Element Method is used in each scale (Zienkiewicz O. C., Taylor R. L., 2000). The evolutionary algorithm (Michalewicz Z., 1992) is used as a global optimization method. The design variables are coded into chromosomes in the form of genes and the evolutionary optimization is used. The optimization of the structures with use of evolutionary algorithms was presented in many papers for different problems e.g. Burczyński T., Osyczka A., 2004. Additionally, in the presented calculations, the grid-based evolutionary algorithm is used (Kuś W., Burczyński T., 2006).

2. MULTISCALE FEM ANALYSIS

The analysis is performed using two scales – macro and micro. The structure is modelled as a macro scale first. A part of the structure with small features is removed from the macro scale and modelled as a microscale. The example of such a structure is presented in Fig. 1.

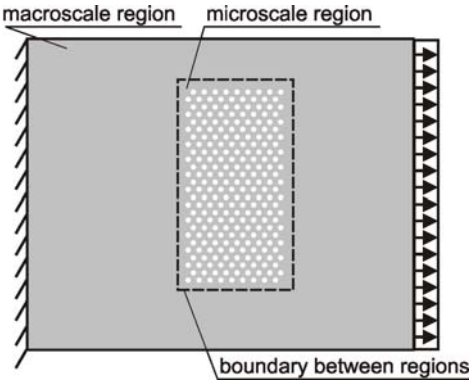


Fig. 1. Macro-micro model of the structure

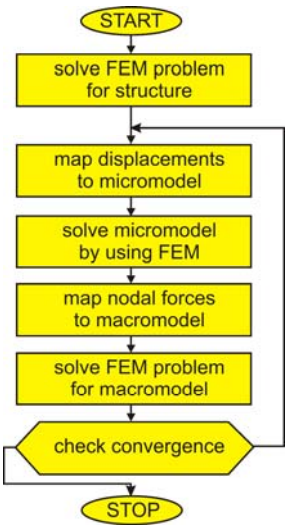


Fig. 2. Algorithm for macro-micro FEM

The "small features" in the example are small circular voids (for example in cooling structure). The analysis of the structure is performed using FEM. The macro and micro regions are computed as shown in the flowchart Fig. 2. The material of regions can be modelled as linear or nonlinear, also combination can be used. The most efficient approach will be use nonlinear model of the material for micro regions and linear material for macro, of course if the nonlinearities occur only in micro zones.

3. EVOLUTIONARY OPTIMIZATION

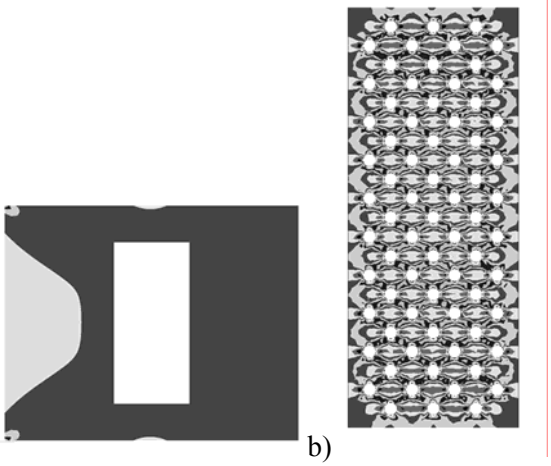
The goal of the evolutionary optimization is to reduce a mass of the considered structure. The genes contain information about thickness of different regions of the shell. The real coding is used in the paper. The constraints on maximum equivalent stresses are imposed. The constraints are introduced as a penalty function (in most cases a chromosome with the described structure with too big stresses is eliminated during the selection process). The Gaussian and uniform mutations, the simple crossover are used. The selection is performed using the ranking selection algorithm.
The number of fitness function evaluations, when the evolutionary algorithm is used, can be in factor of hundreds or even thousands. The most computational time is taken by the FEM analysis. Therefore the parallel evolutionary algorithm is used. The fitness function evaluation is performed in the parallel way. The grid-based evolutionary algorithm is used (Kuś W., Burczyński T., 2006). The algorithm works in parallel, additionally computational grids (Foster I., Kesselman C., 2003) can be used during computations.

4. NUMERICAL RESULTS

The shell shown in Fig. 1. is considered. Two test were performed. The shell was modelled as solid one, without influence of small holes – equivalent stresses are shown in Fig. 3.

Fig. 3. Equivalent stresses plate without considering influence of small features

The second test uses multiscale modelling. The macroscale region is shown in Fig. 4a, the microscale region in Fig. 4b.



a) b)

5. CONCLUSIONS

In the full paper more details about analysis and optimization of shell structures by using multi scale approach will be presented. Additional examples will be presented too.
The micro and macro regions can be both treated as linear, nonlinear or macro as linear and micro as nonlinear. The method shown in the paper allows to optimize structures with regions with small features which significantly influence on the effort of the entire structure.

ACKNOWLEDGEMENTS

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IDENTIFICATION OF MATERIAL MODELS IN HARD SYSTEM OF NANOCOATINGS USING METAMODEL

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Keywords: inverse analysis, metamodel, artificial neural network (ANN)

1. INTRODUCTION

Hard systems of nanocoatings deposited using PVD (physical vapour deposition) are used in various applications. Numerical models of deformation of these coatings are needed for aiding design of new applications of these coatings. Correct determination of nanomaterial parameters is crucial for accuracy of simulations. FEM and ANN (Koker et al., 2007) are often used to obtain parameters of models for various materials. The objective of the present work is identification of material parameters of nanocoatings in hard system using both mentioned methods (Kopernik et al., 2007). The inverse analysis is performed using a metamodel (Kusiak et al., 2005).

2. MODEL OF NANOINDENTATION TEST

Experimental nanoindentation test is performed using a Nano Test System. In the present work deformed 840 nm thick and 2600 nm wide specimen is a system of 3 hard nanocoatings. Two coatings are deposited periodically, respectively coating 1 (elastic, 400 nm thick) is repeated two times and coating 2 (elastoplastic, 40 nm thick) is a single interlayer. Indentation test, which is depth controlled, supplies force versus indentation depth data. Diamond (Young modulus E = 1141 GPa, Poisson ratio ν = 0.07), pyramid, deformable indenter (radius R = 150 nm, pyramid angle α = 70.32º) penetrates into specimen at a depth of 100 nm. Application of the inverse analysis to interpretation of the test results is the objective of the project. Inverse algorithm proposed in (Szeliga et al., 2006) is used. Due to very high computing costs, the concept of the metamodel (Kusiak et al., 2005) is applied in optimization. ANN was used as metamodel. FORGE 2 FEM code is used as direct problem model. Axisymmetric 2D FEM solution is performed. The friction coefficient μ is assumed 0. The following material model is identified:

$$\sigma = K\varepsilon^n \tag{1}$$

where: σ – flow stress, ε - effective strain, K, n –parameters, which are optimization variables. Young modulus E is the third variable. Since testing of the approach is the main objective, the experimental data were generated by the FEM code. Two cases are considered. Two sets were assumed as the real material parameters: I) n = 0.125, E = 380 GPa, K = 290 MPa and II) n = 0.175, E = 400 GPa, K = 270 MPa. 120 simulations were performed to supply data for training ANN, for the following parameters:

a) K = 50, 60, 100, 110, 300, 310 MPa;
b) n = 0.1, 0.15, 0.2, 0.25;
c) E = 330, 350, 370, 390, 410 GPa.

3. METAMODEL AND RESULTS

Approximation of FEM output data is done using MLP - type of ANN with architecture 4-2-1 and logistic functions of transfer in the first and second network layers, and linear function of activation in output network layer. Optimization variables in the inverse analysis (E, K, n) and strain are the input data and the load is the output. 90 training sets of data for n, K and E were used as an input. Each set is composed of 20 values of force versus displacement data.

The network was tested for n = 0.15, E = 370 GPa, K = 100 MPa and the results are shown in

Figure 1. Mean square error for test sets is equal to 40 μN^2 what confirms good predictive capability of the network as the metamodel.

Inverse analysis was performed next. The goal function is the mean square root error between experimental data and network output:

$$\phi(n,E,K)=\frac{1}{N}\sum_{i=1}^{N}\left(F_{exp}(i)-F_{ANN}(n,E,K,d_i)\right)^2$$

where: F_{exp} – experimental force, generated by FEM for the assumed real material parameters, F_{ANN} - force predicted by ANN, d_i – displacement, N - umber of sampling points.

Genetic algorithm is used as optimization algorithm. The results for both cases I and II are presented in Figure 2. Evaluated minimum is found at n = 0.11, E = 384 GPa, K = 280 MPa for case I and n = 0.17, E = 397 GPa, K = 331 MPa for case II. The goal function is respectively ϕ = 34 μN^2 and ϕ = 21 μN^2.

Figure 3 shows results of simulation of strain distribution in the sample, using the material parameters determined from the inverse analysis for the case I.

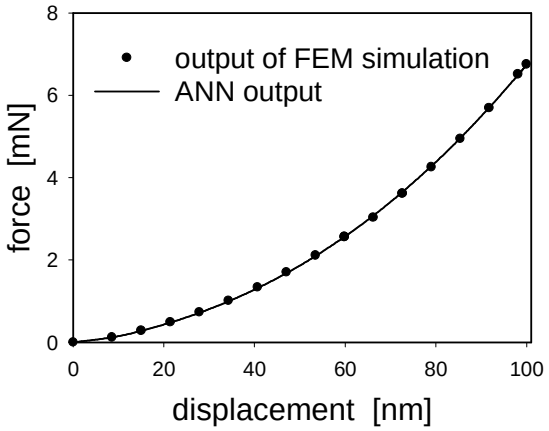

Fig. 1. Results of the network test set for work-hardening curve (n = 0.15, E = 370 GPa, K = 100 MPa).

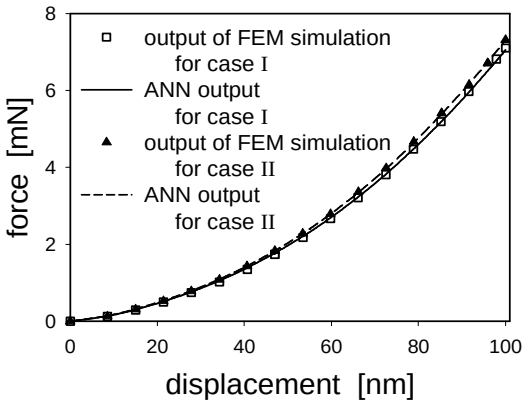

Fig. 2. Results of inverse analysis for the case I and the case II.

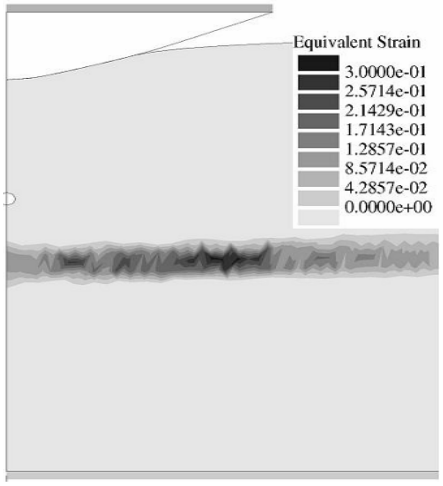

Fig. 3. Strain distribution in the 2D axisymmetric sample for material parameters determined from the inverse analysis for the case I.

6. CONCLUSIONS

Presented approach is useful technique for optimization in problems characterized by high goal function computing costs. The algorithm allows to decrease the number of time-consuming FEM calculations. Presented problem of optimization of flow stress parameters for nanocoatings proved efficiency of the method. Good predictive capability of the trained ANN was confirmed. Low value of the goal function was obtained also in the inverse analysis, but the minimum is weak and problem of uniqueness of the solution exists.

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ELLIPTIC CONTROL BY GENERAL PENALTY TECHNIQUES WITH CONTROL REDUCTION

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Keywords: elliptic control problem, distributed control, penalty method, control reduction

1. PROBLEM AND OPTIMALITY CHARACTERIZATION

In this paper we study the numerical treatment of optimal control problems with bounded distributed controls and elliptic state equations by barrier-penalty methods. Let $\Omega \subset \mathbb{R}^2$ be some bounded convex domain and let be given $q, b \in L_\infty(\Omega)$. Considered is the following optimal control problem

$$\begin{aligned} J(y,u) &:= \frac{1}{2}\int_\Omega (y-q)^2 + \frac{\alpha}{2}\int_\Omega u^2 \to \min! \\ \text{s.t. } -\Delta y &= u \quad \text{in } \Omega, \\ u + \frac{\partial y}{\partial n} &= 0 \quad \text{on } \Gamma := \partial\Omega, \\ u &\in U_{ad}, \end{aligned} \tag{1}$$

where $\alpha > 0$ denotes a regularization parameter and the set of admissible controls is defined by

$$U_{ad} := \{u \in L_2(\Omega) : u \le b \quad \text{a.e.in } \Omega\}. \tag{2}$$

The only one-sided bounds serves to simplify the presentation, but does not principally restrict the considered class of problems. The state equations of the given problem (1) are understood in the weak sense of the Sobolev space $V := H^1(\Omega)$. With the usual bilinear form $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ defined by

$$a(y,v) := \int_\Omega \nabla y \cdot \nabla v + \int_\Gamma yv \quad \forall y, v \in V \tag{3}$$

for any $u \in U_{ad}$ there exists a unique $y \in V$ such that

$$a(y,v) = (u,v) \quad \forall v \in V.$$

With the continuous embedding $V \hookrightarrow L_2(\Omega)$ by $Su := y$ this defines a continuous linear mapping $S : V \to L_2(\Omega)$ and problem (1) can be reduced to its equivalent form

$$\hat{J}(u) := J(Su,u) \to \text{ min! } \quad \text{s.t. } u \in U_{ad}. \tag{4}$$

Since U_{ad} is nonempty, closed and convex and $\hat{J}$ is continuous and strongly convex problem (4) possesses a unique optimal solution $\bar{u}$ and $(S\bar{u}, \bar{u}) \in V \times U_{ad}$ is the unique optimal solution of (1).

Under the made assumptions for the optimality is that the following system necessary and sufficient.

$$\begin{aligned} (\bar{y} - q, y) + a(y, \bar{v}) &= 0 \quad \forall y \in V, \\ a(\bar{y}, v) - (\bar{u}, v) &= 0 \quad \forall v \in V, \\ \alpha(\bar{u}, u - \bar{u}) - (u - \bar{u}, \bar{v}) &\ge 0 \quad \forall u \in U_{ad}, \end{aligned} \tag{5}$$

where the inequality is equivalent to

$$\bar{u} = P(\bar{u} - \sigma(\bar{v} + \alpha\bar{u})) \tag{6}$$

for any $\sigma > 0$, where P denotes the $L_2(\Omega)$-orthoprojection onto U_{ad}. With the particular choice $\sigma = 1/\alpha$ this enables to eliminate $\bar{u}$ from the remaining system. This approach was proposed by Hinze (2) and has the advantage that only $\bar{y}, \bar{v}$ occur that are much smoother than $\bar{u}$. This fact is important for the discretization and leads to optimal convergence rates.

2. GENERAL PENALTIES

The well know idea of barrier-penalty methods is to augment the objective by some term that penalizes either the closedness to the boundary of U_{ad} in case of interior point methods (for the logarithmic barrier see e.g. Weiser/Gänzler/Schiela (3)) or the violation of the constraint in U_{ad} in case of pure penalties. In accordance with the structure of U_{ad} we consider the following barrier-penalty modification

$$\tilde{J}(u,s) := \hat{J}(u) + \int_\Omega \phi(u(x) - b(x), s)dx \tag{7}$$

of the objective. Here $s > 0$ denotes the penalty parameter that has to tend to 0 and $\phi : \mathbb{R} \to \overline{\mathbb{R}}$

denotes some barrier-penalty function that satisfies

$$\frac{\partial}{\partial t}\,\phi(t,s) \;=\; \psi\left(\frac{t}{s}\right)\;\forall t \in \operatorname{dom}\phi(\cdot,s) \qquad (8)$$

with an appropriate function $\psi : \mathbb{R} \to \overline{\mathbb{R}}$.. For finite dimensional optimization problems such a general barrier-penalty class has been discussed in Grossmann/Zadlo (1). Here we restrict us either to the quadratic loss or to the smoothed exact penalty defined by

$$\psi(t) := \max\{0,t\} \text{ and } \psi(t) := \delta\,(1+\frac{t}{\sqrt{1+t^2}}).$$

respectively, were $\delta > 0$ denotes some appropriate constant. For a detailed discussion of the general assumption upon ψ as well as for further types of barrier-penalty functions we refer to Grossmann/Zadlo (1). Under mild additional assumptions holds

Theorem *For any $s > 0$ the penalty problem*

$$\tilde{J}(u,s) \to \textit{ min! } \quad \textit{s.t. } u \in L_2(\Omega) \qquad (9)$$

possesses a unique solution $\bar{u}(s)$ and there holds $\lim_{s\to 0+} \bar{u}(s) = \bar{u}$.

3. CONTROL REDUCTION

The treatment of the restrictions of the controls in (9) by (7) leads to the necessary and sufficient optimality condition

$$\begin{aligned}(\bar{y}-q,y) - a(y,\bar{v}) &= 0 \quad \forall y \in V,\\ -a(\bar{y},v) + (\bar{u},v) &= 0 \quad \forall v \in V,\\ \alpha\bar{u} + \bar{v} + \psi((\bar{u}-b)/s) &= 0 \quad \text{a.e. in } \Omega.\end{aligned} \qquad (10)$$

For any $s > 0$ this system possesses a unique solution $(\bar{y}(s),\bar{v}(s),\bar{u}(s))$. The structure of the considered functions ψ guarantee that from the last equation the optimal control $\bar{u}$ can be determined in dependence of $\bar{v}$. Due to the regularity $\bar{v} \in H^2(\Omega) \hookrightarrow C(\bar{\Omega})$ of the adjoint this can be done by pointwise elimination. Let denote this by $\bar{u}(s) = g(\bar{v}(s),s)$. Thus, (10) leads to a parametric control reduced optimality system

$$\begin{aligned}(\bar{y}(s)-q,y) - a(y,\bar{v}(s)) &= 0 \quad \forall y \in V,\\ -a(\bar{y}(s),v) + (g(\bar{v}(s),s),v) &= 0 \quad \forall v \in V.\end{aligned} \qquad (11)$$

This forms a coupled system of weakly nonlinear partial differential equations. There holds

Theorem *For any $s > 0$ the system (11) possesses a unique solution $(\bar{u}(s),\bar{v}(s)) \in V \times V$ and $\bar{u}(s) := g(\bar{v}(s),s)$ forms the optimal solution of the parametric barrier-penalty problem (9).*

Since the optimal state $\bar{u}$ as well as the optimal adjoint state $\bar{v}$ possess a higher regularity than the optimal control $\bar{u}$ problem (11) allows an efficient treatment by discretization techniques, e.g. by finite elements. However, it has to be noticed that the limit properties of barrier-penalty functions asymptotically lead to ill-conditioned problems for $s \to 0+$. The details of these properties are under investigation.

4. DISCRETIZATION

Conforming finite element discretizations $V_h \subset V$ can be applied to the control reduced system (11). This leads to the finite dimensional system of nonlinear equations

$$\begin{aligned}(\bar{y}_h-q,y_h) - a(y_h,\bar{v}_h) &= 0 \quad \forall y_h \in V_h,\\ -a(\bar{y}_h,v_h) + (g(\bar{v}_h,s),v_h) &= 0 \quad \forall v_h \in V_h.\end{aligned} \qquad (12)$$

Like in the continuous case system (11) defines uniquely the solution $(\bar{y}_h(s),\bar{v}_h(s)) \in V_h \times V_h$. Further, we obtain $\bar{u}_h(s) = g(\bar{v}_h(s),s)$ which unlike in full discretization does not use an a-priori discretization of the space U.

The analysis as well as numerical studies related to this technique are done in cooperation with the diploma students R.Meischner and H.Kunz.

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Goal-oriented adaptive concepts for elliptic optimal control problems in the presence of control and state constraints

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Keywords: Elliptic optimal control problem, control constraints, state constraints, error estimates, goal–oriented adaptivity

1. INTRODUCTION

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a smooth boundary $\partial\Omega$ and corresponding unit outward normal ν. For $U = L^2(\Omega)$ we consider the optimal control problem

$$\min_{u\in U_{ad}} J(y(u),u) = \frac{1}{2}\|y-y_0\|^2_{L^2(\Omega)}+\frac{\alpha}{2}\|u-u_0\|^2_U$$

subject to $y(u)$ solving the elliptic PDE

$$\begin{aligned} Ay &= u \quad \text{in } \Omega \\ \textstyle\sum_{i,j=1}^2 a_{ij} y_{x_i}\nu_j &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

and satisfying the pointwise state constraint $y(x) \le b(x)$ in the whole domain Ω. Further we suppose $U_{ad} = \{u \le d\}$ with d denoting a constant, A to be an elliptic differential operator, $\alpha > 0$, $u_0, y_0 \in H^1(\Omega)$ and $b \in W^{2,\infty}(\Omega)$ are given.

2. FE–DISCRETIZATION

Let $\mathcal{T}_h$ be a triangulation of Ω with vertices $x_1,\dots,x_m$ and let X_h denote the corresponding space of linear, continuous finite elements. The discrete optimization problem reads

$$\min_{u\in U_{ad}} J(y_h(u),u)$$

subject to $y_h(u)$ solving the discrete counterpart of the elliptic PDE and $y_h(x_j) \le b(x_j)$ for $j = 1,\dots,m$. This represents a convex infinite-dimensional optimization problem with only finitely many equality and inequality constraints for the state.

3. LOCAL ERROR INDICATORS

We introduce the dual, control and primal residual functionals ρ^p, ρ^u and ρ^y determined by the discrete solution y_h, u_h, p_h with control and state multipliers λ_h and μ_h. In addition we define the residual functional ρ^μ, respectively steming from the complementarity conditions. We are now in the position to formulate the analogue to (4, Thm. 1) for the state and control constrained case; there holds

$$\begin{aligned} J(y,u) - J(y_h,u_h) &= \frac{1}{2}\rho^p(y - i_h y)+ \\ &+ \frac{1}{2}\rho^y(p - i_h p) + \frac{1}{2}\rho^\mu(y,\mu) + \frac{1}{2}\rho^u(u,\lambda) \end{aligned}$$

with arbitrary quasi–interpolants $i_h y$ and $i_h p \in X_h$. Based on this representation we define appropriate local quantities $\rho^p_T, \rho^y_T, \rho^\mu_T, \rho^u_T$ on every triangle T and obtain the error indicator

$$\eta := \frac{1}{2}\sum_{T\in\mathcal{T}_h} \rho^p_T + \rho^y_T + \rho^\mu_T + \rho^u_T.$$

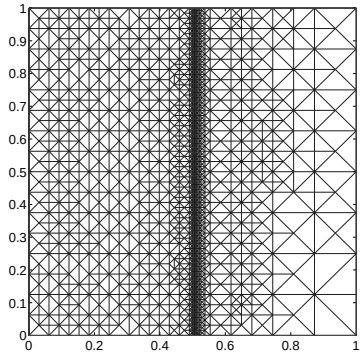

Fig. 1. Adaptive mesh obtained by steering the local refinement process via η.

4. NUMERICAL EXAMPLE

Let $\Omega = (0,1)\times(0,1)$ be the unit square, $U_{ad} = L^2(\Omega)$, $A = -\Delta + Id$ and $\alpha = 1$. The desired control u_0 and state y_0 as well as the *lower*

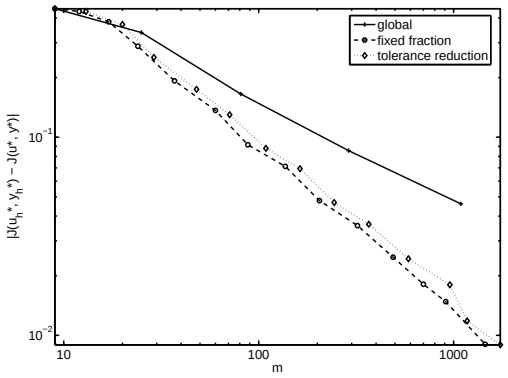

Fig. 2. Error in the objective functional for different refinement strategies and numbers of vertices m.

bound b are taken from (1), where this problem already is investigated for uniform meshes. We simulate the case, where the boundary of the active set $M = \{(\frac{1}{2}, x_2) \in \Omega\}$ is not known a–priori. Therefore we avoid having nodes along M in the initial mesh. As can be seen from figure 1 our estimator provides adaptive meshes in the neighbourhood of M. Furthermore the indicator has the desired property of reducing the error in the objective compared to global refinement (see figure 2).

5. CONCLUSIONS

In order to generate goal-oriented meshes, we extend the DWR concept proposed by Becker and Rannacher for PDE-constrained optimization to the control and / or state constrained case. Using the augmented optimality system we obtain a representation for the error in the objectives. Based on this representation local error indicators are defined. Their performance properties are investigated by means of numerical examples.

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Path-following techniques in PDE-constrained optimization with low multiplier regularity

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Keywords: State and control constraints, primal-dual active set strategy, regularization, semismooth Newton methods

Primal-dual path-following methods for constrained minimization problems in function space with low multiplier regularity are introduced and analyzed. For this purpose let X_1, X_2, and W be real Hilbert spaces with

$$X_1 \hookrightarrow L^2(\omega) \hookrightarrow X_1^*,$$

where X_1^* denotes the dual of X_1 and ω a bounded domain in $\mathbb{R}^m$. Further set $X = X_1 \times X_2$ and let $x = (x_1, x_2)$ denote a generic element in X.

Let $E \in \mathcal{L}(X, W)$, $f \in W$, $\psi_l, \psi_u \in X_1$, and $\phi_l, \phi_u \in X_2$. Further let $J : X \to \mathbb{R}$ denote a quadratic functional such that there exists a constant $\alpha > 0$ with

$$\langle J'(x) - J'(y), x - y\rangle_{X^*,X} \geq \alpha |x - y|_X^2 \quad (1)$$

whenever $E(x - y) = 0$ for $x, y \in X$. Then the problem under consideration is

$$\begin{aligned} &\text{minimize } J(x) \text{ over } x \in X \\ &\text{subject to } Ex = f, \\ &\qquad \psi_l \leq x_1 \leq \psi_u, \\ &\qquad \phi_l \leq x_2 \leq \phi_u, \end{aligned} \quad \text{(P)}$$

where $\leq$ denotes the ordering in $L^2(\omega)$. By duality theory, the Lagrange multiplier associated with the inequality constraint involving x_1 is assumed to exhibit low regularity only, i.e., it does not admit a pointwise interpretation. On the other hand, the multiplier pertinent to $\phi_l \leq x_2 \leq \phi_u$ is supposed to be regular and the mapping x_2-to-adjoint state is assumed to be smoothing.

The regularization employed is of a generalized Moreau-Yosida-type (i.e., including a multiplier shift, which may yield feasibility of the regularized solution with respect to the original constraints) and yields regular approximations to low regularity multipliers of the original problem. First the consistency of the regularization is shown, and then regularity properties of the path are discussed. In particular, under a strict complementarity assumption differentiability with respect to the path/regularization parameter is established. This property is useful in devising highly efficient extrapolation schemes within numerical solution algorithms. Further, the path structure allows us to define approximating models, which are used for controlling the path parameter in an iterative process for computing a solution of the original problem. This strategy turns out to be crucial in avoiding potential ill-conditioning due to a rapid increase of the path/regularization parameter. The Moreau–Yosida regularized subproblems of the new path-following technique are solved efficiently by semismooth Newton methods. Due to the regularization the latter method can be analysed successfully in function space. The overall algorithmic concept is provided, and numerical tests (including a comparison with primal-dual path-following interior point methods) for simultaneously state and control constrained optimal control problems show the efficiency of the new concept.

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Structure Exploitation in Aerodynamic Shape Optimization

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Keywords: aerodynamic shape optimization, parameterization, Hicks-Henne functions, fast optimization, SQP, OneShot optimization

1. Introduction

Recent advances in optimization have reduced the numerical costs of aerodynamic shape optimization considerably. By coupling the optimization with the iterative flow solver in a so called OneShot-Strategy, the cost of the optimization has been reduced to be comparable to a few forward simulation runs. To decrease the costs even further, these studies are now extended to the parameterization of the shape of the aircraft.

Given the background of fast optimization (Gherman and Schulz, 2005), both the convergence speed and the best obtainable optimum solution have to be considered. Because of the conflicting nature of these two criteria, local adaptivity using hierarchical and multi-level parameterizations will be inspected. Out of the multitude of possible parameterizations (nurbs, B-splines, free-form-deformation, ...), special attention is given to the parameterization via Hicks-Henne basis functions. This form of parameterization - which is very often applied in the aerospace industries - possesses inherent smoothing properties, which leads to the surprising behavior of less optimization iterations with more design parameters.

By using an adjoint approach (Gauger, 2003) for the computation of the gradients, the cost does not scale with the number of design parameters. Therefore, a combination of a OneShot optimization strategy (Hazra and Schulz, 2004, 2005) with a high number of Hicks-Henne functions (Hicks and Henne, 1978) and adjoint based gradients produces a very fast optimization routine.

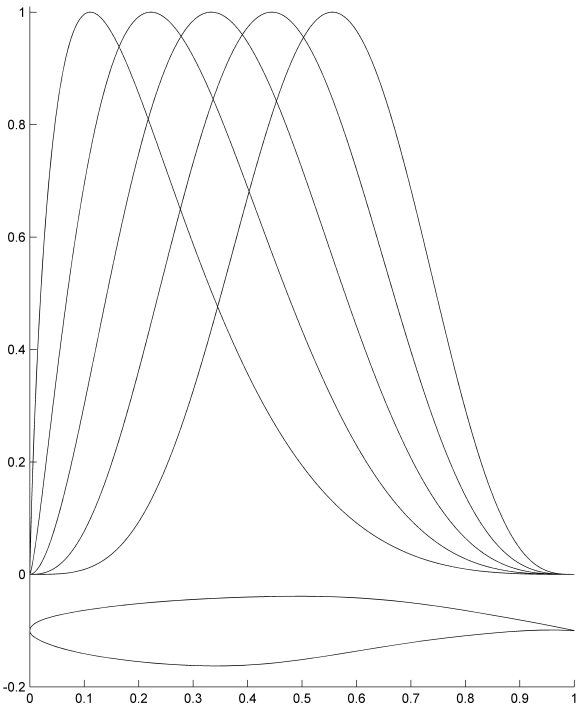

Fig. 1. Hicks-Henne parameterization with 5 basis functions

2. Parameterizations

Out of the multitude of possible parameterizations, special attention is given to the Hicks-Henne functions on the one hand and a free node parameterization on the other hand, because of

- frequent industrial applications
- decrease in optimization iterations with increasing number of design parameters

Here, local adaptivity is a major issue:

Given the optimum solution q_1 of a coarse parameterization level $q_1 \in \mathbb{R}^{n_{q_1}}$, one can reinterpret this as the optimum solution $q_2 = [q_1, \hat{q}]^T$ of a finer level with the additional constraint of $\hat{q} = 0$. The Lagrange-Multiplier of this ad-

ditional constraint, also known as the ”shadow price”, can then be used as a measurement of local adaptivity of the design space. By the use of an adjoint based gradient, this technique has proven to be computationally cheap, since the gradient evaluation on the finer level does not require any new flow solutions.

Using this technique, it is shown, that for the best obtainable optimum solution for the 2D RAE2822 airfoil, as few as 4-5 strategically well placed Hicks-Henne functions are already sufficient.

3. CONCLUSIONS

The parameterization has a major impact on both algorithmic performance and the quality of the obtainable optimum solution. Because of the inverse behavior of the number of design parameters and optimization iterations needed, special attention is given to the Hicks-Henne parameterization and its smoothing properties. Using a hierarchical parameterization with an artificial ”parameterization constraint”, local adaptivity using shadow prices will be shown.

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A trust-region algorithm for nonlinear programming problems with dense constraint Jacobians

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Keywords: Equality Constrained Optimization, Trust Region Algorithms, Dense Constraint Jacobain

For numerous PDE-constraint optimization problems, the underlying application yields very large but also well-structured and sparse derivative matrices. However, there is also a wide range of applications where the derivative matrices have somehow orthogonal characteristics, i.e., they are of rather small size but dense. Examples for such a setting are Periodic Adsorption Processes (PAPs) that consist of vessels or beds packed with solid sorbent. The sorbent is contacted with a multi-component fluid stream to preferentially absorb one of the chemical components onto the solid. Typical tasks for PAPs include vacuum swing adsorption to separate oxygen from air, pressure swing adsorption to separate hydrogen from hydrocarbons in refinery gases and simulated moving bed chromatography to separate two isomers (e.g., glucose and fructose) in the liquid phase. PAPs are typically operated in a cyclic manner with each bed repeatedly undergoing a sequence of steps. These cycle models consist of the bed models, PDAEs in time and space, solved for each step. After a relatively brief start-up period, the adsorption beds run in a cyclic steady state, that is, the bed conditions at the beginning of each cycle match those at the end of the cycle. This fact yields dense constraint Jacobians. As a consequence, the run-time needed for an optimization may be dominated significantly by the computation of the dense Jacobian and its factorization.

This talk presents a trust-region SQP algorithm for the solution of minimization problems with nonlinear equality constraints. The proposed approach does not require the exact evaluation of the constraint Jacobian or an iterative solution of a linear system with a system matrix that involves the constraint Jacobian. Instead the algorithm presented here works only with an approximation of the constraint Jacobian. Hence, it is well suited for optimization problems of moderate size but with a special structure of the constraint Jacobian. The accuracy requirements for the presented first-order global convergence result are based on the feasibility and the optimality of the iterates. The corresponding criteria can be verified easily during the optimization process to adjust the approximation quality of the constraint Jacobian.

Furthermore, we will discuss several possibilities for providing the required derivatie information. This includes a “black-box” application of automatic differentiation to the time integration. As alternative, one may apply semi-automatic approaches combining automatic differentiation and more sophisticated integration algorithms provided for example by CVODES to evaluate the direct sensitivity equation, the adjoint equation and the second order adjoint equation.

Numerical results for various test problems including a simple periodic adsorption process are shown.

Riccati-Based Feedback Stabilization of Flow Problems

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Keywords: Flow control, stabilization, Navier-Stokes equations, Oseen equations, Riccati equation

1. SUMMARY

Our goal is to derive and investigate effective numerical algorithms for the stabilization of flow problems governed by the Navier Stokes equations around an unstable steady state solution w.

Linearizing the Navier Stokes equations for the difference of w and the instationary solution z, we obtain the so-called Oseen equations for $y = z - w$. We want to minimize y by a boundary feedback control. In particular, the control will have a non-zero normal component.

Reformulating the equations allows us to apply Riccati theory and derive an algebraic Riccati equation (ARE) from which we can calculate an optimal control u.

For the numerical solution, we discretize the system by a Galerkin finite element method. For the solution of the ARE, we use a Newton-based algorithm exploiting the structure of the discretized operators.

2. THEORETICAL APPROACH

For the Oseen equations with a given stationary solution w and the instationary solution y that we want to stabilize, we can formulate an optimal boundary control problem as follows:

$$\inf\{J(y,u) :\ (y,u) \text{ fulfill } (1),\ u \in V^{0,0}(\Sigma)\},$$

$$J(y,u) = \frac{1}{2}\int_0^T \int_\Omega |y|^2\, dx\, dt + \frac{1}{2}\int_0^T |u|^2_{V^0(\Gamma)} dt,$$

$$\begin{aligned}
&\partial_t y - \frac{1}{\mathrm{Re}}\Delta y + (y\cdot\nabla)w + (w\cdot\nabla)y + \nabla p = 0,\\
&\operatorname{div} y = 0 \quad \text{in} \quad Q = \Omega\times(0,T),\\
&y = Mu \quad \text{on} \quad \Sigma = \Gamma\times(0,T),\\
&y(0) = \zeta \quad \text{in} \quad \Omega.
\end{aligned} \tag{1}$$

M restricts the control u to a part of the boundary, $T > 0$ can be finite or infinite, the divergence free spaces

$$V^0(\Gamma) = \{u \in L^2(\Gamma) :\ \operatorname{div} u = 0 \text{ in } \Omega,\ < u\cdot n, 1 >_{H^{-1/2}(\Gamma),H^{1/2}(\Gamma)} = 0\},$$

$$V^{0,0}(\Sigma) = L^2(0,T;V^0(\Gamma))$$

allow controls with a nonzero normal component.

Using the orthogonal Helmholtz projection

$$P :\ L^2(\Omega) \to V_n^0(\Omega),$$

$$V_n^0(\Omega) = \{u \in L^2(\Omega) :\ \operatorname{div} u = 0 \text{ in } \Omega,\ u\cdot n = 0\},$$

the Dirichlet operator D_A defined by $D_A w = v$ iff

$$\begin{aligned}
&\lambda v - \frac{1}{\mathrm{Re}}\Delta v + (w\cdot\nabla)v + (v\cdot\nabla)w + \nabla\pi = 0,\\
&\operatorname{div} v = 0 \quad \text{in} \quad \Omega,\\
&v = w \quad \text{on} \quad \Gamma,
\end{aligned}$$

and the boundary projectors

$$\gamma_n u = (u\cdot n)n, \quad \gamma_\tau u = u - \gamma_n u,$$

in (5) Raymond derives the equivalent problem

$$\inf\{I(y,u) :\ (y,u) \text{ fulfill } (2),\ u \in V^{0,0}(\Sigma)\},$$

$$I(y,u) = \frac{1}{2}\int_0^T (|Py|^2_{L^2(\Omega)} + |R_A^{1/2}\gamma_n u|^2_{V^0(\Gamma)} + |\gamma_\tau u|^2_{V^0(\Gamma)})\, dt,$$

$$\begin{aligned} Py' &= APy + BMu \quad \text{in} \quad (0,\infty), \\ Py(0) &= \zeta, \\ (I-P)y &= (I-P)D_A M\gamma_n u, \end{aligned} \tag{2}$$

where

$$Ay = \frac{1}{\mathrm{Re}}\, P\Delta y - P((w\cdot\nabla)y) - P((y\cdot\nabla)w),$$

$B = (\lambda I - A)PD_A$ and
$R_A = MD_A^\star(I-P)D_AM + I.$

To this problem, we can apply Riccati optimal control theory. We solve the ARE

$$A^\star\Pi + \Pi A - \Pi B_\tau M^2 B_\tau^\star \Pi + \Pi B_n M R_A^{-1} M B_n^\star \Pi + I = 0$$

for $\Pi = \Pi^\star \geq 0$, define the feedback control

$$u = -MB_\tau^\star \Pi Py - R_A^{-1} MB_n^\star \Pi Py$$

and get the stabilized solution from (2).

This theory can be extended to the fully nonlinear equation with the additional term $(y\cdot\nabla)y$, and the stabilization can even be made exponential such that, if the initial perturbation $y(0) = \zeta$ is small enough,

$$\exists\, C,\, \omega > 0: \quad ||y(t)|| \leq C\, e^{-\omega t}.$$

3. NUMERICAL REALIZATION

We will demonstrate the Riccati-based approach for a standard benchmark problem in flow control: the backward facing step. Here the goal is to minimize the vorticity behind the step by applying a Dirichlet boundary control.

We are going to use the Taylor-Hood finite element Galerkin space discretization from which we will get n-dimensional approximations of the state equations and the ARE.

Solving the ARE is a numerical challenge due to the size of the solution matrix $\Pi_h \in I\!R^{n\times n}$. We are going to use a low-rank Cholesky approximation $\Pi \approx Z_h Z_h^T$ with $Z_h \in I\!R^{n\times r}, r \ll n$, and compute Z_h by a variant of Newton's method for AREs. Our algorithms exploit the structure of the coefficient matrices by alternating direction iteration methods such that the complexity of each Newton step is reduced from $\mathcal{O}(n^3)$ to the complexity for solving the stationary Stokes problem (3; 4).

For the solution of the differential equations, we use the finite element based solver NAVIER (2). It comprises coupling with energy and species transport, phase change problems and capillary free boundary conditions, for example. There are versions for 2d and 3d.

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Multiperiod risk functionals and their application in electricity risk management

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Keywords: Risk functionals, multi-period, stochastic programming, risk management, electricity

Multiperiod risk functionals for discrete-time stochastic processes with adapted filtration are considered which satisfy monotonocity, translation equivariance and convexity properties. Dual representations of such risk functionals are derived and various examples are discussed (4). The class of polyhedral multiperiod risk functionals, their incorporation into multistage stochastic programs and their stability properties are discussed in more detail (1; 3). Finally, we present a case study for applications of multiperiod risk functionals in electricity risk management (see also (2)).

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ON PRIMAL-DUAL THIRD DEGREE STOCHASTIC DOMINANCE

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1. STOCHASTIC DOMINANCE

In the stochastic dominance approach random variables are compared by pointwise comparison of some performance functions constructed from their distribution functions. Let X be a random variable representing some returns. The first performance function $F_1(X,r)$ is defined as the right-continuous cumulative distribution function itself: $F_1(X,r) = \mathbf{P}[X \leq r]$ for $r \in R$. We say that X weakly dominates Y under the FSD rules ($X \succeq_{FSD} Y$), if $F_1(X,r) \leq F_1(Y,r)$ for all $r \in R$, and X FSD dominates Y ($X \succ_{FSD} Y$), if at least one strict inequality holds. Actually, the stochastic dominance is a stochastic order thus defined on distributions rather than on random variables themselves. Nevertheless, it is a common convention, that in the case of random variables X and Y having distributions P_X and P_Y, the stochastic order relation $P_X \succeq P_Y$ might be viewed as a relation on random variables $X \succeq Y$ (Müller and Stoyan, 2002).

The second degree stochastic dominance relation is defined with the second performance function $F_2(X,r)$ given by areas below the cumulative distribution function itself, i.e.: $F_2(X,r) = \int_{-\infty}^{r} F_1(X,t)dt$ for $r \in R$. Similarly to FSD, we say that X weakly dominates Y under the SSD rules ($X \succeq_{SSD} Y$), if $F_2(X,r) \leq F_2(Y,r)$ for all $r \in R$, while X SSD dominates Y ($X \succ_{SSD} Y$), when at least one inequality is strict. Certainly, $X \succ_{FSD} Y$ implies $X \succ_{SSD} Y$. Function $F_2(X,r)$, used to define the SSD relation can also be presented as follows (Ogryczak and Ruszczyński, 1999): $F_2(X,r) = \mathbf{E}[\max\{r - X, 0\}]$, thus representing the mean below-target deviations from real targets.

Alternatively, the stochastic dominance order can be expressed on the inverse cumulative functions (quantile functions) (Wang and Young, 1998). Namely, for random variable X, one may consider the performance function $F_{-1}(X,p)$ defined as is the left-continuous inverse of the cumulative distribution function $F_1(X,r)$, i.e., $F_{-1}(X,p) = \inf\{\eta : F_1(X,\eta) \geq p\}$. Obviously, X dominates Y under the FSD rules ($X \succ_{FSD} Y$), if $F_{-1}(X,p) \geq F_{-1}(Y,p)$ for all $p \in [0,1]$, where at least one strict inequality holds. Further, the second quantile function (or the so-called *Absolute Lorenz Curve* ALC) is defined by integrating F_{-1} as $F_{-2}(X,p) = \int_0^p F_{-1}(X,\alpha)d\alpha$ for $0 < p \leq 1$. Actually, as shown in (Ogryczak and Ruszczyński, 2002), $F_{-2}(X,p) = \max_{r \in R}[pr - F_2(X,r)]$. Hence, by the theory of convex conjugate (dual) functions, the pointwise comparison of ALCs provides an alternative characterization of the SSD relation in the sense that $X \succeq_{SSD} Y$ if and only if $F_{-2}(X,\beta) \geq F_{-2}(Y,\beta)$ for all $0 < \beta \leq 1$.

If $X \succ_{SSD} Y$, then X is preferred to Y within all risk-averse preference models that prefer larger outcomes. In terms of the expected utility theory the SSD relation represent all the preferences modeled with increasing and concave utility functions. It is therefore a matter of primary importance that a stochastic optimization model be consistent with the second degree stochastic dominance relation. However, in many applications one may deserve stronger risk averse. The classical higher degree stochastic dominance relations no longer maintain the equivalence of the primal and dual (inverse) models. This paper introduces a concept of the

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primal-dual higher degree stochastic dominance which preserve the equivalence of the primal and inverse dominance relations.

2. PRIMAL-DUAL TSD

Classical higher degree stochastic dominance relations depend on performance functions derived by integrating those of lower degrees. The third function $F_3(X,r)$ is given by integrating F_2, i.e.: $F_3(X,r) = \int_{-\infty}^{r} F_2(X,t)dt$ for $r \in R$ and it can also be presented as follows (Ogryczak and Ruszczyński, 2001): $F_3(X,r) = \mathbf{E}[\max\{r - X, 0\}^2]/2$, thus representing the mean square below-target deviations from real targets. The kth function $F_k(X,r)$ is defined as: $F_k(X,r) = \int_{-\infty}^{r} F_{k-1}(X,t)dt$ for $r \in R$. Similarly to FSD and SSD, we say that X weakly dominates Y under the kSD rules ($X \succeq_{kSD} Y$), if $F_k(X,r) \le F_k(Y,r)$ for all $r \in R$. Certainly, $X \succ_{(k-1)SD} Y$ implies $X \succ_{kSD} Y$. One may also consider the higher degree quantile performance functions (Muliere and Scarsini, 1989). In particular, the third quantile function is defined by integrating as $F_{-3}(X,p) = \int_0^p F_{-2}(X,\alpha)d\alpha$ for $0 < p \le 1$, while higher degree functions can respectively be built. Although, already the third degree inverse SD relation, $X \succeq_{TISD} Y$ iff $F_{-3}(X,p) \ge F_{-3}(Y,p)$ for all $0 < p \le 1$, is not equivalent to the primal TSD. Moreover, function F_{-3} is neither monotonic nor convex as already F_{-2} is not always monotonic.

In order to build a primal-dual third degree stochastic dominance concept we need to normalize the corresponding second performance functions prior to their integration. We introduce a nondecreasing performance function $H_2(X,.) : R \to [0,1]$ and its generalized inverse $H_{-2}(X,.) = H_2^{-1}(X,.)$ such that $X \succeq_{SSD} Y$ iff $H_2(X,r) \le H_2(Y,r)$ for all $r \in R$, and equivalently $H_{-2}(X,p) \ge H_{-2}(Y,p)$ for all $0 < p \le 1$. In other words, we introduce alternative performance functions similar to a cdf and its inverse, respectively, but defining the second degree stochastic dominance instead of the FSD. The simplest way to define such performance functions is

$$H_2(X,\eta) = \sup\{p : F_2(X,\eta+\xi) \ge p\xi \ \forall_{\xi \ge 0}\}$$
$$H_{-2}(X,p) = \inf\{\eta : F_{-2}(X,p) \le p\eta \ \}$$

When introducing the set of random variables $Q(\eta,p) = \{Z : \mathbf{P}[Z < \eta] = 0,\ \mathbf{P}[Z \le \eta] \ge p\}$ the functions can be interpreted as follows. $H_2(X,\eta)$ represents then the largest p such that $\hat{X} \succeq_{SSD} X$ for some $\hat{X} \in Q(\eta,p)$ while $H_{-2}(X,p)$ represents the smallest η such that $\hat{X} \succeq_{SSD} X$ for some $\hat{X} \in Q(\eta,p)$.

By integration we get the third degree performance functions $H_3(X,r) = \int_{-\infty}^{r} H_2(X,t)dt$ for $r \in R$ and $H_{-3}(X,p) = \int_0^p H_{-2}(X,\alpha)d\alpha$ for $0 < p \le 1$, respectively. Such functions are convex and they form a pair of conjugate functions. This allows us to define the third degree primal-dual stochastic dominance (TPDSD) as $X \succeq_{TPDSD} Y$ iff $H_3(X,r) \le H_3(Y,r)$ for all $r \in R$, and equivalently $H_{-3}(X,p) \ge H_{-3}(Y,p)$ for all $0 < p \le 1$. Obviously, $X \succeq_{SSD} Y$ implies $X \succeq_{TPDSD} Y$, but not vice versa. Similar approach one may apply to construct higher degree primal-dual stochastic dominance relations.

Various risk averse models can be build by using TPDSD performance functions as optimization criteria. Note that $H_{-2}(X,p) = F_{-2}(X,p)/p$ thus representing the TailVaR risk measures (known also as Average VaR or Conditional VaR). There is no simple formula for $H_2(X,r)$. Nevertheless, for both $H_{-3}(X,p)$ and $H_3(X,r)$ the corresponding integral approximations can be quite easily defined.

This paper presents initial analysis of the TPDSD relation and corresponding risk averse optimization models.

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STOCHASTIC DYNAMIC OPTIMIZATION WITH MULTIVARIATE STOCHASTIC DOMINANCE CONSTRAINTS

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Keywords: Stochastic control, stochastic programming, stochastic orders, risk, utility.

1. INTRODUCTION

In our earlier publications (Dentcheva and Ruszczyński, 2003, 2004) we have introduced and analyzed the following optimization model with stochastic dominance constraints:

$$\begin{aligned} &\max \mathbb{E}\big[H(z)\big] \\ &\text{s.t. } G(z) \succeq_{(2)} Y, \\ &\quad z \in Z_0. \end{aligned}$$

In this problem Z_0 is a convex closed subset of a Banach space $\mathscr{Z}$, and G and H are continuous operators from $\mathscr{Z}$ to the space of integrable random variables $\mathscr{L}_1(\Omega, \mathscr{F}, P)$. The random variable Y plays the role of a benchmark outcome. For example, one may set $Y = G(\bar{z})$, where $\bar{z} \in Z_0$ is some reasonable value of the decision vector, which is currently employed in the system.

The relation $\succeq_{(2)}$ is the stochastic dominance relation of the second order. It is defined as follows: A random variable X dominates another random variable Y in the second order, if

$$\mathbb{E}[u(X)] \geq \mathbb{E}[u(Y)]$$

for every concave nondecreasing function $u(\cdot)$, for which these expected values are finite.

Our objective is to extend this model to a dynamic setting, with $G(z)$ representing a random sequence, rather than a scalar random variable. We are interested in modeling risk aversion in a stochastic control problem for a discrete-time linear dynamic system governed by the equations:

$$s_{t+1} = A_t s_t + B_t v_t + e_t, \quad t = 1, \ldots, T.$$

Here s_t denotes the state vector at time t and v_t denotes the control vector. The vectors e_t and the matrices A_t and B_t are random. The initial state s_1 is given.

Assume that the random outcomes X_t, representing the performance measures of the system at $t = 1, \ldots, T+1$, are scalar and given by

$$\begin{aligned} &X_t(\omega) = g_t(s_t(\omega), v_t(\omega)), \quad \text{for } t = 1, \ldots, T, \\ &X_{T+1}(\omega) = g_{T+1}(s_{T+1}(\omega)), \quad \omega \in \Omega. \end{aligned}$$

The functions $g_t : \mathbb{R}^{n_s} \times \mathbb{R}^{n_v} \to \mathbb{R}$ are concave.

We adopt the convention that larger values of X_t are preferred; for example, X_t may represent profits at time t.

Our goal is to model risk aversion in this problem by using stochastic orders. To this end we compare the multivariate distribution of the rewards $(X_1, X_2, \ldots, X_{T+1})$ with the distribution of some benchmark outcomes $(Y_1, Y_2, \ldots, Y_{T+1})$. We shall add to the problem formulation an appropriate stochastic ordering constraint.

2. STOCHASTIC DOMINANCE FOR RANDOM SEQUENCES

Consider random vectors $(X_1, \ldots, X_{T+1})$ and $(Y_1, \ldots, Y_{T+1})$. The simplest way to define a stochastic ordering relation $X \succeq^{\text{sep}}_{(2)} Y$ between these vectors, is to require the stochastic dominance relation for each coordinate

$$X_t \succeq_{(2)} Y_t, \quad t = 1, \ldots, T+1.$$

The analysis in our earlier paper (Dentcheva and Ruszczyński, 2004) includes this case. This approach, however, ignores the temporal structure and the dependency between the coordinates of the vector $(X_1, \ldots, X_{T+1})$.

Therefore, we are taking a different approach, by considering discounted sums of the rewards, $\sum_{t=1}^{T+1} \varrho_t X_t$, and the corresponding discounted sums of the benchmark: $\sum_{t=1}^{T+1} \varrho_t Y_t$. The sequence of discount factors $\{\varrho_t\}$ is assumed to belong to a compact set $\mathscr{D}$, where

$$\mathscr{D} \subseteq \big\{\varrho \in \mathbb{R}^{T+1} : 1 \geq \varrho_1 \geq \cdots \geq \varrho_{T+1} \geq 0\big\}.$$

DEFINITION. A sequence $(X_1, \ldots, X_{T+1})$ dominates a sequence $(Y_1, \ldots, Y_{T+1})$ in the discounted second order, if for all $\varrho \in \mathscr{D}$ the relation

$$\sum_{t=1}^{T+1} \varrho_t X_t \succeq_{(2)} \sum_{t=1}^{T+1} \varrho_t Y_t$$

is satisfied.

We denote this relation by $X \succeq_{(2)}^{\mathrm{dis}} Y$. The discounted order $\succeq_{(2)}^{\mathrm{dis}}$ neither implies nor is implied by the coordinate order.

3. OPTIMALITY CONDITIONS

We introduce the following stochastic dynamic optimization problem with discounted dominance constraints:

$$\begin{aligned}
\max\ & \sum_{t=1}^{T} \mathbb{E}G_t(s_t, v_t) + \mathbb{E}G_{T+1}(s_{T+1}) \\
\text{s.t. } & s_{t+1} = A_t s_t + B_t v_t + e_t, \quad t = 1, \ldots, T, \\
& (G_1(s_1, v_1), \ldots, G_1(s_T, v_T), G_{T+1}(s_{T+1})) \\
& \qquad \succeq_{(2)}^{\mathrm{dis}} (Y_1, \ldots, T_T, Y_{T+1}) \\
& v_t \in V_t \text{ a.s.}, \quad t = 1, \ldots, T.
\end{aligned}$$

We introduce a class Φ of concave nondecreasing functions $\varphi : \mathbb{R}^{T+1} \to \mathbb{R}$; they will play a role of Lagrange multipliers associated with the ordering constraint. In the talk we shall precisely define the class Φ.

The following functional plays the role of a partial Lagrangian associated with our problem:

$$\begin{aligned}
L(s, v, \varphi) = \mathbb{E}\Big[& \sum_{t=1}^{T} G_t(s_t, v_t) + G_{T+1}(s_{T+1}) \\
& + \Big(\varphi(G_1(s_1, v_1), \ldots, G_T(s_T, v_T), G_{T+1}(s_{T+1})) \\
& \qquad - \varphi(Y_1, \ldots, Y_T, Y_{T+1})\Big)\Big].
\end{aligned}$$

The main contributions of the work are the following.

Under an appropriate constraint qualification condition, the pair $(\hat{s}, \hat{v})$ constitutes the optimal state–control pair of the problem if and only if there exists a utility function $\hat{\varphi} \in \Phi$ such that $(\hat{s}, \hat{v})$ is also the optimal state–control pair in an auxiliary control problem having $L(s, v, \hat{\varphi})$ as its objective functional.

Moreover, a duality relation holds true: the function $\hat{\varphi}$ is the worst among all functions $\varphi \in \Phi$, that is, the maximal value of $L(\cdot, \cdot, \varphi)$ in the auxiliary problem is the smallest, when $\varphi = \hat{\varphi}$.

From these relations one can derive a version of the maximum principle for problems with dominance constraints, and the existence of a random discount process in the original problem.

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STABILITY AND SENSITIVITY OF OPTIMIZATION PROBLEMS WITH STOCHASTIC ORDERING CONSTRAINTS

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Keywords: stochastic programming, stochastic ordering, semi-infinite optimization, chance constraints

1. OPTIMIZATION PROBLEMS WITH STOCHASTIC ORDERING CONSTRAINTS

In stochastic optimization the decisions affect various random outcomes. The relation of *stochastic dominance* is a way to formalize preferences among random outcomes. The notion of stochastic ordering (or *stochastic dominance of first order*) has been introduced in statistics in and further applied and developed in economics. It is defined as follows. For a random variable X we consider its distribution function, $F(X;\eta) = \mathbb{P}[X \leq \eta]$, $\eta \in \mathbb{R}$. We say that a random variable X *dominates in the first order* a random variable Y if

$$F(X;\eta) \leq F(Y;\eta) \quad \text{for all} \quad \eta \in \mathbb{R}.$$

We denote this relation $X \succeq_{(1)} Y$.

Let $g : \mathbb{R}^n \times \mathbb{R}^s \to \mathbb{R}$ be continuous with respect to both arguments, and let V be an s-dimensional random vector, defined on a certain probability space $(\Omega, \mathscr{F}, \mathbb{P})$. For every $z \in \mathbb{R}^n$

$$X_z(\omega) = g(z, V(\omega)), \quad \omega \in \Omega$$

is a random variable. Given a benchmark random variable Y (defined on the same probability space), an optimization model with first order stochastic dominance constraint is formulated as follows:

$$\begin{aligned} &\min\ f(z) \\ &\text{s.t. } X_z \succeq_{(1)} Y, \\ &\quad z \in Z, \end{aligned}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $Z \subset \mathbb{R}^n$. We can express the dominance constraint as a continuum of probabilistic constraints:

$$\mathbb{P}\big[g(z,V) \geq \eta\big] \geq \mathbb{P}\big[Y \geq \eta\big], \quad \eta \in \mathbb{R}.$$

In financial mathematics the corresponding concept is that of *Value-at-Risk* (VaR), which is defined as the maximum loss at a specified confidence level p. It corresponds to the largest p-quantile of the random variable X representing gains, whereas we use here the smallest p-quantile. Our analysis can be adapted in a straightforward way to this case.

Problems with stochastic dominance constraints are new optimization models involving risk aversion introduced in (Dentcheva and Ruszczyński, 2003, 2004). As problems with a continuum of constraints on probability, they pose specific analytical and computational challenges. The probabilistic nature of the problem prevents the direct application of the theory of semi-infinite optimization. On the other hand, the specific structure of dominance constraints is significantly different from the structure of finitely many probabilistic constraints.

2. STABILITY AND SENSITIVITY

We introduce the measures μ_0 on $\mathbb{R}^s$ and ν_0 on $\mathbb{R}$ induced by V and Y. For all Borel sets $A \subset \mathbb{R}^s$ and $B \subset \mathbb{R}$:

$$\begin{aligned} \mu_0(A) &= \mathbb{P}[V \in A], \\ \nu_0(B) &= \mathbb{P}[Y \in B]. \end{aligned}$$

We denote the set of probability measures on $\mathbb{R}^m$ by $\mathscr{P}(\mathbb{R}^m)$.

Furthermore, we introduce the multifunction $H : \mathbb{R}^n \times \mathbb{R} \rightrightarrows \mathbb{R}^s$ defined by

$$H(z,\eta) := \{v \in \mathbb{R}^s : g(z,v) \geq \eta\}.$$

We consider the following parametric optimization problem:

$$\begin{aligned} \min\ & f(z) \\ \text{s.t. } & \mu(H(z,\eta)) - \nu([\eta,\infty)) \geq 0 \quad \forall \eta \in [a,b], \\ & z \in Z, \end{aligned} \tag{1}$$

with parameters $\mu \in \mathscr{P}(\mathbb{R}^s)$ and $\nu \in \mathscr{P}(\mathbb{R})$. The original problem is obtained when $(\mu,\nu) = (\mu_0,\nu_0)$. Our aim is to study the stability of solutions and of the optimal value to (1) under small perturbations of the underlying distributions μ_0 and ν_0.

For this purpose we equip the space $\mathscr{P}(\mathbb{R})$ with the Kolmogorov distance function:

$$\alpha_1(\nu_1,\nu_2) = \sup_{\eta\in\mathbb{R}} |\nu_1([\eta,\infty)) - \nu_2([\eta,\infty))|\,.$$

To introduce a distance function on $\mathscr{P}(\mathbb{R}^s)$, which is appropriate for our problem, we define the family of sets:

$$\mathscr{B} := \{H(z,\eta) : z \in Z, \eta \in [a,b]\} \cup \{v + \mathbb{R}^s_- : v \in \mathbb{R}^s\}.$$

The distance function on $\mathscr{P}(\mathbb{R}^s)$ is defined as the discrepancy

$$\alpha_{\mathscr{B}}(\mu_1,\mu_2) := \sup_{B\in\mathscr{B}} |\mu_1(B) - \mu_2(B)|\,.$$

On the product space $\mathscr{P}(\mathbb{R}^s) \times \mathscr{P}(\mathbb{R})$ we introduce the natural distance:

$$\alpha((\mu_1,\nu_1),(\mu_2,\nu_2)) := \max\{\alpha_{\mathscr{B}}(\mu_1,\mu_2), \alpha_1(\nu_1,\nu_2)\}.$$

Note that α is a metric, because the measures are compared, in particular, on all the cells of form $z + \mathbb{R}^s_-$ and $(-\infty,\eta)$, respectively.

We consider the constraint set mapping $\Phi : \mathscr{P}(\mathbb{R}^s) \times \mathscr{P}(\mathbb{R}) \rightrightarrows \mathbb{R}^n$, which assigns to every parameter (μ,ν) the feasible set of problem (1), i.e.,

$$\Phi(\mu,\nu) := \big\{z \in Z : \mu(H(z,\eta)) - \nu([\eta,\infty)) \geq 0 \quad \forall \eta \in [a,b]\,\big\}.$$

Furthermore, we define the optimal value function, $\varphi : \mathscr{P}(\mathbb{R}^s) \times \mathscr{P}(\mathbb{R}) \to \overline{\mathbb{R}}$, of problem (1) as follows:

$$\varphi(\mu,\nu) := \inf\big\{f(z) : z \in \Phi(\mu,\nu)\big\}.$$

The solution set mapping $\Psi_U : \mathscr{P}(\mathbb{R}^s) \times \mathscr{P}(\mathbb{R}) \rightrightarrows \mathbb{R}^n$ of problem (1) is defined by

$$\Psi(\mu,\nu) := \big\{z \in \Phi(\mu,\nu) : f(z) = \varphi(\mu,\nu)\big\}.$$

W report results from (Dentcheva et.al., 2007) We establish the closedness of the feasible set mapping, and we obtain stability results for the optimal value, for the feasible set, and for the solution set mappings. We analyze the sensitivity of the optimal value function and we obtain bounds for its directional derivatives.

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ABOUT REGULARITY OF OPTIMAL EIGENFUNCTIONS FOR THE LAPLACIAN

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Given a bounded open subset D of R^d, there exists a quasi-open subset of D minimizing the k-th eigenvalue of the Dirichlet-Laplacian operator with prescribed Lebesgue measure. A natural question concerns the regularity of this optimal set and of the corresponding optimal eigenfunction. We will recall the situation for the first eigenvalue in which case regularity essentially holds. The question is harder for the other eigenvalues. We will describe some progress in this direction.

SOME GEOMETRIC INEQUALITIES WITH APPLICATIONS

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1. INTRODUCTION

I will present a common work with Gérard Philippin from Laval University, Québec. In this talk, we are interested in various combinations of moment of inertia with respect to the coordinate axes.

Let Ω be a domain in $\mathbb{R}^N$, Γ its boundary and let us introduce the following notation, where $X = (x_1, x_2, \ldots, x_N)$:

- $J_i(\Omega) := \int_\Omega x_i^2\, dX$ and $j_i(\Gamma) := \int_\Gamma x_i^2\, d\sigma$,
- $J_O(\Omega) := \sum_{i=1}^N J_i(\Omega) = \int_\Omega |X|^2\, dX$ and $j_O(\Gamma) := \sum_{i=1}^N j_i(\Gamma) = \int_\Gamma |x|^2\, d\sigma$,
- $J(\Omega) := \Pi_{i=1}^N J_i(\Omega)$ and $j(\Gamma) := \Pi_{i=1}^N j_i(\Gamma)$.

We are interested in minimizing the four functionals J_O, j_O, J, j on the class of admissible domains with given volume: $\mathcal{O} := \{\Omega \subset \mathbb{R}^N,\ |\Omega| = c\}$.

2. MINIMIZING J_O and j_O

We will show that:
Theorem 1: The ball minimizes J_O.
We use classical rearrangement argument like in [4].

Theorem 2: The ball minimizes j_O.
This is a simple consequence of a more general isoperimetric inequality due to Betta, Brock, Mercaldo, Posteraro, see [1].

3. MINIMIZING J and j

Concerning the products of moment of inertia, we show:
Theorem 3: The ellipsoids minimize J.
This result is due to W. Blaschke, see [2] but can also be recovered by a simple topological derivative argument.

Theorem 4: The disk minimizes j in dimension 2.
We will mainly focus on the proof of this result which seems to be original. Let us remark that the result is unknown in higher dimension.

4. APPLICATION TO A STEKLOV EIGENVALUE PROBLEM

A consequence of Theorem 4 is a new proof of the following Theorem due to J. Hersch, L.E. Payne, M.M. Schiffer, see [3]:
Theorem 5: Let $0 = p_1(\Omega) \leq p_2(\Omega) \leq p_3(\Omega)$ be the first eigenvalues of the Steklov problem:

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \\ \frac{\partial u}{\partial n} = pu & \text{on } \Gamma\,, \end{cases}$$

where Ω is a bounded Lipschitz open set and Γ its boundary.
Then, the disk maximizes the product $p_2(\Omega)p_3(\Omega)$ among plane open sets of given area.

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A level set based shape and topology optimization technique for solving obstacle problems

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Keywords: Level set method, obstacle problem, shape optimization, topological derivative.

Let $\Omega \subset \mathbb{R}^2$ be a bounded and sufficiently smooth domain. Let $\psi \in H^2(\Omega)$ with $0 < \psi \leq M$ on $\partial\Omega$, and let $f \in L^2(\Omega)$. We consider the obstacle problem

$$\begin{array}{l} \text{minimize} \quad \frac{1}{2}\|\nabla y\|_{L^2}^2 - (f,y)_{L^2} \\ \text{subject to } y \in K, \end{array} \tag{1}$$

with

$$K := \{y \in H_0^1(\Omega) : y \leq \psi\}.$$

Above $(\cdot,\cdot)_{L^2}$ denotes the usual $L^2(\Omega)$-inner product. Under these assumption, the first order necessary and sufficient condition for optimality of $y^* \in H_0^1(\Omega)$ is given by

$$\begin{aligned} &-\Delta y^* + \lambda^* = f \text{ in } \Omega, \quad y^* = 0 \text{ on } \partial\Omega, \\ &\lambda^* = \max(0, \lambda^* + c(y^* - \psi)) \text{ a.e. in } \Omega, \end{aligned}$$

where $c > 0$ is arbitrarily fixed. Although λ^* is sufficiently regular, i.e., it admits a pointwise almost everywhere interpretation, algorithms such as semismooth Newton methods exhibit a mesh dependent behavior.

In order to overcome this mesh dependence, we propose a change of paradigm by considering the active and respectively inactive sets

$$\begin{aligned} \mathcal{A}^* &= \{y^* = \psi\}, \\ \mathcal{I}^* &= \Omega \setminus \mathcal{A}^*, \end{aligned}$$

as the unknowns inducing a state y^* with associated Lagrange multiplier λ^*. This allows us to reformulate (1) as a shape respectively topology optimization problem. In fact, we consider

$$\text{minimize} \quad J(\mathcal{A},\mathcal{I}) \text{ over } \mathcal{A},\mathcal{I} \subset \Omega \tag{2}$$

instead of (1), where $J = \alpha_1 J_1 + \alpha_2 J_2 + \alpha_3 J_3$ with positive weights α_i and

$$\begin{aligned} J_1(\mathcal{I}) &= \int_{\mathcal{I}} \max(0,\tilde{u})dx, \\ J_2(\mathcal{A}) &= \int_{\mathcal{A}} \max(0,\tilde{v})dx, \\ J_3(\mathcal{I}) &= \sum_{i=2}^{N} |\mathcal{I}_i|^{-1} \left(\int_{\mathcal{I}_i} g dx\right)^2. \end{aligned}$$

Here we assume $\mathcal{I} = \bigcup_{i=1}^N \mathcal{I}_i$ with $\mathcal{I}_i$ simply connected. Further, $g = f + \Delta\psi$, and $\tilde{u} = u - \psi$, $\tilde{v} = v - \psi$ solve

$$-\Delta u = \bar{g} \text{ in } \mathcal{I}_i, \quad \partial_n \tilde{u} = 0 \text{ on } \partial\mathcal{I}_i,$$

with $\bar{g} = g - |\mathcal{I}_i|^{-1} \int_{\mathcal{I}_i} g dx$ and a suitable modification if $\partial\mathcal{I}_i \cap \partial\Omega \neq \emptyset$, and

$$-\Delta v = -\Delta\psi \text{ in } \mathcal{A}, \quad v = u \text{ on } \partial\mathcal{A}.$$

We employ the concept of topological sensitivity as introduced by Sokolowski and Żochowski (1) in order to compute a descent direction for J. When topological stationarity is reached, the shape gradient is used for locally adjusting the shape of the active set $\mathcal{A}$. Numerically the latter step is realized by employing a level set methodology. Numerical results including a comparison with a primal-dual active set solver will be presented.

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Drag minimisation for stationary, compressible Navier-Stokes equations. Part 1 Existence of optimal shapes, Part 2 Optimality conditions.

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Keywords: Shape optimization, compressible Navier-Stokes equations, drag minimization, transport equations, shape gradient, shape derivative, approximate solutions, shape sensitivity analysis, necessary optimality conditions

1. Introduction

The shape optimization for compressible Navier-Stokes equations is an important branch of the research, e.g. in aerodynamics. The main difficulty in analysis of such problems is the lack of the existence results for inhomogeneous boundary value problems in bounded domains (cf. Plotnikov et al, 2007). The authors proved the existence of an optimal shape for drag minimisation in three spatial dimensions under the Mosco convergence of admissible domains and assuming that the family of admissible domains is nonempty. This is in fact a result on the compactness of the set of solutions to Navier-Stokes equations for the admissible family of obstacles, we refer the reader to Plotnikov et al, 2006a for details. The shape differentiability of solutions with respect to boundary perturbations is shown in Plotnikov et al, 2006b, and leads to the optimality system for the shape optimisation problem under considerations.

2. Compressible, stationary, Navier-Stokes equations.

Inhomogeneous boundary value problems for compressible, stationary Navier-Stokes equations are considered. In particular, the well-posedness for inhomogeneous boundary value problems of elliptic-hyperbolic type is shown. Analysis is performed for small perturbations of the approximate solutions, which are determined from Stokes problem. The existence and uniqueness of solutions close to approximate solution are proved, and in addition, the differentiability of solutions with respect to the coefficients of differential operators is shown. The results on the well-posedness of nonlinear problem are interesting on its own, and are used to obtain the shape differentiability of the drag functional for incompressible Navier-Stokes equations. The shape gradient of the drag functional is derived in the classical and useful for computations form, an appropriate adjoint state is introduced to this end. The shape derivatives of solutions to the Navier-Stokes equations are given by smooth functions, however the shape differentiability is shown in a weak norm. The method of analysis proposed in the paper is general, and can be used to establish the well-posedness for distributed and boundary control problems as well as for inverse problems in the case of the state equations in the form of compressible Navier-Stokes equations. The differentiability of solutions to the Navier-Stokes equations with respect to the data leads to the first order necessary conditions for a broad class of optimization problems.

3. Drag minimisation.

We present an exemple of shape optimization in aerodynamics. Mathematical analysis of the drag minimization problem for compressible Navier-Stokes equations can be found in Plotnikov et al., 2006a, 2006b.

PDE model. We assume that the viscous gas occupies the double-connected domain $\Omega = B \backslash S$, where $B \subset \mathbb{R}^3$, is a hold-all domain with the smooth boundary $\Sigma = \partial B$, and $S \subset B$ is a compact obstacle. Furthermore, we assume that

the velocity of the gas coincides with a given vector field $\mathbf{U} \in C^\infty(\mathbb{R}^3)^3$ on the surface Σ. In this framework, the boundary of the flow domain Ω is divided into the three subsets, inlet Σ_{in}, outgoing set Σ_{out}, and characteristic set Σ_0, which are defined by the equalities

$$\Sigma_{\text{in}} = \{x \in \Sigma : \mathbf{U} \cdot \mathbf{n} < 0\},$$
$$\Sigma_{\text{out}} = \{x \in \Sigma : \mathbf{U} \cdot \mathbf{n} > 0\},$$
$$\Sigma_0 = \{x \in \partial\Omega : \mathbf{U} \cdot \mathbf{n} = 0\},$$

where $\mathbf{n}$ stands for the outward normal to $\partial\Omega = \Sigma \cup \partial S$. In its turn the compact $\Gamma = \Sigma_0 \cap \Sigma$ splits the surface Σ into three disjoint parts $\Sigma = \Sigma_{\text{in}} \cup \Sigma_{\text{out}} \cup \Gamma$. The problem is to find the velocity field $\mathbf{u}$ and the gas density ϱ satisfying the following equations along with the boundary conditions

$$\Delta\mathbf{u} + \lambda\nabla\text{div}\,\mathbf{u} = R\varrho\mathbf{u}\cdot\nabla\mathbf{u} + \frac{R}{\epsilon^2}\nabla p(\varrho) \quad \text{in} \quad \Omega,$$
$$\text{div}\,(\varrho\mathbf{u}) = 0 \quad \text{in} \quad \Omega,$$
$$\mathbf{u} = \mathbf{U} \quad \text{on} \quad \Sigma, \quad \mathbf{u} = 0 \quad \text{on} \quad \partial S,$$
$$\varrho = \varrho_0 \quad \text{on} \quad \Sigma_{\text{in}},$$

where the pressure $p = p(\varrho)$ is a smooth, strictly monotone function of the density, ϵ is the Mach number, R is the Reynolds number, λ is the viscosity ratio, and ϱ_0 is a positive constant.

Drag minimization. One of the main applications of the theory of compressible viscous flows is the optimal shape design in aerodynamics. The classical sample is the problem of the minimization of the drag of airfoil travelling in atmosphere with uniform speed $\mathbf{U}_\infty$. Recall that in our framework the hydro-dynamical force acting on the body S is defined by the formula,

$$\mathbf{J}(S) = -\int_{\partial S} (\nabla\mathbf{u} + (\nabla\mathbf{u})^*$$
$$+(\lambda - 1)\text{div}\,\mathbf{u}\mathbf{I} - \frac{R}{\epsilon^2}p\mathbf{I})\cdot\mathbf{n}dS\ .$$

In a frame attached to the moving body the drag is the component of $\mathbf{J}$ parallel to $\mathbf{U}_\infty$,

$$J_D(S) = \mathbf{U}_\infty \cdot \mathbf{J}(S), \tag{2}$$

and the lift is the component of $\mathbf{J}$ in the direction orthogonal to $\mathbf{U}_\infty$. For the fixed data, the drag can be regarded as a functional depending on the shape of the obstacle S. The minimization of the drag and the maximization of the lift are between shape optimization problems of some practical importance.

We present first of all the result on the existence of the optimal shape in three spatial dimensions. Then we show the shape differentiability of the drag functional with respect to the boundary variations. The proof of the results are given in Plotnikov et al. 2006a and 2006b.

4. CONCLUSIONS

The modelling and shape optimization for the compressible Navier-Stokes equations is a new field of applications for the theory of non linear PDE's. We present some new results for the stationary case.

We point out the following aspects of proposed method of analysis of compressible Navier-Stokes equations which seems to be our original contribution.

- Extended form of the governing equations which allows to cope with the so-called mass control problem.
- The splitting of the boundary value problem for the transport equation into two parts: the local problem in the vicinity of inlet, and the global problem with the modified vector field $\tilde{\mathbf{u}}$ and the empty inlet $\tilde{\Sigma}_{in}$.
- The estimates of solutions to the model problem for the transport in the fractional Sobolev spaces, which can not be obtained by the interpolation method.
- The very weak formulation of linearized equations introduced to assure the existence of shape derivatives.

In this way we obtain the shape gradients of the drag functional for compressible Navier-Stokes equations.

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Free Material Optimization for Plates and Shells

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1. MOTIVATION

Free Material Optimization (FMO) has proven to be an efficient approach to the problem of finding the ultimatively best material for an elastic continuum structure subjected to given loads and boundary conditions (1), (2). Due to the underlying physical model describing the elastic behaviour of solid bodies, the original FMO approach is not applicable to thin-walled structures, as they frequently appear in the optimization of airplanes and cars. In this paper Free Material Optimization based on an elastic shell model is proposed.

2. SINGLE LOAD PROBLEM

The elastic behaviour of the shell body is described by Naghdi's shell model (3). The shell is interpreted as a surface ω with a director vector attached to each point. Two types of displacements are considered: the displacement of the point at the surface $u \in \left[H^1(\omega)\right]^3$ and the rotation of the director vector $\theta \in \left[H^1(\omega)\right]^2$. Rotations of the director vector around it's own axis are not taken into account:

$$U(\xi_1,\xi_2,\xi_3) = u(\xi_1,\xi_2) + \xi_3\theta_\lambda(\xi_1,\xi_2)a^\lambda(\xi_1,\xi_2)$$

where ξ_i, $i = 1,2,3$ are the curvilinear coordinates of the shell surface and a^λ, $\lambda = 1,2$ is the contravariant basis. The boundary Γ of the design space is divided into two parts: $\Gamma = \overline{\Gamma}_0 \cup \overline{\Gamma}_1$, where $\Gamma_0 \cap \Gamma_1 = \emptyset$. The set of admissible displacements is given by

$$\begin{aligned}\mathcal{U} := \big\{(u,\theta) \in H^1(\omega;\mathbb{R}^3)\big| \\ \theta \cdot a_3 = 0\,;\; u = \theta = 0 \text{ on } \Gamma_0\}\end{aligned}$$

It is now possible to deduce the formulas for the appearing membrane, bending and shear strains

$$\begin{aligned}\gamma_{\alpha\beta}(u) &= \frac{1}{2}\left(u_{\alpha|\beta} - u_{\beta|\alpha}\right) - b_{\alpha\beta}u_3\,, \\ \chi_{\alpha\beta}(u,\theta) &= \frac{1}{2}\Big(\theta_{\alpha|\beta} - \theta_{\beta|\alpha} - b^\lambda_\beta u_{\lambda|\alpha} \\ &\qquad - b^\lambda_\alpha u_{\lambda|\beta}\Big) + c_{\alpha\beta}u_3\,, \\ \zeta_\alpha(u,\theta) &= \frac{1}{2}\left(\theta_\alpha + u_{3,\alpha} + b^\lambda_\alpha u_\lambda\right)\,.\end{aligned}$$

In the plate case the midsurface ω has no curvature, hence $b_{\alpha\beta}$ and $c_{\alpha\beta}$ vanish (4). Thus the potential energy of the Naghdi shell reads as

$$\begin{aligned}&\Pi((u,\theta),(C^{\alpha\beta\mu\lambda},D^{\alpha\lambda})) := \\ &\quad\frac{1}{2}\int_\omega \Big[t\gamma_{\alpha\beta}C^{\alpha\beta\mu\lambda}\gamma_{\mu\lambda} + \frac{t^3}{12}\chi_{\alpha\beta}C^{\alpha\beta\mu\lambda}\chi_{\mu\lambda} \\ &\quad + t\zeta_\alpha D^{\alpha\lambda}\zeta_\lambda\Big]\,dS - \int_{\Gamma_1}(g\cdot u + m\cdot\theta)dl\end{aligned}$$

where $C^{\alpha\beta\mu\lambda}$ and $D^{\alpha\lambda}$ are the elasticity tensors of the shell, t is its thickness and g and m are applied forces and moments, respectively. Body forces are neglected. The potential energy can be reformulated by writing material and strain tensors as matrices and vectors:

$$\begin{aligned}\Pi((u,\theta),(C,D)) = \int_\omega \Big[&\frac{t}{2}\gamma^\top C\gamma + \frac{t^3}{24}\chi^\top C\chi \\ &+ \frac{t}{2}\zeta^\top D\zeta\Big]\,dS - \int_{\Gamma_1}(g\cdot u + m\cdot\theta)dl\end{aligned}$$

The minimum of the potential energy indicates the equilibrium state

$$\min_{(u,\theta)\in\mathcal{U}} \Pi((u,\theta),(C,D))$$

Now the optimization problem can be formulated. The stiffest structure possible is found

by minimizing the compliance $J((u,\theta),(C,D))$, which is given by the negative potential energy:

$$\min_{(C,D)\in\mathcal{C}} \max_{(u,\vartheta)\in\mathcal{U}} J((u,\theta),(C,D)) = -\frac{1}{2}\int_\omega \left[t\gamma^\top C\gamma + \frac{t^3}{12}\chi^\top C\chi + t\zeta^\top D\zeta \right] dS + \int_{\Gamma_1} (g\cdot u + m\cdot\theta) dl$$

The admissible elasticity tensors $(C,D) \in L^\infty(\omega)$ have to be symmetric and positive semidefinite: $C = C^\top \succeq 0$, $D = D^\top \succeq 0$, are subjected to a resource limit $\int_\omega \operatorname{tr}(C(x)) + \operatorname{tr}(D(x))\, dx \le V$ and have to satisfy the constraints $\operatorname{tr}(C(x)) \le c^+$, $\operatorname{tr}(D(x)) \le d^+$ preventing arbitrarily stiff material at singular points. A Minimax-Theorem guaranties the existence of an optimal point, which is a saddle point of the compliance functional J. Due to strong duality one can pass to the dual problem (5).

3. NUMERICAL TREATMENT

To solve this problem numerically the midsurface ω is partitioned into M elements ω_m. $C(x)$ and $D(x)$ are approximated by elementwise constant matrices $(C_1,\dots,C_M)$ and $(D_1,\dots,D_M)$. The displacements take the following form

$$U = \sum_{i=1}^{n} \lambda_i(r,s)\left(u^{(i)} + z\frac{t}{2}\theta^{(i)}\right)$$

where the $\lambda_i(r,s)$ are bilinear Lagrangean shape functions and n is the number of nodes (6). For each element one defines

$$A_m^\gamma = \sum_{i,j\in K} \int_{\omega_m} B_j^\gamma U U^\top (B_i^\gamma)^\top dx$$

where K is the index set of nodes associated with the element m and B_i^γ is the discretized membrane strain matrix. Matrices A_m^χ and A_m^ζ are defined analogously. According to this the discretized dual Single Load Problem takes the form of a convex semidefinite programm (7)

$$\begin{aligned} \max_{\substack{(u,\theta)\in\mathcal{U}\\ \alpha\in\mathbb{R}_+\\ \beta_u^C,\beta_u^D\in\mathbb{R}_+^M}} \quad & \int_{\Gamma_1} (g\cdot u + m\cdot\theta) dl - V\alpha \\ & - \int_\omega (c^+\beta_u^C + d^+\beta_u^D) dS \\ \text{subject to} \quad & \frac{t}{2}A_m^\gamma + \frac{t^3}{24}A_m^\chi - (\alpha+\beta_u^C)\mathbf{1} \preceq 0 \\ & \frac{t}{2}A_m^\zeta - (\alpha+\beta_u^D)\mathbf{1} \preceq 0 \end{aligned}$$

As a numeric test example the design of a clamp is optimized. In Fig. 1 the problem setting is shown, the resulting "density function" $\operatorname{tr}(C) + \operatorname{tr}(D)$ is displayed in Fig. 2.

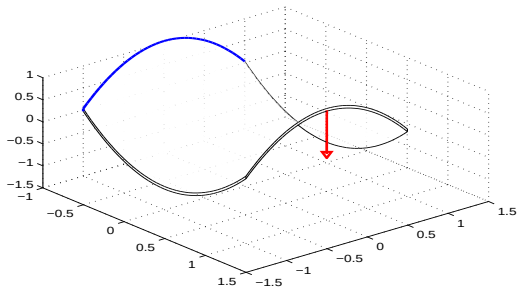

Fig. 1. Shell (hyperbolic paraboloid) with thickness $t = 0.03$, Dirichlet boundary conditions at $x = -1$ and a downward force at $x = 1$, $y = 0$

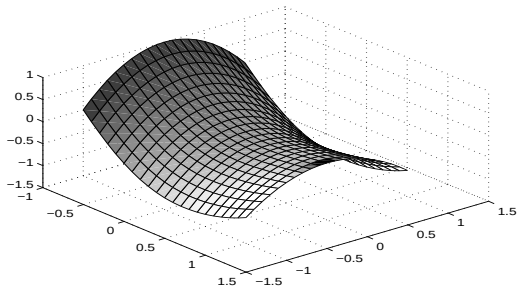

Fig. 2. "density function" of the deformed shell

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INVERSE PROBLEMS AND SELF-ADJOINT EXTENSIONS OF LAPLACIAN

A. LAURAIN AND K. SZULC

Let Ω and ω, with $0 \in \omega$, $0 \in \Omega$ two open subsets of $\mathbb{R}^2$ with smooth boundaries. Let $\varepsilon > 0$ be a small parameter and h a vector of $\mathbb{R}^2$. We define the perturbed domains Ω_ε^h and ω_ε^h in the following way: $\omega_\varepsilon = \{x \in \mathbb{R}^2,\ x = \varepsilon\xi,\ \xi \in \omega\}$ and $\Omega_\varepsilon = \Omega \setminus \omega_\varepsilon$, $\omega_\varepsilon^h = \{x = y + h,\ y \in \omega_\varepsilon\}$ and $\Omega_\varepsilon^h = \Omega \setminus \omega_\varepsilon^h$. We consider the following perturbed problem in $\mathbb{R}^2$, with f in $L^2(\Omega)$:

$$-\Delta v_h(x,\varepsilon) = f(x) \quad \text{in } \Omega_\varepsilon^h, \tag{1}$$

$$v_h(x,\varepsilon) = 0 \quad \text{on } \partial\Omega, \tag{2}$$

$$v_h(x,\varepsilon) = 0 \quad \text{on } \partial\omega_\varepsilon^h. \tag{3}$$

For $h = 0$, the self-adjoint extension of the Laplace operator is defined as follows: let $\mathcal{A}_0$ be the Laplacian operator $-\Delta_x$ in $L_2(\Omega)$ with the domain of definition

$$\mathcal{D}(\mathcal{A}_0) = \left\{v \in C_0^\infty(\overline{\Omega} \setminus \{0\}),\ v = 0 \text{ sur } \partial\Omega\right\} \tag{4}$$

The closure $\overline{\mathcal{A}_0}$ and the adjoint $\mathcal{A}_0^*$ of the operator $\mathcal{A}_0$ are given by the differential expression $-\Delta_x$, with the respective domain of definition:

$$\mathcal{D}(\overline{\mathcal{A}_0}) = \left\{v \in H^2(\Omega),\ v(0) = 0,\ v = 0 \text{ on } \partial\Omega\right\} \tag{5}$$

and

$$\mathcal{D}(\mathcal{A}_0^*) = \left\{v\ :\ v(x) = \chi_\delta(x)(-\frac{a}{2\pi}\log r + b) + \bar{v}(x),\ \bar{v} \in \mathcal{D}(\overline{\mathcal{A}_0}),\ a, b \in \mathbb{R}\right\} \tag{6}$$

There exists a family of self-adjoint operators $\mathcal{A}$, such that $\mathcal{A}_0 \subset \mathcal{A} \subset \mathcal{A}_0^*$ and the domain of definition $\mathcal{D}(\mathcal{A})$ contains all the required singular solutions for the Dirichlet problem in Ω.

Theorem 1. *Let* $\mathbf{A}$ *be the restriction of the operator* $\mathcal{A}_0^*$ *to the vector space*

$$\mathcal{D}(\mathbf{A}) = \{v \in \mathcal{D}(\mathcal{A}_0^*)\ :\ b = Sa\}$$

where $S = S(\varepsilon) = (2\pi)^{-1}(\log\varepsilon + L)$, L *is a constant which depends on the shape of* ω. *Then* $\mathbf{A}$ *is a self-adjoint operator and the following equation admits a unique solution* $\mathbf{v} \in \mathcal{D}(\mathbf{A})$.

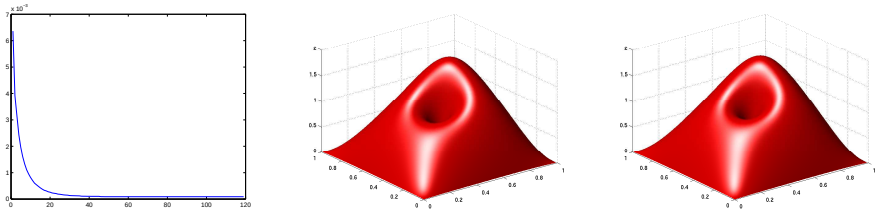
$$\mathbf{A}\mathbf{v} = f \in L_2(\Omega)$$

Actually, the function $\mathbf{v}$ is given by:

$$\mathbf{v}(x) = v^0(x) + \lambda(h)G(x,h)v^0(h), \quad \forall x \in \Omega, \tag{7}$$

with

$$\lambda(h) = \left(\frac{\log\varepsilon + L}{2\pi} + \mathcal{G}(h,h)\right)^{-1}. \tag{8}$$



$\mathcal{J}$ (left), $\mathbf{v}$ (center) and z (right) after 119 iterations.

where $v^0 \in H^2$ is the solution of the problem in Ω described as

$$\begin{aligned} -\Delta v^0(x) &= f(x) \quad \text{in} \quad \Omega \\ v^0(x) &= 0 \qquad \text{on} \quad \partial\Omega \end{aligned} \tag{9}$$

where G is the Green function and $\mathcal{G}$ is the regular part of the Green function.

From now on, the domain ω is assumed to be a ball of radius 1. We want to minimize the cost functional

$$\min_{h\in\Omega} \mathcal{J}(h) := \frac{1}{2}\int_{\Omega_2} (\mathbf{v}(x) - z(x))^2 dx \tag{10}$$

where z is a given observation in $L^2(\Omega_2)$. To this end we compute the gradient of $\mathcal{J}$ with respect to h.

$$\nabla\mathcal{J}(h) = \int_{\Omega_2} (\mathbf{v}(x) - z(x))\nabla_h \mathbf{v}(x) dx \tag{11}$$

The gradient $\nabla_h \mathbf{v}(x)$ takes the form:

$$\begin{aligned} \nabla_h \mathbf{v}(x) = \lambda(h)\left[v^0(h)\left(\frac{x-h}{2\pi r_h^2} - \nabla_y \mathcal{G}(x,h)\right) + G(x,h)\nabla v^0(h)\right] \\ - \lambda(h)^2 G(x,h) v^0(h)[\nabla_x \mathcal{G}(h,h) + \nabla_y \mathcal{G}(h,h)]. \end{aligned}$$

where $r_h = \|x-h\|$, and $\nabla_x\mathcal{G}$ and $\nabla_y\mathcal{G}$ are the gradients with respect to the first and second variables of $\mathcal{G}$, respectively.

For the numerical example we use the usual Polak-Ribière algorithm of conjugate gradient and we take $\Omega = [0,1]\times[0,1]$, $\Omega_1 = B((0.5,0.5),0.25)$ and $f = 100x^2y+10$. The observation z is artificial, which means that we know *ad hoc* the location of the hole h^* but we start the procedure from another value of h. We use finite differences with a Shortley-Weller approximation to discretize the Laplacian on the boundary of the ball Ω_1. The exact position h^* of the hole to be found is $h^* = (0.5, 0.5)$. The initial and final values of $\mathcal{J}$ and h are reported below. After 119 iterations with 255×255 elements on the grid, we converge to the following value of h and $\mathcal{J}$

	initialization	after 119 iterations
h	$(0.65, 0.65)$	$(0.50011, 0.50003)$
$\mathcal{J}$	$6.36024.10^{-3}$	$8.88902.10^{-5}$

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NUMERICAL METHOD FOR INVERSE PROBLEMS OF DETECTION OF IMPERFECTIONS WITH TOPOLOGICAL DERIVATIVES AND NEURAL NETWORKS

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1. SHAPE OPTIMIZATION

In the present paper the method of indentification of the coordinates and the radius of a small hole [1] is extended to the case of a finite number of imperfections. We consider a vector of locations $y_j \in \Omega$ and radiuses ρ_j, $j = 1, \ldots, M$ of small holes $B_j(y_j) = \{x : |x - y_j| < \rho_j\}$ which are included in Ω_0. The procedure of such an identification is based on the values of shape functionals $J_i(\Omega)$, $i = 1, \ldots, N$ defined by

$$J_i(\Omega_j) = \int_{\Omega_j} F_i(x, u(x), \nabla u(x))dx, \quad (1)$$

$$i = 1, \ldots, N,$$

which depend on the solutions $u(x)$, $x \in \Omega$, of the boundary value problem

$$\begin{cases} \triangle u = f & \text{in} \quad \Omega_j, \\ u = g & \text{on} \quad \Gamma_1, \\ \frac{\partial u}{\partial n} = h & \text{on} \quad \Gamma_2, \\ \frac{\partial u}{\partial n} = 0 & \text{on} \quad \Gamma_3, \end{cases} \quad (2)$$

$$\Gamma_3 = \cup_{k=1}^{j} \partial B_k(y_k) = \partial\Omega_j \setminus (\Gamma_1 \cup \Gamma_2).$$

in the domains $\Omega_j := \Omega_{j-1} \setminus \overline{B_j(\Omega_j)}$, $j - 1, \ldots, N$. Here we denote by Ω_0 i.e., for $j = 0$ the domain without any hole, $\Omega_1 = \Omega_0 \setminus \overline{B_1(y_1)}$ the domain with one hole and for each $j \geq 2$, Ω_j is the domain with j holes.

By the proposed identification procedure we can compute the coordinates $y_j \in \Omega_0$ of the holes $B_j(y_j)$ as well as the radiuses ρ_j such that given values of observation from physical model denoted by $J_{1j}, \ldots, J_{Nj}$, $j = 1, \ldots, M$ coincide approximately with the values $J_i(\Omega_j)$, $i = 1, \ldots, N$, $j = 1, \ldots, M$ obtained from the mathematical model.

For the case of one small hole the method is described in [1]. In the present paper the problem consists in identification of several holes. Therefore, we are interested from numerical point of view, in the inverse of the mapping

$$\mathcal{G}_j : \mathbf{R}^{3j} \to \mathbf{R}^N,$$

$$\mathcal{G}_j(y_1, \rho_1, \ldots, y_j, \rho_j) = \{\mathcal{J}_1(\Omega_j), \ldots, \mathcal{J}_N(\Omega_j)\}. \quad (3)$$

In the method we construct its approximation in the form

$$\mathcal{G}_{ij}(y_1, \rho_1, \ldots, y_j, \rho_j) \cong \mathcal{J}_i(\Omega_j) + \sum_{k=1}^{j} \frac{\rho_k^2}{2} \mathcal{T}_{\Omega_0} \mathcal{J}_i(y_k) \quad (4)$$

and determine the generalized inverse of this approximation, instead of the inverses of mappings $\mathcal{G}_j$. From the mathematical point of view, the inverse mapping $\mathcal{G}_j^{-1}$ is difficult to evaluate. In this case we can use, as it is proposed in [1], artificial neural networks to determine the generalized inverse of mapping (4). The numerical method can be described briefly as follows. We are going to generate a learning set consists of patterns formed by the values of shape functionals and targets formed by the coordinates and the radiuses of holes. We restrict ourselves to particular case of domain with three holes. Let us denote the learning set by J_i^k, (y_j^k, ρ_j^k), $i = 1, \ldots, 12$, $j = 1, \ldots, 3$, $k = 1, \ldots, K$ where K is a size of learning set.

2. NEURAL NETWORKS

A learning set created in this way cantains the degraded values calculated based on the random sets of triples holes. A neural network is an approximator of the conditional expectation θ_0. It

is the conditional expectation of the exact vector of set of triples holes $Y^k = (Y_1^k, \ldots, Y_9^k)$, $k = 1, \ldots, K$ - completely unknown, where:
$(Y_1^k, Y_2^k)-$ the coordinates of first hole's center, Y_3^k- the radius of first hole,
$(Y_4^k, Y_5^k)-$ the coordinates of second hole's center, Y_6^k- the radius of second hole,
$(Y_7^k, Y_8^k)-$ the coordinates of third hole's center, Y_9^k- the radius of third hole;
given the value of random generated vector of set of triples holes $X^k = (X_1^k, \ldots, X_9^k)$, $k = 1, \ldots, K$, where:
$(X_1^k, X_2^k) = y_1^k-$ the coordinates of first hole's center, $X_3^k = \rho_1^k-$ the radius of first hole,
$(X_4^k, X_5^k) = y_2^k-$ the coordinates of second hole's center, $X_6^k = \rho_2^k-$ the radius of second hole,
$(X_7^k, X_8^k) = y_1^k-$ the coordinates of third hole's center, $X_9^k = \rho_3^k-$ the radisus of third hole.
For the vector X^k we calculate, using the function $\mathcal{G}$, the shape functionals J_i^k, $i = 1, \ldots, 12$, $k = 1, \ldots, K$. The shape functionals are the elements of the learning set and they are the input vectors for neural network as the vectors corresponding to the set of triples holes.

The conditional expectation we denote the following formula

$$\theta_0(X^k) = E(Y^k|X^k),$$

$$for\ k \in \{1, \ldots, K\},$$

where a size of learning set $K \to \infty$.

We learn the neural network composed of 13 inputs (the vector of shape functionals + bias) and 9 outputs (the vektor conditional expectations of triples holes). Moreover the neural network contains 4 hidden layers composed of q_1, q_2, q_3, q_4 neurons.

We define a function space Θ containing θ_0. Created neural network is capable of arbitrarily accurate approximation to elements of space Θ. Let θ be neural network described earlier. $\theta \in \Theta$. We construct a sequence of „sieves" $\{\Theta_K\}$ for $K = 1, 2, \ldots$. Θ_K is a function space containing neural networks learnt based on $K-$ elements learning set. The number of neurons in hidden layers of neural network depends on a size of learning set and increases with increase of K, i.e. $q_1 \underset{K\to\infty}{\longrightarrow} \infty$, ..., $q_4 \underset{K\to\infty}{\longrightarrow} \infty$.

3. CONCLUSIONS

We define „connectionist sieve estimator" as a solution to the least squares problem (appropriate for learning $E(Y^k|X^k)$)

$$\min_{\theta\in\Theta_K} K^{-1} \sum_{k=1}^{K} [Y^k - \theta(X^k)]^2,$$

$$for\ K = 1, 2, \ldots \quad .$$

We show, that by some assumptions, there exists sieve estimator $\tilde{\theta}_K$ such that

$$\frac{1}{K}\sum_{k=1}^{K}[Y^k - \tilde{\theta}_K(X^k)]^2 = \min_{\theta\in\Theta_K} \frac{1}{K}\sum_{k=1}^{K}[Y^k - \theta(X^k)]^2,$$

for $K = 1, 2, \ldots$. Further $d(\tilde{\theta}_K, \theta_0) \xrightarrow{P} 0$, where $d-$ a measure of distance between functions and convergence is in measure.

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Modeling of geometrical imperfections Topological derivatives in nonsmooth domains

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1. INTRODUCTION

Topological derivatives are used in order to model the influence of geometrical imperfections or singularities of small size on the integral functionals evaluated for solutions of PDE's, ((Argatov et.al, 2003), (Fulmaści et.al, 2006), (Jackowska et.al, 2002), (Lewiński et.al, 2003), (Nazarov et.al, 2003), (Nazarov et.al, 2004), (Nazarov et.al, 2006), (Sokołowski et.al, 1999), (Sokołowski et.al, 2001), (Sokołowski et.al, 2003)). In the paper we present a mathematical model in the case of the Signorini problem on the crack and the numerical method for approximating such solutions and evaluating topological derivatives.

Actually, in the paper, a numerical method for the evaluation of topological derivatives is proposed for specific integral functionals which can be minimized for the resolution of some inverse problems. The method can be applied to a class of nonlinear contact problems on cracks, i.e. for the problems with nonpenetration conditions prescribed on the crack faces. Such boundary value problems in theory of elasticity can be formulated in smooth geometrical domains with the inequality constraints included in a convex set (Khludnev et.al, 2004). From the numerical point of view, it means, that all computations can be performed in the domain without any cut (crack). However, we should take into account the presence of the crack in the function space in the formulation of the unilateral problem under considerations, in another words the unilateral conditions are included in the convex set of test functions.

Numerical analysis of the variational inequality considered here is performed in (Belhachmi et.al, 2003). Our paper is in fact a continuation of the research in the direction of applications, in numerical methods for shape optimisation problems in the domains with cracks. In such a case, we should be able to evaluate the shape and topological derivatives of shape functionals and to solve the shape optimization problem by an application of e.g., the level set method Fulmaści et.al (2006). In the present paper, we focus on the evaluation of topological derivatives for the integral shape functionals in view of applications to inverse problems, see Jackowska et.al (2002) for this type of applications in smooth domains.

The outline of the paper is the following. In section 2, the mathematical formulation of the Signorini problem is presented. The model includes the Poisson equation in the domain Ω, and the inequality type boundary conditions on the crack faces $\Gamma_c^{\pm}$. The existence of a unique weak solution u for the boundary value problem is assured and the so-called smooth formulation of the problem is introduced for the purposes of numerical methods.

In section 3, related shape optimization problems for the integral shape functionals are considered. Some sufficient conditions for the existence of an optimal shape are given. We restrict ourselves to the computation of topological derivatives. Numerical solution of the related shape optimization problems is the subject of a forthcoming paper.

In section 4, the shape differentiability of the energy functional is shown. We provide the form of shape derivatives for the variations of external boundary as well as the crack faces. The notion of topological derivative is introduced and its form is derived.

Finally, in section 5 the numerical method for

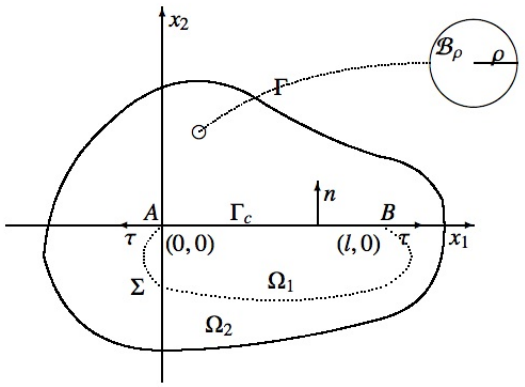

Fig. 1. The domain Ω

evaluation of topological derivatives is described and some numerical results are given.

2. VARIATIONAL INEQUALITY IN NONSMOOTH DOMAINS

We consider variational inequalities in the geometrical domain with the cut Γ_c. The set Γ_c is called a crack, if some specific boundary conditions for solutions of boundary value problems are prescribed on both faces $\Gamma_c^{\pm}$ of the cut Γ_c.

Let D be a bounded domain in $\mathbf{R}^2$ with smooth boundary Γ, and $\Gamma_c \subset D$ be a smooth curve without self-intersections.

We assume that Γ_c can be extended to a closed smooth curve $\Sigma \subset D$, with Σ of class $C^{1,1}$, and $D = \Omega^1 \cup \Sigma \cup \Omega^2$ is divided into two sub-domains Ω^1, Ω^2, (see Figure 1). In this case, $\Sigma = \partial\Omega^1$ is the boundary of Ω^1 and $\Sigma \cup \Gamma = \partial\Omega^2$ is the boundary of Ω^2. Let Ω be the domain $D \setminus \overline{\Gamma_c}$. Then Γ_c is called a crack in the elastic body of the reference configuration Ω. We restrict ourselves to the case of an elastic membrane, the generalization to an elastic body in two or three spatial dimensions is straightforward. The static equilibrium problem for the elastic membrane in the domain Ω with the interior crack Γ_c can be formulated as follows. Find u such that

$$\begin{array}{rcl} -\Delta u = f & \text{in} & \Omega \\ u = 0 & \text{on} & \Gamma \\ [u] \geq 0, \left[\frac{\partial u}{\partial \nu}\right] = 0, [u]\,\frac{\partial u}{\partial \nu} = 0 & \text{on} & \Gamma_c \\ \frac{\partial u}{\partial \nu} \leq 0 & \text{on} & \Gamma_c^{\pm} \end{array} \tag{1}$$

where f is a given function in $L^2(\Omega)$. The jump of the solution u on Γ_c is denoted by $[u] = u^+ - u^-$, where $u^{\pm} = u|_{\Gamma_c^{\pm}}$ are the traces of u on $\Gamma_c^{\pm}$.

Boundary value problem (1) can be considered as a free boundary problem since the coincidence set $\Xi = \{x \in \Gamma_c | [u] = 0\}$ is an unknown part of the solution. For the modelling of such problems in the framework of linear elasticity, similar boundary conditions arise in the crack theory for elastic bodies ((Khludnev et.al, 2004) (Lewinski et.al, 2000)). In such a case, the inequality type boundary conditions are imposed on Γ_c to describe the mutual non-penetration between the crack faces. It is the so-called frictionless contact problem on the crack ((Khludnev et.al, 2004), (Sokołowski et.al, 1992)). If the small ball $\mathcal{B}_\rho(\vartheta)$ is a *hole* in Ω, the performed domain $\Omega_\rho = \Omega \setminus \overline{\mathcal{B}_\rho(\vartheta)}$ is obtained, and the Neumann boundary conditions are prescribed in addition on $\partial\mathcal{B}_\rho(\vartheta)$. The solution u_ρ is given by the following boundary value problem,

$$\begin{array}{rcl} -\Delta u_\rho = f & \text{in} & \Omega_\rho \\ u_\rho = 0 & \text{on} & \Gamma \\ \left[u_\rho\right] \geq 0, \left[\frac{\partial u_\rho}{\partial \nu}\right] = 0, \left[u_\rho\right]\frac{\partial u_\rho}{\partial \nu} = 0 & \text{on} & \Gamma_c \\ \frac{\partial u_\rho}{\partial \nu} \leq 0 & \text{on} & \Gamma_c^{\pm} \\ \frac{\partial u_\rho}{\partial \nu} = 0 & \text{on} & \partial B_\rho(\vartheta) \end{array} \tag{2}$$

Problems (1) and (2) admit variational formulations in Ω and Ω_ρ, respectively.

Let us consider the boundary value problem in Ω. The variational problem in Ω_ρ can be formulated in the same way. It is well-known that (1) admits a unique weak solution which minimizes, with respect to $\mathrm{v} \in \mathbf{C}(\Gamma_c)$, the energy functional

$$\mathcal{E}(\mathrm{v}) = \frac{1}{2}\int_\Omega |\nabla \mathrm{v}|^2\,dx - \int_\Omega f\mathrm{v}\,dx \geq \mathcal{E}(u)\,. \tag{3}$$

The closed convex cone $\mathbf{C}(\Gamma_c)$ includes all functions in the Sobolev space $H^1(\Omega)$ which vanish on Γ and satisfies the unilateral condition $[\mathrm{v}] \geq 0$ on Γ_c,

$$\mathbf{C}(\Gamma_c) = \{\mathrm{v} \in H^1(\Omega) | \mathrm{v} = 0 \text{ on } \Gamma, [\mathrm{v}] \geq 0 \text{ on } \Gamma_c\}. \tag{4}$$

We introduce the mixed formulation of the variational inequality. To this end we denote by $V = V(\Omega)$ the space $L^2(\Omega)$, to indicate the dependence on the domain Ω, and introduce the space

$\mathbf{X} = \mathbf{X}(\Omega)$ of vector functions

$$\mathbf{X} = \left\{ \mathbf{q} \in L^2(\Omega)^2 \mid \operatorname{div} \mathbf{q} \in L^2(\Omega) \right\}. \quad (5)$$

$\mathbf{X}(\Omega)$ is a Hilbert space equipped with the norm

$$\|\mathbf{q}\|_{\mathbf{X}} = \left(\|\mathbf{q}\|^2_{(L^2(\Omega))^2} + \|\operatorname{div} \mathbf{q}\|^2_{L^2(\Omega)} \right)^{\frac{1}{2}} . \quad (6)$$

Let $\mathbf{K}(\Omega) \subset \mathbf{X}(\Omega)$ denote the convex set

$$\mathbf{K} = \{ \mathbf{q} \in \mathbf{X} \mid [\mathbf{q}.\nu] = 0 \text{ on } \Gamma_c,\ (\mathbf{q}.\nu)^{\pm} \leq 0 \text{ on } \Gamma_c^{\pm} \} , \quad (7)$$

which is defined by using the dual order in the fractional Sobolev space $(H^{\frac{1}{2}}_{00}(\Gamma_c))'$ for the inequality condition on $\Gamma_c^{\pm}$. We refer the reader to (Adams et.al, 1975) for the definition and properties of the Sobolev spaces. Here $[\cdot]$ denotes the jump across Γ_c and ν is the unit normal vector pointing to the exterior of Ω_1 (see Figure 1). The mixed formulation of boundary value problem (1) can be written in the form of variational problem. Find $(\mathbf{p}, u) \in \mathbf{K}(\Omega) \times V(\Omega)$ such that

$$\begin{cases} \int_\Omega \mathbf{p}\,(\mathbf{q} - \mathbf{p})\,dx \\ \quad + \int_\Omega u\,(\operatorname{div}\mathbf{q} - \operatorname{div}\mathbf{p})dx \geq 0, & \forall \mathbf{q} \in \mathbf{K}(\Omega), \\ - \int_\Omega \operatorname{div} \mathbf{p}\, v\, dx = \int_\Omega f\, v\, dx, & \forall v \in V(\Omega) \end{cases} \quad (8)$$

Note that $(\nabla u, u)$ is the solution of problem (1).

The smooth domain formulation of (1) in D, useful for numerical methods, is introduced (Khludnev et.al, 2004) as follows.
Find $(\mathbf{p}, u) \in \mathbf{K}(D) \times V(D)$ such that

$$\begin{cases} \int_D \mathbf{p}\,(\mathbf{q} - \mathbf{p})\,dx \\ \quad + \int_D u\,(\operatorname{div}\mathbf{q} - \operatorname{div}\mathbf{p})dx \geq 0, & \forall \mathbf{q} \in \mathbf{K}(D), \\ - \int_D \operatorname{div} \mathbf{p}\, v\, dx = \int_D f\, v\, dx, & \forall v \in V(D). \end{cases} \quad (9)$$

The smooth domain formulation of (8) means that the functions $\mathbf{p}$ and u which are defined in Ω are extended to the entire domain $D = \Omega \cup \Gamma_c$. Hence, the closed problem formulation (9) is obtained by replacing Ω with D in (7), with the obvious modification of the function spaces are defined now over D, and are denoted by $\mathbf{X} = \mathbf{X}(D)$ and $V = V(D)$.
The well-posedness of smooth domain formulation (9) is proved in (Khludnev et.al, 2004) with the arguments based on the regularization technique. This means that the solution is defined in D, the crack is present only in the definition of the set of test functions $\mathbf{K}(\Omega)$.

3. SHAPE OPTIMIZATION IN NONSMOOTH DOMAIN

Our aime is to prepare numerical method of analysis of variational inequalities, which can be used for numerical solutions of relate shape optimisation or inverse problems. Shape optimization problems can be solved numerically e.g. by an application of the level set method combined with the shape derivatives and the topological derivatives (Fulmaści et.al, 2006). We introduce the shape and topological derivatives for the maximization of integral shape functionals, to fix ideas. Similar expressions for shape and topological derivatives can be obtained for a broad class of integral shape functionals ((Sokołowski et.al, 2001), (Sokołowski et.al, 2003)). We present numerical results for some exemples in section 4. As an example, let us consider the energy functional

$$J(\Omega) := \mathcal{E}(u) = \inf_{v \in \mathbf{C}(\Gamma_c)} \left\{ \frac{1}{2} \int_\Omega |\nabla v|^2 - \int_\Omega f v \right\}. \quad (10)$$

Shape optimization problem which can be considered for functional (10) is e.g. the maximization of $J(\Omega) := \mathcal{E}(u_\Omega)$ with the respect to the geometrical domain Ω. It is supposed that the volume of Ω is fixed and the crack Γ_c is included in the family $\mathcal{U}_{ad}$ of admissible domains. A regularisation term for the shape functional can be introduced in order to assure the existence of an optimal shape (Fulmaści et.al, 2006). To solve the shape optimization problems one usually needs the so-called shape derivatives (Khludnev et.al, 2004). We briefly recall the different sorts of shape derivatives which can be derived for the energy functional. We refer to (Slimane et.al, 2004) for all details of such a derivation. In numerical methods of shape optimization, the shape gradients are used for the change of domain by means of boundary variations, and the topological derivatives are useful for creating small holes. Proofs of the formulae given below can be founded e.g. in (Sokołowski et.al, 2001) (Sokołowski et.al, 2003), (Sokołowski et.al, 1992).

The shape derivatives of the energy functionals

$$J(\Omega) := \mathcal{E}(u). \quad (11)$$

which can be obtained with respect to the variations of the boundary $\partial\Omega$ include:

1. boundary variations, (Sokołowski et.al, 1992) of $\Gamma = \partial D$ for the vector field V with $suppV \cap \overline{\Gamma_c} = \emptyset$ are given by the expression

$$dJ(\Omega; \mathrm{v}) = \frac{1}{2}\int_{\Gamma} \|\nabla u\|^2 V \cdot n d\Gamma(x) \qquad (12)$$

2. variations of the proposition of the crack tip for the constant vector field V in direction of the tangent vector to the crack and such that $suppV \cap \Gamma = \emptyset$

$$\begin{aligned} dJ(\Omega; \mathrm{v}) = \; & -\tfrac{1}{2}\int_{\Omega}(\vartheta_{x_1}(u_{x_1}^2 - u_{x_2}^2) + 2\vartheta_{x_2}u_{x_1}u_{x_2}) \\ & -\int_{\Omega}(\vartheta f)_{x_1}u \end{aligned} \qquad (13)$$

where $\vartheta \in C_0^{\infty}(D)$ is any function (Khludnev et.al, 2004) such that $\vartheta = 1$ in the neighbourhood of the tip $(l; 0)$, $l > 0$ (see Figure 1.)

3. topological variations of the energy functional resulting from the creation of a small hole $\mathcal{B}_\rho(\vartheta)$. This leads to the topological derivative denoted by $\mathcal{T}_\Omega(\vartheta)$. The derivative is defined using the asymptotic expansion of the energy functional with respect to the small parameter ρ

$$J(\Omega_\rho) = J(\Omega) + \rho^2\mathcal{T}_\Omega + o(\rho^2), \qquad (14)$$

where $\Omega_\rho = \Omega \setminus \overline{B_\rho(\vartheta)}$, $\vartheta \in \Omega$, $\overline{B_\rho(\vartheta)} \cap \overline{\Gamma_c} = \emptyset$

The topological derivative $\mathcal{T}_\Omega(\vartheta)$ is given by two equivalent expressions, see (Sokołowski et.al, 2001), (Sokołowski et.al, 2003) for the results in the case of contact problems.

- The first expression is the line integral :

$$\mathcal{T}_\Omega(\vartheta) = -\frac{1}{\pi R^6}\left[\left(\int_{\Gamma_R} ux_1\right)^2 + \left(\int_{\Gamma_R} ux_2\right)^2\right] \qquad (15)$$

where Γ_R is a contour outside of $\mathbf{B}_\rho(O)$, i.e. $\mathbf{B}_\rho(O) \subset \mathbf{B}_R(O) \subset \Omega_\rho$ and $\Gamma_R = \partial\mathbf{B}_R(O)$.

- The second expression includes the value of the gradient $\|\nabla u(O)\|^2$ at the center O of the hole, where u is the solution of unperturbed problem (1). The equivalent expression is obtained in (Nazarov et.al, 2006) for the expansion of the energy functional and for $\rho > 0$, ρ small enough,

$$\mathcal{E}(\Omega_\rho) = \mathcal{E}(\Omega) + \frac{\rho^2\pi}{2}|\nabla u(\Omega; O)|^2 + O(\rho^{3-\delta}) \qquad (16)$$

for some $0 < \delta < 1$. For the derivation of (16), the asymptotics of solutions to the boundary value problem defined in Ω_ρ are used, with respect to the small parameter $\rho > 0$, $u_\rho \in H^1(\Omega_\rho)$.

4. NUMERICAL EVALUATION OF TOPOLOGICAL DERIVATIVES BY SMOOTH DOMAIN METHOD

In order to determine the shape and topological derivatives we need a numerical solution to the variational inequality under considerations. We describe the numerical procedure for solutions of variational inequalities in Ω. Let $h > 0$ denotes the parameter of discretization by the finite element method. We denote by $\sigma > 0$ the regularization parameter. The discrete problem for (8) is defined in the following way:
Find $(u_h, \mathbf{p}_h) \in V_h \times \mathbf{K}_h$ such that

$$\begin{cases} a_\delta(u_h, v_h) + b(v_h, p_h) = (f, v_h) & \forall v_h \in V_h \\ -b(u_h, \mathbf{q}_h - \mathbf{p}_h) + g(\mathbf{p}_h, \mathbf{q}_h - \mathbf{p}_h) \geq 0 & \forall \mathbf{q}_h \in \mathbf{K}_h \end{cases} \qquad (17)$$

There is a unique solution $(u_h, \mathbf{p}_h)$ to (17) for $h > 0$. The energy functional over the convex set $V \times \mathbf{K}$ is given by

$$\mathcal{J}(v, \mathbf{q}) = \frac{1}{2}a_\delta(v, v) - (f, v) - b(v, \mathbf{q}) + \frac{1}{2}g(\mathbf{q}, \mathbf{q}). \qquad (18)$$

Solution of problem (17) is equivalent to the minimization of functional (18)

$$\mathcal{J}(u, \mathbf{p}) = \min_{(v,\mathbf{q}) \in V \times \mathbf{K}} \mathcal{J}(v, \mathbf{q})\,. \qquad (19)$$

The linear constraints in the definition of $\mathbf{K}$ can be imposed by the duality using the closed convex cone

$$M = \left\{\mu \in H^{\frac{1}{2}}(\Gamma_c);\ \mu \geq 0\right\}, \qquad (20)$$

thus the variational formulation for problem (17) can be rewritten as follows:
Find $(u_h, \mathbf{p}_h, \lambda_h) \in V_h \times \mathbf{X}_h \times M_h$ such that

$$\begin{cases} a_\delta(u_h, v_h) + b(v_h, \mathbf{p}_h) = (f, v_h) & \forall v_h \in V_h\,, \\ -b(u_h, \mathbf{q}_h) + g(\mathbf{p}_h, \mathbf{q}_h) & \\ \quad + \int_{\Gamma_c}(\lambda_h)(\mathbf{q}_h.\nu)\,d\sigma = 0 & \forall \mathbf{q}_h \in \mathbf{X}_h\,, \\ \int_{\Gamma_c}(\mu_h - \lambda_h)(\mathbf{p}_h.\nu)\,d\sigma \leq 0 & \forall \mu_h \in M_h\,, \end{cases} \qquad (21)$$

where M_h is a specific multiplier set, (Belhachmi et.al, 2003), which can be defined by the following approximation

$$M_h^0 = \left\{\mu_h \in W_h^0(\Gamma_c),\ \mu_h \geq 0,\ \text{on}\ \Gamma_c\right\}, \qquad (22)$$

and the choice of $W_h^1(\Gamma_c)$ leads to the following two approximation sets, Belhashmi et al. (2003)

$$M_h^1 = \left\{\mu_h \in W_h^1(\Gamma_c),\ \mu_h \geq 0,\ \text{on}\ \Gamma_c\right\}, \qquad (23)$$

or

$$M_h^{1,*} = \begin{array}{l}\left\{\mu_h \in W_h^1(\Gamma_c),\right. \\ \left.\int_{\Gamma_c} \mu_h \psi_h \, d\Gamma \geq 0,\ \forall \psi_h \in M_h^1\right\}.\end{array} \qquad (24)$$

Here W_h^0 or W_h^1 means the approximation piecewise constant and piecewise linear respectively.

In order to perform the computations, the matrix formulation of problem (21) is used. It is readily checked that $(u_h, \mathbf{p}_h, \lambda_h) \in V_h \times \mathbf{X}_h \times M_h$ is a solution of (21) if and only if $(u_h, \mathbf{p}_h, \lambda_h)$ is a saddle-point of the Lagrangian defined on $V_h \times \mathbf{X}_h \times M_h$ by

$$\mathcal{L}(\mathrm{v}_h, \mathbf{q}_h, \mu_h) = \mathcal{J}(\mathrm{v}_h, \mathbf{q}_h) + \int_{\Gamma_c} \mu_h.(\mathbf{q}_h.\mathrm{v}) \, d\sigma \qquad (25)$$

which means that $(u_h, \mathbf{p}_h, \lambda_h)$ satisfies

$$\begin{array}{rll}\mathcal{L}(u_h, \mathbf{p}_h, \mu_h) & \leq \mathcal{L}(u_h, \mathbf{p}_h, \lambda_h) & \forall (\mathrm{v}_h, \mathbf{q}_h) \in V_h \times \mathbf{X}_h, \\ & \leq \mathcal{L}(\mathrm{v}_h, \mathbf{q}_h, \lambda_h), & \forall \mu_h \in M_h.\end{array} \qquad (26)$$

Let $\mathbf{V}$, $\mathbf{U}$ denote the vectors with the entries given by the nodal values of the functions $(\mathrm{v}_h, \mathbf{q}_h)$ and $(u_h, \mathbf{p}_h)$, respectively. Let M and Λ be the vectors with the entries given by the nodal values of μ_h and λ_h, respectively, for the three different choices of the space M_h, namely $M_h = M_h^1$, $M_h = M_h^{1,*}$ or $M_h = M_h^0$. Therefore, the saddle-point problem for Lagrangian (25) can be rewritten in finite dimensional setting :
Find $\mathbf{U} = (u_h, \mathbf{p}_h)$ and Λ, defined by the following max-min condition

$$\max_{S\,M \geq 0} (\min_{\mathbf{V}} \frac{1}{2} {}^t\mathbf{V}\mathbf{K}\mathbf{V} - {}^t\mathbf{V}\mathbf{F} + ({}^t\mathbf{V}\,\mathbf{L})S\,M), \qquad (27)$$

where $\mathbf{K}$ denotes the stiffness matrix, $\mathbf{F}$ is the vector corresponding to the external loading and the matrix S expresses the sign conditions for multipliers (22)-(24) and L is the coupling matrix defined below.

Given a triangularization $\mathcal{T}_h$ of Ω, let N denote the number of nodes in Ω and N_T the number of elements in $\mathcal{T}_h$. Denote by $(w_i)_{i=1}^N$, the Lagrange finite element basis of V_h and let $(\mathbf{\Phi}_i)$ stand for the basis in the space $\mathbf{X}_h$. Each vector function $\mathbf{\Phi}_i$ is either of the form $(w_i, 0)$, $1 \leq i \leq N$, $(b_i, 0)$, $1 \leq i \leq N_T$, or it is given by $(0, w_i)$, $1 \leq i \leq N$, $(0, b_i)$, $1 \leq i \leq N_T$, respectively, where by b_i is denoted a bubble function. Then the matrix K is defined by

$$\mathbf{K} = \begin{pmatrix} A_\delta & {}^tB_1 & {}^tB_2 \\ -B_1 & G_1 & 0 \\ -B_2 & 0 & G_2 \end{pmatrix} \qquad (28)$$

and the right hand side takes the form

$$\mathbf{F} = \begin{pmatrix} D\,F \\ 0 \\ 0 \end{pmatrix},$$

with $F = (f_i)_i$, $D = (\int_\Omega w_i \, w_j \, dx)_{ij}$, $i, j = 1, \ldots, N$ and $A_\delta = \delta\, D$. The matrices B_1 and B_2 are defined by $(B_1)_{ij} = (\int_\Omega w_j \partial_1 \mathbf{\Phi}_i^{(1)} \, dx)_{ij}$ and $(B_2)_{ij} = (\int_\Omega w_j \partial_2 \mathbf{\Phi}_i^{(2)} \, dx)_{ij}$, $j = 1, \ldots, N$, $i = 1, \ldots, N + N_T$. Finally

$$G_1 = G_2 = \begin{pmatrix} D & (\int_\Omega w_i \, b_j \, dx)_{ij} \\ (\int_\Omega b_i \, w_j \, dx)_{ij} & (\int_\Omega b_i^2 \, dx)\delta_{ij} \end{pmatrix},$$

where δ_{ij} is the Kronecker symbol.

Let N_c denote the number of nodes on Γ_c and let us denote by $(\psi_i)_i$, $1 \leq i \leq N_c$ the basis in the space $W_h^1(\Gamma_c)$ and by $(\phi_i)_i$ the basis of $W_h^0(\Gamma_c)$, $1 \leq i \leq N_c - 1$. We have a specific form of S for each particular choice of M_h, namely

- if M_h is M_h^0 or M_h^1 then S is given by the identity matrix.
- if $M_h = M_h^{1,*}$, then S is given by $S_{ij} = \int_{\Gamma_c} \psi_i \, \psi_j \, d\Gamma$, $1 \leq i, j \leq N_c$.

Finally, the *coupling* matrix $L = (0, L_1, L_2)$' is defined in the following way
If $M_h = M_h^1$ or $M_h = M_h^{1,*}$, then

$$(L^1)_{ij} = \begin{cases} \int_{\Gamma_c} \psi_j \, ((w_i, 0).\nu) \, d\Gamma, & \begin{array}{l}1 \leq i \leq N, \\ 1 \leq j \leq N_c,\end{array} \\ 0, & \begin{array}{l}1 \leq i \leq N_T, \\ 1 \leq j \leq N_c,\end{array} \end{cases}$$

and

$$(L^2)_{ij} = \begin{cases} \int_{\Gamma_c} \psi_j \, ((0, w_i).\nu) \, d\Gamma, & \begin{array}{l}1 \leq i \leq N, \\ 1 \leq j \leq N_c,\end{array} \\ 0, & \begin{array}{l}1 \leq i \leq N_T, \\ 1 \leq j \leq N_c,\end{array} \end{cases}$$

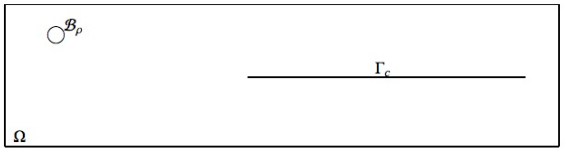

Fig. 2. Domain Ω with a crack Γ_c and a defect $\mathcal{B}_\rho$

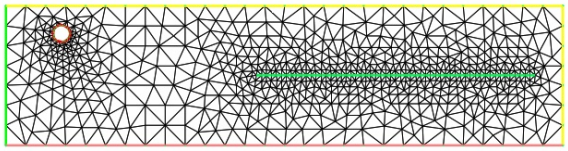

Fig. 3. Finite element approximation

If $M_h = M_h^0$, then

$$(L^1)_{ij} = \begin{cases} \int_{\Gamma_c} \phi_j\,((w_i, 0).\nu)\,d\Gamma, & 1 \le i \le N, \\ & 1 \le j \le N_c - 1, \\ 0, & 1 \le i \le N_T, \\ & 1 \le j \le N_c, \end{cases}$$

and

$$(L^2)_{ij} = \begin{cases} \int_{\Gamma_c} \phi_j\,((0, w_i).\nu)\,d\Gamma, & 1 \le i \le N, \\ & 1 \le j \le N_c - 1, \\ 0, & 1 \le i \le N_T, \\ & 1 \le j \le N_c \end{cases}$$

The solution $(\mathbf{U}, \Lambda)$ of (27) satisfies the saddle-point conditions and we have

$$\mathbf{U} = \mathbf{K}^{-1}(\mathbf{F} - L\,S\,\Lambda). \tag{29}$$

Therefore, for $\Phi = S\Lambda$, the saddle-point problem (27) can be rewritten as a quadratic programming problem

$$\min_{\Phi \ge 0}\left(\frac{1}{2}{}^t\Phi\,{}^tL\mathbf{K}^{-1}L\Phi - {}^t\Phi\,{}^tL\mathbf{K}^{-1}\mathbf{F} + \frac{1}{2}{}^t\mathbf{F}\mathbf{K}^{-1}\mathbf{F}\right). \tag{30}$$

If $\overline{\Phi}$ is the solution of (30), then $\Lambda = S^{-1}\overline{\Phi}$. The solution $\mathbf{U}$ is obtained by solving (29). For all the proofs on well posedness of numerical scheme we refer the reader to (Belhachmi et.al, 2003).

5. NUMERICAL EXAMPLE

We present numerical results for topological derivatives of the energy functional for Signorini problem on the crack. Let us consider a rectangle $\Omega = (2, 4) \times (0, 0.5)$ with the crack $\Gamma_c = (2.9, 3.9) \times 0.25$ and the small hole with center in $x_0 = (2.2, 0.4)$ and radius $\rho = 0.03$.

In the domain Ω we solve the variational inequality

$$\begin{aligned} -\Delta u &= 1 \quad \text{in} \quad \Omega \\ u &= 0 \quad \text{on} \quad \Gamma \\ [u] \ge 0, \left[\tfrac{\partial u}{\partial \nu}\right] = 0, [u]\,\tfrac{\partial u}{\partial \nu} &= 0 \quad \text{on} \quad \Gamma_c \\ \tfrac{\partial u}{\partial \nu} &\le 0 \quad \text{on} \quad \Gamma_c^{\pm} \end{aligned} \tag{31}$$

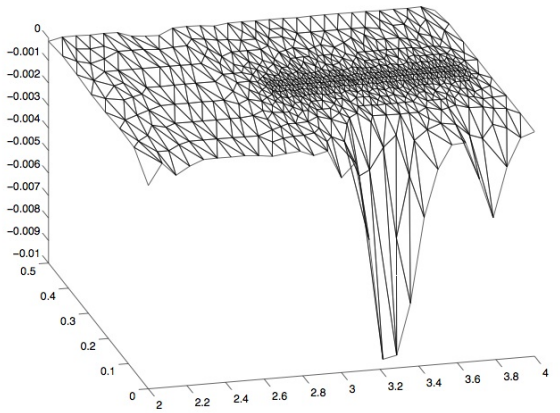

Fig. 4. Topological derivative of the energy functional in the domain with the crack Γ_c

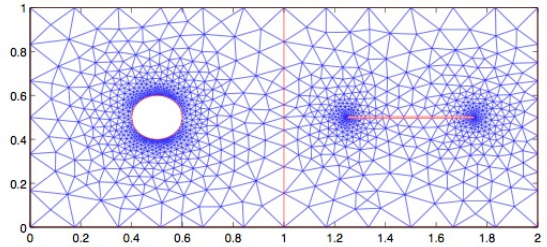

Fig. 5. Topological derivative of the energy functional in the domain with the crack.

using the method presented in (Belhachmi et.al, 2003). The topological derivative of the energy functional is given by the formula

$$\mathcal{T}_\Omega(x_0) = \left[-|\nabla u(x_0)|^2 + u(x_0)\right]\pi\rho^2 \tag{32}$$

in function of the point $x_0 \in \Omega$ Results of computations are presented by the following figures

Let us consider another example. In Fig. 6 the actual geometrical domain with a crack and a hole is presented. In Fig. 7 the topological derivative of the energy functional is visualized. The results of computations confirm that the topological derivative can be evaluated using the finite element method proposed in the paper.

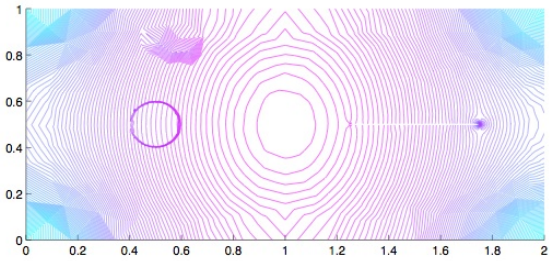

Fig. 6. Topological Derivative

6. CONCLUSIONS

We present a numerical method for evaluating topological derivatives. Some numerical results obtained by the method are presented. The next step will be the use of level set method in shape optimization for numerical solution of the associated shape optimization problems. The topological derivatives can be also used for numerical solutions of inverse problems of identification of small imperfection.

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THE *FREE MATERIAL DESIGN* REVISITED

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1. INTRODUCTION

The free material design (FDM) approach was proposed by Bendsøe et al.(1994), see also the recent paper by Kočvara and Stingl(2007). In this approach the Hooke tensor **C** is viewed as the design variable to minimize the compliance of the structure optimized. The isoperimetric condition is usually put on the trace of this tensor or on its Frobenius norm. Within such formulation the resulting optimal material occurs to be isotropic with zero Poisson ratio. The aim of the present paper is to reformulate this problem by using the representation theorem of Rychlewski (1984) and additional theorems by Blinowski et al.(1996). According to this representation theorem Hooke's tensor in two dimensions is decomposed as follows:

$$\mathbf{C} = \lambda_1 \mathbf{P}_1 + \lambda_2 \mathbf{P}_2 + \lambda_3 \mathbf{P}_3 .$$

The moduli λ_i are called Kelvin moduli according to Rychlewski's suggestion. The tensors $\mathbf{P}_i$ are projectors given by tensorial products $\mathbf{P}_i = \boldsymbol{\omega}_i \otimes \boldsymbol{\omega}_i$, i=1,2,3. The components of tensors (called proper states) $\boldsymbol{\omega}_i$ in the Cartesian basis $\mathbf{e}_\alpha \otimes \mathbf{e}_\beta$ can be expressed as follows

$$\boldsymbol{\omega}_i^{\alpha\beta} = f^{\alpha\beta}(\psi_i, \theta_i),$$

where the functions $(x,y) \to f^{\alpha\beta}(x,y)$ are defined below

$$f^{11}(x,y) = \cos x \cos^2 y + \sin x \sin^2 y ,$$
$$f^{12}(x,y) = (\cos x - \sin x) \sin y \cos y ,$$
$$f^{22}(x,y) = \cos x \sin^2 y + \sin x \cos^2 y ,$$

where $f^{12}(x,y) = f^{21}(x,y)$; Greek indices assume values 1,2. The quantities ψ_i, θ_i determine certain angles characterizing geometry of the underlying microstructure. These angles are linked by three formulae which will not be reported here. The Kelvin moduli and the above angles will be treated as design variables. We shall express the free material problem in terms of these variables and pose the minimum compliance problem in a new manner imposing the isoperimetric condition on the Kelvin moduli. A new derivation with new assumptions will be given for the resulting zero Poisson ratio effective material.

2. REFORMULATION OF THE FREE MATERIAL DESIGN

Consider 2D elasticity within a domain Ω, parameterised by Cartesian system (x_1, x_2). Let $\varepsilon_{\alpha\beta}(\mathbf{u})$ be a symmetric part of $\nabla\mathbf{u}$, where $\mathbf{u} = (u_1, u_2)$ is the displacement vector, an element of the space U of kinematically

admissible displacements. Let $f(\mathbf{v})$ represent the work of the loading on the trial displacement fields $\mathbf{v}$. The elastic potential

$$J(\mathbf{C},\mathbf{u})=\frac{1}{2}\int_{\Omega}\sum_{\alpha,\beta,\lambda,\mu}C^{\alpha\beta\lambda\mu}(x)\varepsilon_{\alpha\beta}(\mathbf{u})\varepsilon_{\lambda\mu}(\mathbf{u})dx-f(\mathbf{u})$$

is treated as dependent on the tensor $\mathbf{C}$ and field $\mathbf{u}$. We shall assume that the cost of the plate depends on the Kelvin moduli. Let

$$\Psi(\mathbf{C})=\|\boldsymbol{\lambda}\|_p,$$

where

$$\boldsymbol{\lambda}=(\lambda_1,\lambda_2,\lambda_3) \text{ and } \|\boldsymbol{\lambda}\|_p=(\sum_{i=1}^{3}|\lambda_i|^p)^{1/p}.$$

The minimum compliance problem is put in the form discussed in Bendsøe et al.(1994) as

$$\max_{\substack{\text{admissible } \mathbf{C} \text{ such that}\\ \int_\Omega \Psi(\mathbf{C})dx\le V}}\ \min_{\mathbf{u}\in U} J(\mathbf{C},\mathbf{u}),$$

which leads to

$$\max_{\rho\in G}\min_{\mathbf{u}\in U}\left\{\int_\Omega W(\mathbf{u})dx-f(\mathbf{u})\right\}$$

where G is the set of admissible densities being non-negative, bounded, whose integral over the given domain is smaller than V. The potential W is given by

$$2W(\mathbf{u})=\max_{\substack{\text{admissible } \mathbf{C} \text{ such that}\\ \Psi(\mathbf{C})\le\rho}}\sum_{\alpha,\beta,\lambda,\mu}C^{\alpha\beta\lambda\mu}\varepsilon_{\alpha\beta}(\mathbf{u})\varepsilon_{\lambda\mu}(\mathbf{u})$$

where we can write now

$$\sum_{\alpha,\beta,\lambda,\mu}C^{\alpha\beta\lambda\mu}\varepsilon_{\alpha\beta}(\mathbf{u})\varepsilon_{\lambda\mu}(\mathbf{u})=\sum_{i=1}^{3}\lambda_i a_i(\mathbf{u})$$

with

$$a_i(\mathbf{u})=\sum_{\alpha,\beta}\left(f^{\alpha\beta}(\psi_i,\theta_i)\varepsilon_{\alpha\beta}(\mathbf{u})\right)^2.$$

Define $\mathbf{a}=(a_1,a_2,a_3)$. Let us note that the choice

$$\lambda_i=\rho\left(\|\mathbf{a}\|_q\right)^{-q/p}a_i(\mathbf{u})^{q/p},\quad q^{-1}+p^{-1}=1,$$

is optimal. The local problem reduces to

$$2W(\mathbf{u})=\rho\max_{\text{admissible }\theta_i,\psi_i}\|\mathbf{a}(\mathbf{u})\|_q$$

If $q>1$, $p>0$, maximum is realized for the angles ψ_i,θ_i chosen such that

$$f^{\alpha\beta}(\psi_1,\theta_1)=\varepsilon_{\alpha\beta}(\mathbf{u})/\|\boldsymbol{\varepsilon}\|_2$$

$$\sum_{\alpha,\beta}f^{\alpha\beta}(\psi_2,\theta_2)\varepsilon_{\alpha\beta}(\mathbf{u})=0,\sum_{\alpha,\beta}f^{\alpha\beta}(\psi_3,\theta_3)\varepsilon_{\alpha\beta}(\mathbf{u})=0$$

where $\|\boldsymbol{\varepsilon}\|_2=\left(\sum_{\alpha,\beta}(\varepsilon_{\alpha\beta})^2\right)^{1/2}$. Then

$a_1=(\|\boldsymbol{\varepsilon}\|_2)^2$, $a_2=0$, $a_3=0$, which gives

$$2W(\mathbf{u})=\rho(\|\boldsymbol{\varepsilon}\|_2)^2$$

This means that the optimal Hooke tensor has the components $\rho I^{\alpha\beta\lambda\mu}$, which refers to isotropy and zero Poisson ratio; here $\mathbf{I}$ is the unit tensor. This proves that the problem of minimization of the compliance with the isoperimetric condition imposed on the distribution of the norm $\|\boldsymbol{\lambda}\|_p$ does not depend on p if $p>0$ and coincides with the results of the paper by Bendsøe et al.(1994) for $p=1$, $p=2$.

3. THE *SAMP* METHOD

The second aim of the paper is to generalize the SIMP method for 2D anisotropic elasticity problems (now called SAMP) with the artificial density as a design variable. It will be proved that the case of two Kelvin moduli being equal implies orthotropy and leads to isotropy upon optimization. The case of three different Kelvin moduli lead to essentially new optimal layouts. The numerical results to be presented were found by Svanberg's Method of Moving Asymptotes, the equilibrium problems being solved with using a version of Meshless Method called the Radial Point Interpolation Method.

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OPTIMAL SAMPLE TIME ESTIMATION FOR THE FINITE–DIMENSIONAL DISCRETE DYNAMIC COMPENSATOR IMPLEMENTED AT THE "SOFT PLC" PLATFORM

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Keywords: parabolic systems, discrete dynamic feedback, sample time assign.

1. THE EXPERIMENTAL HEAT OBJECT AND ITS MODEL

In the paper we deal with a one dimensional experimental heat object, shown in Figure 1. The main part of the object is a thin copper rod with an electric heater at one end and a temperature sensor at the other end. The input $u(t)$ and the output $y(t)$ of this object are electric signals. The length of the heater equals x_u and the length of the temperature sensor is equal to $\Delta x = x_2 - x_1$.

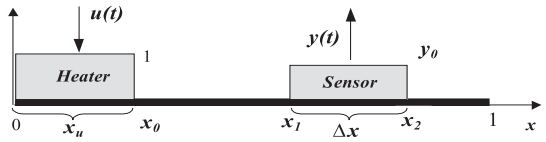

Figure 1. The one dimensional heat object.

The temperature along the rod can be described by a discrete state space equation (obtained after the discretization of time t):

$$\begin{aligned} &\Theta(k+1) = A^{+}\Theta(k) + B^{+}u^{+}(k) \\ &\Theta(0) = 0, \quad k = 0,1,2,\ldots \\ &y^{+}(k) = C^{+}\Theta(k) \end{aligned} \tag{1}$$

$\Theta(k)$ denotes the temperature at the moment k,
$A^{+} = diag\left\{\lambda_0^{+}, \lambda_1^{+}, \lambda_2^{+}, \ldots\right\}$ - state operator,
$B^{+} = \left[b_0^{+}\ b_0^{+}\ b_0^{+}\ \ldots\right]^{T}$ - control operator,
$C^{+} = \left[c_0^{+}\ c_1^{+}\ c_2^{+}\ \ldots\right]$ - output operator.
The above operators are expressed as follows:

$$A^{+} = e^{AT_s},\ B^{+} = \int_0^{T_s} e^{At} B dt \tag{2}$$

$$C^{+} = C$$

where T_s denotes the sample time for the system.

2. THE FINITE-DIMENSIONAL DISCRETE DYNAMIC COMPENSATOR

For the system (1) described in the previous section the following finite–dimensional discrete feedback can be proposed (see Fig. 2):

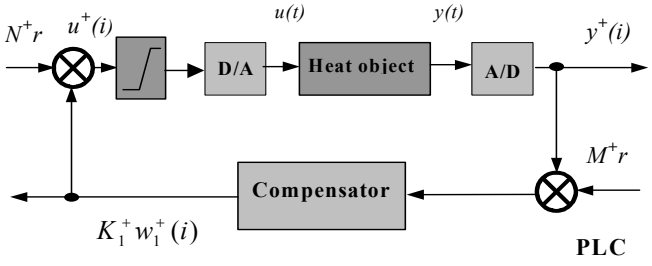

Figure 2. The closed-loop control system with dynamic discrete compensator.

The discrete compensator is described as follows:

$$\begin{aligned} &\begin{bmatrix} w_1^{+}(i+1) \\ w_2^{+}(i+1) \end{bmatrix} = A_k^{+} \cdot \begin{bmatrix} w_1^{+}(i) \\ w_2^{+}(i) \end{bmatrix} + B_k^{+}\left[y^{+}(i) + M^{+}r\right] \\ &u^{+}(i) = K_1^{+} w_1^{+}(i) + N^{+}r \end{aligned} \tag{3}$$

where

$$A_k^+ = \begin{bmatrix} A_1^+ - G_1^+ C_1^+ + B_1^+ K_1^+ & -G_1^+ C_2^+ \\ B_2^+ K_1^+ & A_2^+ \end{bmatrix}$$

$$B_k^+ = \begin{bmatrix} G_1^+ \\ 0 \end{bmatrix}$$

The dimension of matrix A_1^+ is $m < +\infty$ and the dimension of matrix A_2^+ is $p < +\infty$ (see Mitkowski 1991, p. 232).

The matrices G_1^+ and K_1^+ are selected such that $|\lambda(A_1^+ - G_1^+ C_1^+)| < 1$ and $|\lambda(A_1^+ + B_1^+ K_1^+)| < 1$.

Denote the spectrum of the closed–loop system from Figure 2 by Λ_c^+ :

$$\Lambda_c^+ = \{\lambda_0^+, \lambda_1^+, \lambda_2^+, \ldots\} \tag{4}$$

The spectrum (4) is dependent on sample time T_s. Let T_r denotes a control time such that $\|\Theta(T_r)\| < \varepsilon$ (see (1)), $\varepsilon > 0$ is suitably small. If the eigenvalues of the matrices $A_1^+ - G_1^+ C_1^+$ and $A_1^+ + B_1^+ K_1^+$ equal zero, then $\varepsilon \approx 0$ and thus $T_r \approx (m+p)T_s$.

The closed-loop control system with dynamic discrete compensator (see Figure 2) was implemented on the "soft PLC" platform built with the use of SIEMENS SIMATIC components.

3. AN OPTIMAL SAMPLE TIME SELECTION PROBLEM AND PROPOSITION OF ITS SOLUTION.

A proper selection of the value of the sample time T_s is a crucial problem in the construction of discrete control system.

We are not able to give an exact analytical relation between the sample time T_s and the control time T_r, but some points of this relation are known from experiments.

The proposed algorithm of selection of an estimate for the optimal sample time consists of the following steps:

1. Experimentally determine some points of the function: $T_r = f(T_s)$.
2. Make a polynomial interpolation $W(T_s)$ of function f.
3. Find a minimum of function W. The sample time, which minimizes W is the estimate we are looking for.

Results obtained by the above algorithm are presented in Figure 3.

For the above example the following second order polynomial was used:

$$W(T_s) = a_2 T_s^{\,2} + a_1 T_s + a_0 \tag{5}$$

where

$a_2 = 0.00002600000000$

$a_1 = -0.03720000000000$

$a_0 = 61.23999999999997$

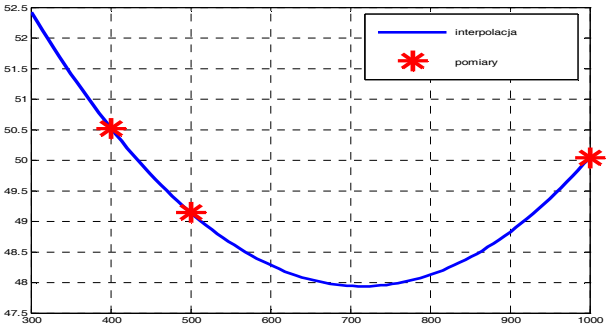

Figure 3. Control time T_r as a function of sample time T_s.

An estimation of the optimal sample time is presented in the Table 1. For a comparison, in the same table the experimentally tested control time for the optimal sample time is given:

Table 1. Estimated and tested control times:

Estimation of optimal sample time T_s^{min} [ms]	715
The estimated minimal control time T_r^{min} [s]	47.94
The experimentally selected control time for T_s^{min} [s]	48.17

4. CONCLUSIONS

The main conclusion is that the proposed approach can be useful for selecting the optimal sample time T_s in most of real situations, when we are not able to use analytical methods to that purpose.

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ASYMPTOTIC ANALYSIS AND TOPOLOGICAL DERIVATIVES FOR LINEAR ELASTICITY

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Keywords: shape optimization, topological derivative, shape derivative, shape functional, asymptotic analysis.

Asymptotic analysis with respect to singular perturbations of geometrical domains is used in shape optimization in order to improve the performance of numerical methods, in particular of the level set method. The first term of asymptotic expansion of a given shape functional with respect to small parameter which measures the size of the perturbation is called *topological derivative* of the shape functional under study. Such notion is introduced in (2) for elliptic boundary value problems, and it is based on the works of Russian school on the asymptotic analysis of PDE's in the sense of Il'in as well as of Mazja, Nazarov and Plamenievskii, the list of references can be found e.g., in (4).

We present a general framework for construction of asymptotic expansions of shape functionals in two dimensional case. We restrict ourselves to the case of plane elasticity and singular geometrical perturbations of the domain of integration. The method of analysis of elasticity boundary value problems is based on complex variable approach developed by Muskhelishvili. In this way we are able to construct explicit solutions of elasticity boundary value problems in a ring and perform the asymptotic analysis of the solutions with respect to the radius of the interior hole, when the radius tends to zero.

The asymptotic analysis results in expansions of arbitrary order with respect to the small parameter which measures the size of the small opening inserted into the domain of integration, i.e. of the small hole in an elastic body. The results are given not only in an explicit form, but also in the form useful for numerical methods. The presented formulae can be used in shape and topology optimization in structural mechanics. This means that we are able to derive the form of higher order topological derivatives in linearized elasticity, which seems to be new in the literature on the subject. Roughly speaking, the first order topological derivative indicates the place where a small hole can be injected in order to improve the value of the shape functional, and the second order topological derivative indicates the size of the hole, we refer to the presentation of A. Novotny in our minisymposium for the results in this direction in the case of the Laplacian.

Some numerical results are also included in our presentation.

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COMPUTATIONAL ANALYSIS OF LAYERED LAMINATES IN TWO-DIMENSIONAL ELASTICITY PROBLEMS

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Keywords: extremal properties, two-dimensional, layered laminates, L-closure.

1. INTRODUCTION

We are interested in finding representations of effective constitutive tensors of composites assembled from two basic materials whose physical characteristics are described by Hooke's tensors, that belong to two-element set $U = \{\mathbf{A}, \mathbf{B}\}$. Total volumes of both materials in the mixture are given; they amount to m and $1-m$ respectively. We introduce the notion of L_mU for the set under consideration.

Mathematical structure of L_mU in the frame of two-dimensional elasticity problem is due to [Lurie and Cherkaev (1986)] where the set L_mU is described as the result of an iterative process

$$L_mU = \lim_{k\to\infty} \Lambda_k \tag{1}$$

where Λ_k stands for the set of all layered laminates of kth rank obtained by single lamination of two arbitrary (k-1)th rank laminates in the direction determined by vector $\mathbf{n}_k$. By the notion of "layering" it is stated that laminated materials can be assumed to be homogeneous at each step of forming the laminate. Another key feature is the monotonicity of lamination process, namely $U \equiv \Lambda_0 \subset ... \subset \Lambda_k \subset ... \subset L_mU$.

Laminate composites prove they utility in such problems as the description of G_mU, i.e. the set of all composites being an arbitrary mixture of basic materials or certain structural design problems solutions such as the compliance minimization problem of plates, see [Lewiński and Telega (2000)]. In the latter the optimal energy density of the composite is locally attained on the set of so-called sequential laminates, i.e. layered laminates obtained by consecutive lamination with pure material. The set of such laminates is well examined, see for instance [Avellaneda 1987], but comparing the theoretical results of the last-mentioned paper and these concerning the explicit description of G_mU we conclude that for the purpose of covering this last set layered laminates need to be considered in the analysis. This in turn may open the way to obtain optimal laminate topologies in elasticity problems different from those based on local energy minimization.

2. THE SCOPE OF THE WORK

The research of explicit characterization of G_mU or the problem of attainability of its boundary ∂G_mU on finite laminate microstructures can be more precisely directed or narrowed thanks to certain elasticity problems solutions, that describe some subsets of G_mU or its estimates P_mU, such that $G_mU \subset P_mU$. In this work we seek the microstructural parameters of kth rank layered laminate $\mathbf{H}_{*k} \in \Lambda_k \subset L_mU$, $k \to \infty$ whose moduli optimally approximate some $\mathbf{H} \in \partial G_mU$ or $\mathbf{H} \in P_mU$.

Formula for effective tensor of two-phase layered laminate, see [Lurie et al. (1984)], reads

$$\mathbf{H}_{*k} = m_1\mathbf{H}_1 + m_2\mathbf{H}_2 - m_1m_2(\Delta\mathbf{H})\boldsymbol{\Pi}\left[\boldsymbol{\Pi}^{\mathrm{T}}(m_1\mathbf{H}_2 + m_2\mathbf{H}_1)\boldsymbol{\Pi}\right]^{-1}\boldsymbol{\Pi}^{\mathrm{T}}(\Delta\mathbf{H}) \tag{2}$$

where:
$\mathbf{H}_{*k}$ – kth rank laminate constitutive tensor,
$\mathbf{H}_1$, $\mathbf{H}_2$ – (k-1)th rank laminate constitutive tensors, $\Delta\mathbf{H} = \mathbf{H}_2 - \mathbf{H}_1$.
$\mathbf{\Pi}$ – projector on the space of possibly discontinuous components of second order tensor appearing in the description of the elasticity problem. The discontinuity line Γ separates material $\mathbf{H}_1$ from $\mathbf{H}_2$. The lamination direction vector $\mathbf{n}_k$ is perpendicular to that line.
m_1, m_2 – volumes of materials $\mathbf{H}_1$ and $\mathbf{H}_2$ in the kth rank lamination, $m_1 + m_2 = 1$.

The algorithm of the procedure for finding optimal tensor $\mathbf{H}_{*k}$ consists of the following
Step 0:
- Let $\mathbf{A}$, $\mathbf{B}$ be basic Hooke's tensors and $\mathbf{H}$ the approximated one.
- Let k be the lamination rank. We set $k = 1$.
- Let

$$\begin{aligned} \mathbf{n}_0 &= [\varphi_{r1}, \varphi_{r2}, ..., \varphi_{ri_r}] \\ \mathbf{m}_0 &= [m_{r1}, m_{r2}, ..., m_{ri_r}] \end{aligned} \tag{3}$$

where $i_r = 2^{k-r}$, $r = 1...\ k$, denote vectors of initial values of lamination direction angles and material volumes in consecutive laminations respectively. Here m_{ri} is the volume of one of the (r-1)th rank laminate in ith laminate of rth rank; volume of the second laminate in this lamination amount to 1– m_{ri}. Total volumes of basic materials in kth rank laminate are given as m and 1–m.
- Effective tensors of laminates of ranks 1 to k are given by $\mathbf{n}_0$, $\mathbf{m}_0$ and (2).
Step 1:
If for fixed ε

$$\left\| \mathbf{H} - \mathbf{H}_{*k} \right\| < \varepsilon \tag{4}$$

holds, we terminate the procedure, otherwise we proceed to the second step.
Step 2a:
- We compute the new values of lamination direction angles and material volumes and we define vectors $\mathbf{n}_1$, $\mathbf{m}_1$ similarly to (3). If for fixed δ we have

$$\begin{aligned} &\max_{i=1,...,d} \left| (\mathbf{n}_0 - \mathbf{n}_1)_i \right| > \delta \vee \max_{i=1,...,d} \left| (\mathbf{m}_0 - \mathbf{m}_1)_i \right| > \delta \\ &d = \sum_{i=1}^{k} 2^{k-i} \end{aligned} \tag{5}$$

then we use $\mathbf{n}_1$, $\mathbf{m}_1$ and (2) for effective tensor, we set $\mathbf{n}_0 := \mathbf{n}_1$, $\mathbf{m}_0 := \mathbf{m}_1$ and we pass to the first step.
Step 2b:
If (5) does not hold we set $k := k + 1$ and we pass to step 0.
Notice 1:
The internal structure of tensor $\mathbf{H}$ can be restricted by additional symmetry constraints, e.g. isotropy. For dealing with such additional property two ways of approximation are available. Namely, not only "the best approximate laminate" can be determined but also the one whose constitutive tensor is subject to the same restrictions as $\mathbf{H}$. In the modified procedure for the latter problem the representation of $\mathbf{H}_{*k}$ is controlled by checking the required symmetry in its first step and restricting the update of $\mathbf{n}$ and $\mathbf{m}$ in step 2a. Symmetry criteria for two-dimensional Hooke's tensors are easy to analyze by using the isotropic decomposition of these tensors and by determining the set of its independent invariants. Vanishing of certain invariants means "the passage" of the tensor to the higher symmetry class, see [Blinowski et al. (1996)].
Notice 2:
The procedure can be easily modified also to deal with the problem of characterization of the set Λ_k for any fixed k.

3. ACKNOWLEDGEMENT

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SHAPE OPTIMIZATION AND THE PONTRYAGIN PRINCIPLE

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Keywords: Pontryagin maximum principle, shape optimization

1. PROBLEM FORMULATION

Let us consider a physical system which the state equation is of the form

$$\frac{dx}{d\xi} = f(x, u, \xi), \tag{1}$$

where $x(\xi) \in \mathbb{R}^n$, $u(\xi) \in U_{ad} \subset \mathbb{R}$, $\xi \in [\xi_0, \xi_1]$, f is a vector function that is differentiable in x and ξ with continuous derivatives. The equation (1) with the boundary conditions

$$x(\xi_0) = x^0, \quad x(\xi_1) = x^1 \tag{2}$$

can describe statics and kinematics of the system. In such situation the vector x represents geometrical variables along the section $[\xi_0, \xi_1]$, U_{ad} stands for the set of admissible controls and it is usually determined by geometrical and strength constraints. Existence of the contraints secures the solutions of (1) the proper physical meaning.

One wishes to determine the function u defined in $[\xi_0, \xi_1]$, which minimizes the cost function J:

$$J(u) = \int_{\xi_0}^{\xi_1} f_0(x, u) d\xi. \tag{3}$$

Here f_0 is a given function from the same class as f. The cost function may represent displacement of a chosen point, volume of an element, etc.

In order to solve the formulated problem we can use the Pontryagin maximum principle, see Boltianski [2], Pontryagin et al. [4] and also Gorecki [3], Mitkowski [5]. In this approach the key role plays the Hamiltonian

$$H(\lambda, x, u) = \sum_{i=0}^{n} \lambda_i f_i(x, u), \tag{4}$$

where the vector of adjoint variables $\lambda = [\lambda_0, \lambda_1, \ldots, \lambda_n]$ is such that

$$\frac{d\lambda_i}{d\xi} = -\frac{\partial H(\lambda, x, u)}{\partial x_i}, \quad i = 1, 2, \ldots, n \tag{5}$$

and

$$\frac{d\lambda_0}{d\xi} = -f_0(x, u). \tag{6}$$

The principle states that the Hamiltonian (4) must be maximized over U_{ad}. If x^*, u^* is a solution of the optimal control problem, then

$$H(\lambda^*, x^*, u^*) \geq H(\lambda, x, u) \tag{7}$$

for all $u \in U_{ad}$.

2. PRELIMINARY RESULTS

In the previous section the optimization problem has been formulated. The problem consists of finding a pair consisting of the optimal control $u^*(\xi)$ and the corresponding optimal trajectory $x^*(\xi)$. It will be shown that such approach can be applied to shape optimization of many mechanical systems. See also the works of Atanackovic [1], Mitkowski and Skruch [6], Skruch [7], Szefer and Mikulski [8, 9].

There are several limitations concern convergence, uniqueness, stability and existence of solution. A general proof is very often impossible. Therefore the main focus in this paper will be put on the numerical solutions and methods that can be used to solve the shape optimal control problem. The computer program has been designed in MATLAB-Simulink environment. Using this program we will try to find optimal shapes for beams and arches.

3. EXAMPLE

To illustrate our theory we consider a single span beam with rectangular cross-section working under self-weight (Fig. 1). The height of the cross-section is taken as the control variable. The deflection at the end point is the optimality criterion. Side conditions concern strength constrains and geometry are imposed on the dimensions of the cross-section. The statics and the kinematics of the beam can be written using equations (1), (2). The deflection of the end point can be expressed by the cost function (3).

The Pontryagin method can be used for solving

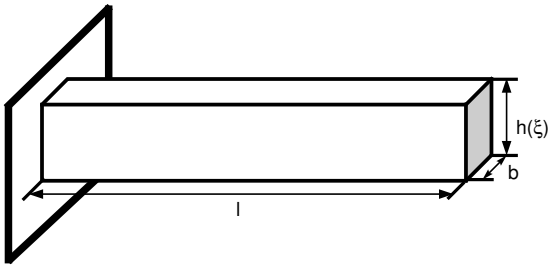

Fig. 1. Single span beam under self-weight

the formulated tasks of optimization. To find effectively the optimal control $u(\xi) = h(\xi)$, it is necessary to solve the system which consists of nonlinear ordinary differential equations of the first order with the boundary conditions defined at initial and end points, i.e. for $\xi = 0$ and $\xi = l$ (see Mitkowski and Skruch [6], Skruch [7], Szefer and Mikulski [8]). The solution of this system is possible only in a numerical way.

The algorithm of the numerical solution of the problem has be design using MATLAB-Simulink environment. The written program has been used in a series of computations. The results of these computations are presented in Fig. 2.

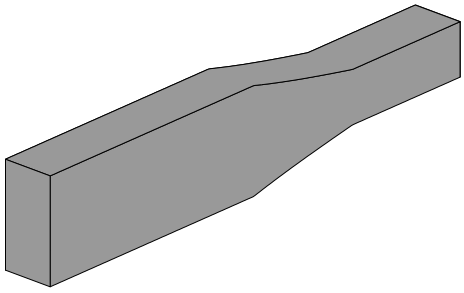

Fig. 2. Optimal shape of the beam

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ON THE SECOND ORDER TOPOLOGICAL ASYMPTOTIC

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Keywords: topological asymptotic expansion, second order topological derivative

1. INTRODUCTION

The topological sensitivity analysis [1, 4] gives the topological asymptotic expansion of a cost functional with respect to an infinitesimal domain perturbation. However, for practical applications, it is necessary to deal with perturbations of finite size. This issue was addressed in our previous work [2], where we have introduced a definition for the second order topological derivative, which provides a good estimation for the cost functional even for very large holes. Therefore, as a natural sequence of our work, in the present paper we calculate first and second order topological derivative for inclusions.

Let us consider an open bounded domain $\Omega \subset \mathbb{R}^2$, with a smooth boundary $\partial\Omega$. If the domain Ω is perturbed by introducing a small inclusion represented by B_ε, which is a ball of radius ε centered at point $\hat{\mathbf{x}} \in \Omega$, we have a perturbed domain $\Omega_\varepsilon \cup B_\varepsilon$, where $\Omega_\varepsilon = \Omega - B_\varepsilon$. Then, the topological asymptotic expansion of a given cost functional ψ may be expressed as

$$\begin{aligned} \psi(\Omega_\varepsilon \cup B_\varepsilon) &= \psi(\Omega) + f_1(\varepsilon) D_T\psi \\ &+ f_2(\varepsilon) D_T^2\psi + \mathcal{R}(f_2(\varepsilon)) \,, \end{aligned} \quad (1)$$

where $f_1(\varepsilon) \to 0$, $f_2(\varepsilon) \to 0$ when $\varepsilon \to 0^+$, $f_2(\varepsilon) \in o(f_1(\varepsilon))$ and $\mathcal{R}(f_2(\varepsilon)) \in o(f_2(\varepsilon))$. Thus, $D_T\psi$ and $D_T^2\psi$ are the first and second order topological derivative of ψ, respectively.

In this work, we apply the Topological-Shape Sensitivity Method developed in [3] to calculate $D_T\psi$ and $D_T^2\psi$ for the total potential energy associated to the Laplace equation in two-dimensional domain. Finally, we present some numerical experiments showing the influence of the second order term in the topological asymptotic expansion for different values of the thermal conductivity coefficient of the inclusion.

2. TOPOLOGICAL ASYMPTOTIC FOR THE LAPLACE EQUATION

The variational formulation for the Laplace equation associated to the perturbed domain $\Omega_\varepsilon \cup B_\varepsilon$ can be stated as: find $u_\varepsilon \in \mathcal{U}_\varepsilon$, such that

$$\int_{\Omega_\varepsilon \cup B_\varepsilon} k_\delta \nabla u_\varepsilon \cdot \nabla \eta + \int_{\Gamma_N} \bar{q}\eta = 0 \quad \forall \eta \in \mathcal{V}_\varepsilon \,, \quad (2)$$

where $\mathcal{U}_\varepsilon$ and $\mathcal{V}_\varepsilon$ are defined by

$$\begin{aligned} \mathcal{U}_\varepsilon &= \{u_\varepsilon \in H^2(\Omega_\varepsilon \cup B_\varepsilon) : u_\varepsilon|_{\Gamma_D} = \bar{u}\} \\ \mathcal{V}_\varepsilon &= \{\eta \in H^2(\Omega_\varepsilon \cup B_\varepsilon) : \eta|_{\Gamma_D} = 0\} \,, \end{aligned}$$

and Γ_D and Γ_N are the Dirichlet and Neumann boundaries, such that $\partial\Omega = \Gamma_D \cup \Gamma_N$, with $\Gamma_D \cap \Gamma_N = \emptyset$; $\bar{u}$ and $\bar{q}$ are the temperature and heat flux prescribed on Γ_D and Γ_N, respectively. In addition, the material property k_δ is defined, for $\delta \in \mathbb{R}^+$, as

$$k_\delta = k \;\forall \mathbf{x} \in \Omega_\varepsilon \;\text{ and }\; k_\delta = \delta k \;\forall \mathbf{x} \in B_\varepsilon \,. \quad (3)$$

Taking the associated total potential energy as cost functional, that is

$$\psi(\Omega_\varepsilon \cup B_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon \cup B_\varepsilon} k_\delta \left|\nabla u_\varepsilon\right|^2 - \int_{\Gamma_N} \bar{q} u_\varepsilon \,. \quad (4)$$

and after applying the Topological-Shape Sensitivity Method we get the following results for $f_1(\varepsilon) = \pi\varepsilon^2$ and $f_2(\varepsilon) = \pi\varepsilon^4$

$$D_T\psi = -k\frac{1-\delta}{1+\delta}\left|\nabla u\left(\widehat{\mathbf{x}}\right)\right|^2, \quad (5)$$

$$D_T^2\psi = \frac{1}{2}k\frac{1-\delta}{1+\delta}\det\nabla\nabla u\left(\widehat{\mathbf{x}}\right), \quad (6)$$

where function u is solution of eq. (2) for $\varepsilon = 0$.

3. NUMERICAL EXPERIMENTS

Let us consider a body represented by $\Omega = (0,1) \times (0,1)$, with $\bar{u} = 0$ on $\overline{\Gamma_{D_1} \cup \Gamma_{D_2}}$, and

$\bar{q}_1 = 1$ on Γ_{N_1}, $\bar{q}_2 = 2$ on Γ_{N_2} and $\bar{q} = 0$ on the remainder boundary, as shown in fig. (1, where $a = 0.2$). This body is perturbed by introducing inclusions with center at $\mathbf{x}^* = (0.5, 0.5)$, where $\delta \in \{1/16, 1/4, 1/2, 2, 4, 16\}$ and $k = 1$. Then, for each value of δ, we take $\varepsilon \in \{0.01, 0.02, 0.04, 0.08, 0.16\}$. From these values of ε and δ, we compute the topological asymptotic expansion associated to the domain Ω at $\mathbf{x}^*$ considering the following estimates

$$\psi(\Omega_\varepsilon \cup B_\varepsilon) \approx \psi(\Omega) + f_1(\varepsilon) D_T \psi \, . \qquad (7)$$

$$\psi(\Omega_\varepsilon \cup B_\varepsilon) \approx \psi(\Omega) + f_1(\varepsilon) D_T \psi + f_2(\varepsilon) D_T^2 \psi \, . \quad (8)$$

Then, in order to compute the cost functional $\psi(\Omega_\varepsilon \cup B_\varepsilon)$, we effectively insert the inclusions with center at $\mathbf{x}^*$. Finally, from these results, we can compare the accuracy obtained from both estimates given by eqs. (7, 8).

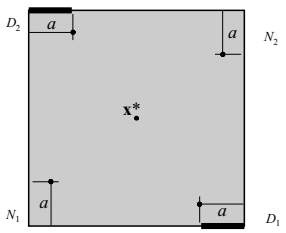

Fig. 1. example.

The behavior of the topological asymptotic expansion as a function of ε, evaluated at $\mathbf{x}^*$, is shown in figs. (2-4) for different values of δ.

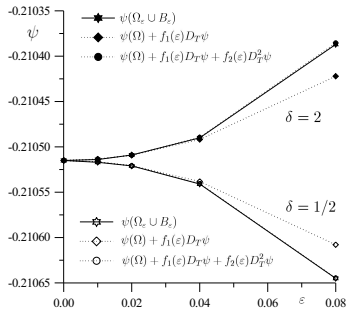

Fig. 2. Estimate of $\psi(\Omega_\varepsilon \cup B_\varepsilon)$ for $\delta \in \{1/2, 2\}$.

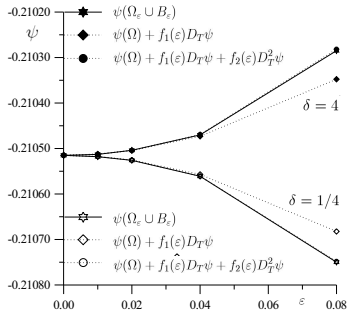

Fig. 3. Estimate of $\psi(\Omega_\varepsilon \cup B_\varepsilon)$ for $\delta \in \{1/4, 4\}$.

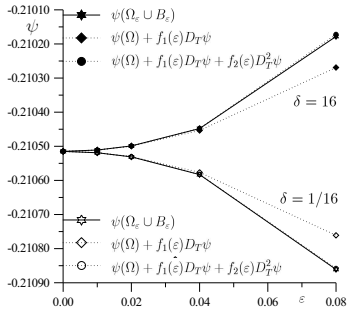

Fig. 4. Estimate of $\psi(\Omega_\varepsilon \cup B_\varepsilon)$ for $\delta \in \{1/16, 16\}$.

4. CONCLUSIONS

In this work, we have calculated the first and second order topological derivatives for the total potential energy associated to the Laplace equation in two-dimensional domain, which was perturbed through the insertion of a small inclusion. Then, we have presented some numerical experiments showing that the estimate considering the second order topological derivative remains precise even for very large inclusions, allowing to deal with perturbations of finite size.

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DECAY OF ENERGY FOR EVOLUTION EQUATIONS WITH MEMORY DAMPING

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Keywords: viscoelasticity, stabilization of PDE's

We study stabilization properties of viscoelastic materials. For these materials, the feedback law is of memory type, that is the feedback appears as a convolution operator with respect to time. We prove stabilization properties such as exponential or polynomial decay for general abstract hyperbolic equations with applications to various models such as wave equation, anisotropic elasticity.

DYNAMIC PROGRAMMING FOR INFINITE HORIZON BOUNDARY CONTROL PROBLEMS FOR PDEs WITH AGE STRUCTURE

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Keywords: Boundary control of PDEs, Hamilton–Jacobi–Bellman equations in Hilbert spaces, Vintage Capital Models, Age structured systems

1. INTRODUCTION

We develop the dynamic programming approach for a family of infinite horizon boundary control problems with linear state equation and convex cost. We prove that the value function of the problem is the unique regular solution of the associated stationary Hamilton–Jacobi–Bellman equation and use this to prove existence and uniqueness of feedback controls. The idea of studying this kind of problem comes from economic applications, in particular from models of optimal investment with vintage capital. Such family of problems has already been studied in the finite horizon case in (S. Faggian, 2005, 2007). The infinite horizon case is more difficult to treat and it is more interesting from the point of view of economic applications, where what mainly matters is the behavior of optimal trajectories and controls in the long run. The study of infinite horizon is here performed through a non-trivial limiting procedure from the corresponding finite horizon problem.

2. THE ECONOMIC PROBLEM

We motivate the study of the (abstract) optimal control problem by means of the application to optimal investment with vintage capital. Such an applied problem can be described as follows: the state variable is the amount of capital goods (technologies) implied to obtain some product to be sold on the market; controls are investments in technologies; the problem of the firm is that of choosing investments (both in new and older technologies), in order to maximize their profits over a infinite interval of time.

The crucial assumption, with respect to applied problems of the same kind, is that capital goods depend on two variables, namely time and age, as introduced by (E. Barucci, F. Gozzi). The state equation representing the capital accumulation process is then a linear PDE, with both distributed and boundary controls (resp., investments in older and new capital goods). For (τ, s) in $]t, +\infty[\times]0, \bar{s}]$

$$\frac{\partial y(\tau,s)}{\partial \tau} + \frac{\partial y(\tau,s)}{\partial s} + \mu y(\tau,s) = u_1(\tau,s),$$

where the unknown $y(\tau, s)$ represents the amount of capital goods of age s accumulated at time τ, $\mu > 0$ is a depreciation factor, and $u_1 : [t, +\infty[\times[0, \bar{s}] \to R$ is the investment at time τ in capital goods of age s (hence, the distributed control). The equation is coupled with some boundary condition

$$y(\tau, 0) = u_0(\tau), \quad \tau \in]t, +\infty[$$

where $u_0 : [t, +\infty[\to R$ is the investment in new capital goods (u_0 is the boundary control), and some initial condition

$$y(t, s) = x(s),$$

for $s \in [0, \bar{s}]$ with $t > 0$ the initial time, $\bar{s} \in [0, +\infty]$ the maximal allowed age, and $x \in L^2(0, \bar{s})$ the initial amount of capital goods.

The problem is then reformulated into abstract terms, yielding a linear ODE in Hilbert spaces and the associated infinite dimensional Hamilton–Jacobi–Bellman equation, and to which the following class of problems apply:

$$y'(\tau) = Ay(\tau) + Bu(\tau), \quad \tau \in]t, +\infty[$$

with initial condition

$$y(t) = x \in H$$

where H is the state space ($L^2(0, \bar{s})$ in the application), y is the trajectory, U is the control space

and u is the control ($u = (u_0, u_1)$ in the application), $A : D(A) \subset H \to H$ is the infinitesimal generator of a strongly continuous semigroup of linear operators $\{e^{\tau A}\}_{\tau \geq 0}$ on H, and the control operator B is linear and *unbounded*, say $B : U \to [D(A^*)]'$. The objective functional is of type

$$J_\infty(t, x, u) = \int_t^{+\infty} e^{-\lambda\tau} \left[g_0 \left(y(\tau) \right) + h_0 \left(u(\tau) \right) \right] d\tau$$

g_0 and h_0 both convex functions, and the associate HJB equation is then of type

$$-\lambda\psi(x) + (\psi'(x) \mid Ax)_H + \\ -h_0^*(-B^*\psi'(x)) + g(x) = 0, \ x \in H$$

(h_0^* indicates the Légendre transform of the convex function h_0.)

It is worth remarking that the presence of the boundary control yields an unbounded control operator in the abstract state equation and a discontinuous Hamiltonian.

3. THE LIMITING PROCEDURE

The problem with infinite horizon is discussed by means of an associated family of finite horizon problems, so that we make use of the results proved in (S. Faggian, 2005, 2007), and a non trivial limiting procedure. The technique is not new, as Barbu and Da Prato introduced it in the case of distributed control, but the discontinuities caused by the presence of boundary controls plus the non analiticity of the semigroup involved in the state equation make the job harder.

4. CONCLUSIONS

The main results that we were able to obtain are the following: 1) the value function of the optimal control problem is the unique *regular* solution of the associated HJB equation, and it is obtained as the limit of the value functions of finite horizon problems; 2) there exists a unique optimal feedback strategy, which we can write in terms of the gradient of the value function. Moreover we are able to establish the connections between finite and infinite horizon value functions. WE also intend, in the near future, to apply the results to the study of quality properties of both optimal strategies and trajectories in the particular case of optimal investment with vintage capital, possibly deriving some meaningful economic interpretation.

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LUR'E FEEDBACK SYSTEMS: WELL–POSEDNESS and STABILITY USING NONLINEAR SEMIGROUPS

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Keywords: infinite–dimensional control systems, semigroups, Lyapunov functionals, circle criterion

1. INTRODUCTION

Consider the Lur'e feedback control system in Figure 1, which consists of a linear part described by

$$\left\{ \begin{array}{rcl} \dot{x}(t) & = & A[x(t)+du(t)] \\ y(t) & = & c^{\#}x(t) \end{array} \right\}, \qquad (1)$$

and a scalar static controller nonlinearity $f : \mathbb{R} \to \mathbb{R}$. It is assumed that:

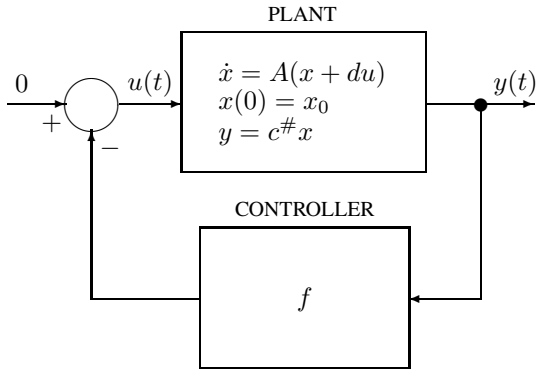

Fig. 1. Lur'e feedback system

- $A : (\mathcal{D}(A) \subset \mathrm{H}) \longrightarrow \mathrm{H}$ generates a linear exponentially stable (**EXS**), C_0–semigroup $\{S(t)\}_{t\geq 0}$ on a Hilbert space H with a scalar product $\langle \cdot, \cdot \rangle_{\mathrm{H}}$,
- y is a scalar output defined by an A–bounded linear observation functional $c^{\#}$ (bounded on $\mathcal{D}_A$, i.e the space $\mathcal{D}(A)$ equipped with the graph norm of A, here equivalent to $\|x\|_A := \|Ax\|_{\mathrm{H}}$). The restriction of $c^{\#}$ to $\mathcal{D}(A)$ is representable as $c^{\#}x = \langle h, Ax \rangle_{\mathrm{H}}$ for every $x \in \mathcal{D}(A)$ and some $h \in \mathrm{H}$, or shortly $c^{\#}\big|_{\mathcal{D}(A)} = h^*A$.
- $d \in \mathcal{D}(c^{\#}) \subset \mathrm{H}$ is a factor control vector, $u \in \mathrm{L}^2(0,\infty)$ is a scalar control function.

The closed–loop system is described by the abstract nonlinear differential equation

$$\dot{x}(t) = A\left\{x(t) - df\left[c^{\#}x(t)\right]\right\} \qquad (2)$$

2. WELL–POSEDNESS

We examine conditions under which the nonlinear semigroups theory applies to (2).

Theorem 2.1. Assume that there exist k_1, $k_2 \in \mathbb{R}$ such that:

(i) $f : \mathbb{R} \longrightarrow \mathbb{R}$ satisfies the incremental sector condition

$$\begin{aligned} &-\infty < k_1 < \frac{f(y_1)-f(y_2)}{y_1-y_2} < k_2 < \infty \\ &\forall y_1, y_2 \in \mathbb{R}, \quad f(0) = 0 \end{aligned} \qquad (3)$$

(ii) with

$$\begin{aligned} &q := k_1k_2, e := -\frac{k_1+k_2}{2} + k_1k_2c^{\#}d, \\ &\delta := (1-k_1c^{\#}d)(1-k_2c^{\#}d) = \\ &= 1 + 2ec^{\#}d - q\left(c^{\#}d\right)^2 \geq 0 \end{aligned}$$

the *linear operator inequality*

$$\begin{aligned} &\left[\begin{array}{cc} \left(A^{-1}\right)^*\mathcal{H} + \mathcal{H}A^{-1} - qhh^* & \mathcal{H}d - eh \\ d^*\mathcal{H} - eh^* & -\delta \end{array} \right] \\ &\leq 0 \end{aligned} \qquad (4)$$

holds for some $\mathcal{H} \in \mathbf{L}(\mathrm{H})$, $\mathcal{H} = \mathcal{H}^* \geq \eta I > 0$.

Then the *single–valued* operator

$$\begin{aligned} &\mathcal{A}x := A\left[x - df(c^{\#}x)\right], \\ &\mathcal{D}(\mathcal{A}) = \left\{x \in \mathcal{D}(c^{\#}) : x - df(c^{\#}x) \in \mathcal{D}(A)\right\}, \end{aligned} \qquad (5)$$

in the RHS of (2), is *dissipative* with respect to an *equivalent* scalar product $\langle x_1, x_2\rangle_e := \langle x_1, \mathcal{H}x_2\rangle_{\mathrm{H}}$ and, if additionally, $c^{\#}$ is admissible and the transfer function of (1) $\hat{g}$ is in $\mathrm{H}^\infty(\mathbb{C}^+)$, then it satisfies the range condition

$$\mathcal{R}(\lambda I - \mathcal{A}) = \mathrm{H} \qquad \forall \lambda > 0 \ . \tag{6}$$

Furthermore, $\mathcal{A}$ is *demiclosed* and *densely defined*, i.e. $\overline{\mathcal{D}(\mathcal{A})} = \mathrm{H}$. Finally, for $x_0 \in \mathcal{D}(\mathcal{A})$, (2) has a unique strong solution $x \in \mathrm{W}^{1,\infty}([0,\infty),\mathrm{H})$ (the Sobolev space of absolutely continuous functions $x(t) \in \mathrm{H}$ with both x and $\dot{x}$ in $\mathrm{L}^\infty((0,\infty),\mathrm{H})$) and the output y of the Lur'e feedback system of Figure 1 is in $\mathrm{L}^\infty(0,\infty)$.

Next we give a criterion of solvability of the linear operator inequality (4) in the *nonsingular* case $\delta > 0$.

Lemma 2.1. If the observation functional $c^{\#}$ is admissible and exactly observable, $\hat{g} \in \mathrm{H}^\infty(\mathbb{C}^+)$ and there exist k_1, $k_2 > k_1$ such that the frequency–domain inequality of the *circle–type* holds,

$$\begin{aligned} &1 + (k_1 + k_2)\,\mathrm{Re}\big[\hat{g}(j\omega)\big] + \\ &+k_1 k_2 \big|\hat{g}(j\omega)\big|^2 \geq \eta > 0 \quad \forall \omega \in \mathbb{R} \end{aligned} \tag{7}$$

then there exists $\mathcal{H} \in \mathbf{L}(\mathrm{H})$, $\mathcal{H} = \mathcal{H}^* \geq \eta I > 0$, satisfying (4).

3. STABILITY: coercive case

Our results lead to a "coercive" version of a circle criterion.

Theorem 3.1. Let the assumptions of Lemma 2.1 hold and let for the given k_1 and $k_2 \in \mathbb{R}$ the incremental sector condition (3) be satisfied. Moreover let d be an admissible factor control vector. Then the null equilibrium of (2) is globally strongly asymptotically stable.

This result, up to some extent, coincides with that of (Grabowski and Callier, 2006).

4. STABILITY: non-coercive case

The *resolvent* of the closed–loop operator $\mathcal{A}$ has a representation

$$(\lambda I - \mathcal{A})^{-1} z = \underbrace{(\lambda I - A)^{-1} z}_{\text{linear part}} - \underbrace{\big[\lambda(\lambda I - A)^{-1} d - d\big]\, f \circ \big[I_{\mathbb{R}} + \hat{g}(\lambda) f\big]^{-1} \left\{h^* \left[\lambda(\lambda I - A)^{-1} z - z\right]\right\}}_{\text{nonlinear part}}$$

i.e. it splits into the infinite–dimensional part, the resolvent of an open–loop linear operator A and the nonlinear part, given by the second component. Hence, the resolvent $(\lambda I - \mathcal{A})^{-1}$ of $\mathcal{A}$ is compact, provided that A^{-1} is a compact operator, or equivalently A has a compact resolvent.

We are in position to recall the result of (Dafermos and Slemrod, 1973, Theorem 3).

Lemma 4.1 (Dafermos and Slemrod). If A^{-1} is a compact operator then all closed–loop trajectories, starting from $\mathcal{D}(\mathcal{A})$ are *precompact*.

A "noncoercive" version of the circle criterion involves the LaSalle invariance principle – see Grabowski and Callier (2007) for more details.

Theorem 4.1. Let the assumptions (**i**) and (**ii**) of Theorem 2.1 hold, $c^{\#}$ is admissible, the transfer function of (1) $\hat{g}$ is in $\mathrm{H}^\infty(\mathbb{C}^+)$, and A^{-1} is a compact operator. Then the null equilibrium of (2) is globally strongly asymptotically stable.

5. CONCLUSION

We have considered a SISO infinite–dimensional Lur'e feedback control system. Elegant and self-contained proofs were obtained by using nonlinear semigroups and reciprocal systems, giving Theorem 2.1 (well-posedness of the Lur'e feedback system), Lemma 2.1 (solvability of the linear operator inequality (4), and Theorem 3.1 (global strong asymptotic stability of the null state of the Lur'e feedback system in the coercive case). Moreover LaSalle's invariance principle enabled us to handle stability in the non-coercive case – Theorem 4.1.

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LONG-TERM DYNAMICS OF A NONLINEAR STRUCTURAL ACOUSTIC MODEL WITH THERMOELASTIC WALL

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Keywords: Coupled PDE system, global attractor, fractal dimension

1. INTRODUCTION

This lecture will report on the study of the long-time behaviour of the solutions to a nonlinear system of partial differential equations (PDE) describing the interactions between a vibrating plate and an enclosed acoustic field. Central issues such as (i) well-posedness of the composite PDE model, (ii) existence of a global attractor, and (iii) finiteness of its fractal dimension will be dealt with. The results achieved benefit from recent developments in the analysis of the long-time behaviour of evolution equations with nonlinear damping by I. Chueshov and I. Lasiecka, which combine effectively the theory of (infinite-dimensional) dynamical systems with techniques and tools pertaining to control theory.
(The lecture is based on joint work with Igor Chueshov, Kharkov University, Ukraine).

2. THE PROBLEM

Let $\Omega \subset \mathbb{R}^n$ ($n = 2$ or 3) be an open bounded domain with boundary Γ. Γ consists of two connected parts: the active wall Γ_0, which is *flat* and whose dynamics is described by a thermoelastic Berger plate ($n = 3$) or beam ($n = 2$) equation; and the 'hard' wall Γ_1. The PDE system under consideration consists of the wave equation in the variable z,

$$\begin{cases} z_{tt} + g(z_t) - \Delta z + f(z) = 0 & \text{in } \Omega \times (0,T) \\ \dfrac{\partial z}{\partial \nu} = 0 & \text{on } \Gamma_1 \times (0,T) \\ \dfrac{\partial z}{\partial \nu} = \alpha\kappa\, v_t & \text{on } \Gamma_0 \times (0,T)\,, \end{cases} \tag{1}$$

and an elastic equation representing the displacement of the wall subject to thermal effects,

$$\begin{cases} v_{tt} - \gamma\Delta v_{tt} + \Delta^2 v + \Big[Q - \displaystyle\int_{\Gamma_0} |\nabla v|^2 dx\Big]\,\Delta v \\ \qquad +\beta\kappa z_t|_{\Gamma_0} + \Delta\theta = p_0 & \text{in } \Gamma_0 \times (0,T) \\ \theta_t - \Delta\theta = \Delta v_t & \text{in } \Gamma_0 \times (0,T) \\ v = \Delta v = 0\,;\ \theta = 0 & \text{on } \partial\Gamma_0 \times (0,T)\,, \end{cases} \tag{2}$$

to be supplemented with initial data (in the natural energy space). In the above system (1)–(2), $g(s)$ is a nondecreasing function describing the dissipation which affects the wave component, while $f(z)$ represents a nonlinear force; ν is the outer normal vector, α and β are positive constants. The parameter $0 \le \kappa \le 1$ enables us to deal as well with the case of non-interacting wave and plate equations ($\kappa = 0$). In subsystem (2), the real parameter Q describes in-plane forces applied to the plate, while $p_0 \in L_2(\Omega)$ represents transversal forces; the boundary term $\beta\kappa z_t|_{\Gamma_0}$ describes the acoustic pressure. It is well known that the parameter $\gamma > 0$ (or $\gamma = 0$), corresponding to the presence (or absence) of rotational moments, results in a hyperbolic-like (or parabolic, respectively) character of the thermoelastic system. Notice that the model considered does not display additional (viscous, or structural) mechanical damping on the active wall Γ_0.

The lecture will deal with the long-term behaviour of the coupled PDE system (1)-(2). Accordingly, the following questions will be addressed: (i) existence and uniqueness of the solution, (ii) existence of a global attractor, (iii) finite dimensionality of the attractor, (iv) smoothness of the attractor. It must be emphasized in particu-

lar the central importance of property (iii), which means that the permanent observed regime depends on a finite number of degrees of freedom. Indeed, the finite dimensionality of the attractor is established under suitable growth conditions on the nonlinearities g and f, which significantly allow the semilinear term f to be of *critical exponent*. The technical key of this result is a specific *stabilizability estimate*, inspired to the ones encountered in control theory, which enables us to invoke the recent novel achievements concerning the dimension of invariant sets; see, e.g., [2, Ch. 4]. This method, developed by the authors of [2], has been successfully used in the previous work [1], dealing with the isothermal case.

It should be noted that the aforesaid estimate holds uniformly with respect to the parameters γ and κ; this brings about, e.g., bounds for the attractor's dimension which are independent of both parameters—even though the dynamics of the thermolastic system are different in the two cases $\gamma > 0$ or $\gamma = 0$.

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NULL CONTROLLABILITY RESULTS FOR DEGENERATE PARABOLIC EQUATIONS

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Keywords: degenerate parabolic equations, null controllability, Carleman estimates, Hardy type inequality

1. ABSTRACT

The null controllability of parabolic operators in bounded domains, with both boundary or locally distributed controls, is a well-established property, see, e.g., (Bensoussan et al., 1993) and (Fattorini, 1998). Such a property brakes down, however, for degenerate parabolic operators even when degeneracy occurs on "small" subsets of the space domain, such as subsets of the boundary.

This talk will discuss some null controllability results that have been recently obtained for degenerate parabolic operators via new global Carleman estimates. It will be also explained why, in such a context, the use of suitable Hardy-type inequalities becomes essential.

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On-line reconstruction of inputs to a class of distributed parameter systems

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keywords: Input reconstruction, deconvolution, holomorphic semigroups

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Reconstruction of input signals to linear dynamical systems is an important problem. In fact, in the time invariant case, it is a special instance of the deconvolution problem. Several algorithms have been proposed to achieve this goal, which can be classified in two large classes: off-line and on-line deconvolution algorithms. Off-line deconvolution algorithms accumulate all the available pieces of information and, after the process has come to an end, these pieces of information are elaborated so to obtain an estimate of the input signal. An example of this is Tikonov method. On-line deconvolution methods instead at the time t produce an estimate $v(t)$ of the unknown input u at the time t solely on the basis of observations taken at previous times. Of course, solely the algorithms in this class can be used for regulation and control purposes, see applications in [2, 3] for the case of finite dimensional systems.

In this talk we present an extension of the algorithm proposed in [1] (a paper concerned with finite dimensional systems) to the on-line identification of inputs to a class of distributed systems. The class of systems we consider in this talk is described in the time domain

$$\dot{x} = Ax + Bu\,, \qquad y = Cx$$

and we want to mimic thermal processes, i.e. we assume $A = A^*$ generates a contraction semigroup and B is a bounded linear operator from $\mathbf{R}$ (i.e. scalar input to the state space X. Input and outputs are "colocated". In the usual sense, this would mean $C = B^*$ which in particular implies internal observation, not physically feasible. More in general our results cover the case

$$y = B^*(-A)^\sigma x\,.$$

In concrete cases, this means that the output y is an average, on a part of the boundary, of the heat flux.

We shall present an algorithm for the on-line reconstruction of u based on measures taken on the output y. In the ideal case of noiseless observations, the algorithm constructs a function v_α which converges to u in $L^2(0,T)$ for every $T > 0$ for $\alpha \to 0+$ (the case of noisy measures is considered too). This is a "consistency results" which justifies the choice of v_α, with

small α, as an approximation of the unknown input u.

As a first step, the proof is naturally performed in the time domain, i.e. state space techniques, under quite restrictive assumptions. A second step will remove such restrictive assumptions using a frequency domain type of proof. It is thanks to these frequency domain arguments that we can prove consistency of the algorithm in the case of boundary observations.

An interesting observation is that the frequency domain proof depends on the fact that a certain transfer function is positive real, and this shows a connection of the on-line reconstruction problem with the quadratic regulator theory.

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SOME RESULTS OF NULL CONTROLLABILITY OF PARABOLIC EQUATIONS IN THE CASE OF NON-SMOOTH COEFFICIENTS

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Null controllability results of semilinear parabolic equations can be obtained by means of global Carleman estimates and a fix-point method. Such a Carleman estimate for the heat equation with smooth coefficients was derived by Fursikov and Imanuvilov [5]. The fix-point approach was introduced for semilinear equations simultaneously by Barbu [1] and Fernandez-Cara and Zuazua in [4] to treat superlinear terms. It was generalized by Doubova et al. in [2] to treat a non-linear terms that involve both the state and the gradient.

In Doubova et al. [3], the authors treat the case of piecewise regular coefficients and introduce non-smooth Carleman weight functions assuming that they satisfy the *same transmission condition as the solution*. To obtain observability, they have to add some assumption on the monotonicity of the coefficients: observability is proved in the case where the control is supported in the region where the diffusion coefficient is the 'lowest'.

We shall show how the monotonicity condition can be relaxed in dimension one and obtain a Carleman estimate with a regularity of the coefficient in the principal part as low as BV. We shall also prove a null controllability result for the heat equation in dimension greater than two in the case of stratified media, by means of the technique of Lebeau and Robbiano [6], thus proving that regarding controllability of parabolic equations the monotonicity condition introduced above [3] is not optimal. We shall present open problems.

Part of this work is in collaboration with Assia Benabdallah and Yves Dermenjian.

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BOUNDARY CONTROL OF PARABOLIC-HYPERBOLIC SYSTEMS WITH TIME DELAYS

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Abstract

Keywords: boundary control, parabolic-hyperbolic system, integral time delays, Neumann problem, quadratic programming method, Hilbert space

In this paper, we consider optimal boundary control problems for parabolic-hyperbolic systems in which time delays appear in the integral form in the state equations. The right-hand side of the state equation and the initial and boundary conditions are not continuous functions usually, but they are measurable functions belonging into L^2 or L^∞ spaces. Therefore we shall look the solution of the time delay parabolic-hyperbolic equation in some Sobolev spaces (Lions and Magenes, 1972).

Sufficient conditions for the existence of a unique solution of the time delay parabolic – hyperbolic equation with the Neumann boundary condition are proved – Theorem 1.

Consequently, we formulate the optimal control problem. The performance functional has the quadratic form. The time horizon is fixed. Finally, we impose some constraints on the boundary control.

The necessary and sufficient conditions of optimality with the quadratic performance functional and constrained control are derived for the Neumann problem -Theorem 2.

We must notice that the conditions of optimality derived above (Theorem 2) allow us to obtain an analytical formula for the optimal control in particular cases only (e.g. there are no constraints on the controls). This results from the following: the determining of the adjoint variable $p(v_0)$ in the maximum condition from the adjoint equation is possible if and only if we know the state variable y_0 which corresponds to the control v_0. These mutual connections make the practical use of the derived optimization formulae difficult. Therefore we resign from the exact determining of the optimal control and we use approximation methods (Kowalewski, 2001).

As an example, a quadratic programming method in a Hilbert space, which can be used in solving certain optimization problems for time delay parabolic-hyperbolic systems is also presented.

The results presented in the paper can be treated as an extension of the results obtained by Lions (1971) onto the case of additional time delays appearing in the integral form in the state equations.

In this paper we have considered the optimal time delay parabolic-hyperbolic systems with

the Neumann boundary conditions. We can also consider optimal control problems for parabolic-hyperbolic systems with the Neumann boundary conditions involving time delays.

We can also obtain estimates and a sufficient condition for the boundedness of solutions for time delay parabolic-hyperbolic systems with specified forms of feedback control.

The ideas mentioned above will be developed in forthcoming papers.

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Two-person zero-sum differential games

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Keywords: Linear quadratic differential game, saddle point, value of a game, Riccati differential equation, open loop and closed loop strategies, conjugate point, blow-up time

In *differential zero-sum two-player games* the first player tries to minimize and the second player to maximize a utility function that depends on a state variable whose dynamics is governed by a system of differential equations. Two classical approaches are via *open loop* and *closed loop strategies* for the players. In this paper, we shall mainly restrict ourselves to the open loop case and a perfect knowledge of the *state*.

(M. C. Delfour and S. K. Mitter 1969) studied the dynamical Min-Sup problem for the following perturbed control process in $\mathbb{R}^n$

$$\frac{dx}{dt}(t) = A(t)\,x(t) + f(t,u(t)) + g(t,v(t)), \quad (1)$$

where $A(t)$ is a $n \times n$ measurable and bounded matrix on $[0,T]$, f is in C^1 in $\mathbb{R}^{1+m}$ and g is in C^1 in $\mathbb{R}^{1+k}$ (n, m, and k are integers ≥ 1), and furthermore, (i) the initial state x_0 at time 0 is given, (ii) the admissible controllers $\mathcal{F}$ consist of all Lebesgue measurable functions $t \mapsto u(t)$ on the compact interval $[0,T]$ such that $u(t) \in U$, (almost everywhere on $[0,T]$), where U is a compact set in $\mathbb{R}^m$, (iii) the admissible disturbances $\mathcal{G}$ consist of all Lebesgue measurable functions $t \mapsto v(t)$ on the compact interval $[0,T]$ such that $v(t) \in V$, almost everywhere on $[0,T]$, where V is a compact set in $\mathbb{R}^k$, (iv) the cost function for each admissible u and v is given by $C(u,v) = G(x(T))$, where G is a continuous function in $\mathbb{R}^n$.

The fundamental theory of closed loop two-player zero-sum LQ games was given in (P. Bernhard 1979) followed by the seminal book in 1991 of (T. Başar and P. Bernhard 1995) that covered the H^∞-theory. They considered two-player zero-sum game over the finite time interval $[0,T]$ characterized by the quadratic *utility function*

$$C_{x_0}(u,v) \stackrel{\text{def}}{=} Fx(T)\cdot x(T) + \int_0^T Q(t)x(t)\cdot x(t) + |u(t)|^2 - |v(t)|^2\,dt, \quad (2)$$

where x is the solution of the linear differential system, the so-called *state equation*

$$\frac{dx}{dt}(t) = A(t)x(t) + B_1(t)u(t) + B_2(t)v(t) \quad \text{a.e. in } [0,T], \qquad x(0) = x_0, \quad (3)$$

x_0 is the *initial state* at time $t = 0$, $u \in L^2(0,T;\mathbb{R}^m)$, $m \geq 1$, is the strategy of the first player, and $v \in L^2(0,T;\mathbb{R}^k)$, $k \geq 1$, is the strategy of the second player. F is an $n \times n$-matrix and A, B_1, B_2, and Q are matrix-functions of appropriate order that are measurable and bounded almost everywhere in $[0,T]$. Moreover, $Q(t)$ and F are positive semi-definite.

Given an initial state x_0 in $\mathbb{R}^n$ at time $t = 0$, the game is said to achieve its *open loop lower value* if

$$v^-(x_0) \stackrel{\text{def}}{=} \sup_{v\in L^2(0.T;\mathbb{R}^k)} \inf_{u\in L^2(0.T;\mathbb{R}^m)} C_{x_0}(u,v)$$

is finite. It is said to achieve its *upper value* if

$$v^+(x_0) \stackrel{\text{def}}{=} \inf_{u\in L^2(0.T;\mathbb{R}^m)} \sup_{v\in L^2(0.T;\mathbb{R}^k)} C_{x_0}(u,v)$$

is finite. By definition $v^-(x_0) \leq v^+(x_0)$. The game is said to achieve its *open loop value* if its open loop lower value $v^-(x_0)$ and upper value $v^+(x_0)$ are finite and $v^-(x_0) = v^+(x_0)$. The *open loop value* of the game will be denoted by $v(x_0)$. A pair $(\bar{u},\bar{v})$ in $L^2(0,T;\mathbb{R}^m) \times$

$L^2(0,T;\mathbb{R}^k)$ is an *open loop saddle point* of $C_{x_0}(u,v)$ in $L^2(0,T;\mathbb{R}^m)\times L^2(0,T;\mathbb{R}^k)$ if for all u in $L^2(0,T;\mathbb{R}^m)$ and all v in $L^2(0,T;\mathbb{R}^k)$ $C_{x_0}(\bar{u},v)\leq C_{x_0}(\bar{u},\bar{v})\leq C_{x_0}(u,\bar{v})$. An open loop saddle point coincides with the classical notion of a *Nash equilibrium*.

The very nice work of (P. Zhang 2005-1) established the equivalence between the finiteness of the open loop value of a two-player zero-sum LQ game and the finiteness of its open loop lower and upper values *without a priori positive semidefiniteness assumption* on the matrices entering in the utility function, that is $Q(t)$ and F are not necessarily positive semi-definite. It means that the *duality gap*, that is the difference between the upper and the lower values of the game, is either 0 or $+\infty$. The reader is referred to the above references for a detailed bibliography of the vast and rich literature on dynamical games.

In a recent paper (M. C. Delfour 2007) completed and sharpened the results of (P. Zhang 2005-1) for the finiteness of the lower value of the game by providing a set of necessary and sufficient conditions that emphasizes the *feasibility condition*: $(0,0)$ is a solution of the open loop lower value of the game for the zero initial state.

Then he shows that, under the assumption of an open loop saddle point in the time horizon $[0,T]$ for all initial states, there is an open loop saddle point in the time horizon $[s,T]$ for all initial times s, $0\leq s<T$, and all initial states at time s. From this he gets an *optimality principle*, adapts the *invariant embedding approach* to construct the decoupling symmetrical matrix function $P(s)$, and shows that it is an $H^1(0,T)$ solution of the matrix Riccati differential equation. Thence an open loop saddle point in $[0,T]$ yields closed loop optimal strategies for both players.

Furthermore, a necessary and sufficient set of conditions for the existence of an open loop saddle point in $[0,T]$ for all initial states is the convexity-concavity of the utility function and the existence of an $H^1(0,T)$ symmetrical solution to the matrix Riccati differential equation. As an illustration of the cases where the open loop lower/upper value of the game is $-\infty/+\infty$, two informative examples of solutions to the Riccati differential equation with and without blow-up time are worked out.

In this paper we first go back to the case where the lower value of the game is finite and the upper value is infinite. In general, it is difficult to make sense of a Riccati differential equation. Yet, (P. Bernhard 1979) studied a family of games where it is still possible to get such an equation provided escape times are allowed at a finite number of times. For that family there is a closed loop-closed loop saddle point. Some thoughts and hopefully new insights will be presented.

Finally, we shall extend the above results to infinite dimensional parabolic systems. For related work the reader is referred to (I. Lasiecka and R. Triggiani 2000) and their bibliography.

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AN ECONOMIC MODEL WITH VINTAGE CAPITAL: DYNAMIC PROGRAMMING APPROACH.

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Keywords: Endogenous growth, Vintage capital, AK model, Dynamic programming.

1. INTRODUCTION

This paper deals with an endogenous growth model with vintage capital and, more precisely, with the AK model proposed in Boucekkine et al (2005). In endogenous growth models the introduction of vintage capital allows to explain some growth facts but strongly increases the mathematical difficulties. So far, in this approach, the model is studied by the Maximum Principle; here we develop the Dynamic Programming approach to the same problem by obtaining sharper results and we provide more insight about the economic implications of the model. We explicitly find the value function, the closed loop formula that relates capital and investment, the optimal consumption path and the long run equilibrium. The short run fluctuations of capital and investment and the relations with the standard AK model are analyzed. Moreover we discuss possible extensions of the model.

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Mild Solutions of Semilinear Stochastic Equations with Fractional Noise

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Keywords: Semilinear stochastic equations, fractional Brownian motion, stochastic partial differential equations, mild solutions

1. Introduction

The solutions of a family of semilinear stochastic equations in a Hilbert space with a fractional Brownian motion are investigated. The nonlinear term in these equations has primarily only a growth condition assumption. An arbitrary member of the family of fractional Brownian motions can be used in these equations. Existence and uniqueness for both weak and mild solutions are obtained for some of these semilinear equations. The weak solutions are obtained by a measure transformation that verifies absolute continuity with respect to the measure for the solution of the associated linear equation. Some examples of stochastic differential and partial differential equations are given that satisfy the assumptions for the solutions of the semilinear equations.

Evolution equations with a fractional noise have been studied in recent years by several authors, e.g. Duncan, Maslowski and Pasik-Duncan; Grecksh and Ash; Maslowski and Nualart; Hu, Oksendal and Zhang; and others.

Fractional Brownian motion denotes a family of Gaussian processes with continuous sample paths that are indexed by the Hurst parameter $H \in (0,1)$ and that have properties that appear empirically in a wide variety of physical phenomena, such as hydrology, economic data, telecommunications, and medicine. Since some physical phenomena are naturally modeled by stochastic partial differential equations and the randomness can be described by a fractional Gaussian noise, it is important to study the problems of the solutions of stochastic differential equations in a Hilbert space with a fractional Brownian motion. A significant family of these stochastic equations is the set of semilinear equations, so it is important to investigate the existence and the uniqueness of the solutions of the equations and the sample path properties of the solutions.

2. Main Topics

The mild solutions are obtained for various semilinear stochastic equations with a fractional Brownian motion. The cases $H \in (0, 1/2)$ and $H \in (1/2, 1)$ are treated separately.

The following semilinear stochastic equation is considered:

$$dX(t) = (AX(t) + F(X(t)))\, dt + \Phi dB(t) \tag{1}$$

where $t \in R_+$, $X(t)$, $X_0 \in V$, $(B(t), t \geq 0)$ is a standard cylindrical fractional Brownian motion with the Hurst parameter $H \in (0,1)$, $\Phi \in \mathscr{L}(V)$, $A : Dom(A) \to V$, $Dom(A) \subset V$, and A is the infinitesimal generator of a strongly continuous semigroup $(S(t), t \geq 0)$ on V. The function $F : V \to V$ is nonlinear and for the applications to stochastic partial differential equations it is more useful to assume that F is only defined on a (dense) subspace of V. So, let $(E, \|\cdot\|_E)$

be a separable Banach space that is continuously embedded in V and $F : E \to V$ with $X_0 \in E$. Subsequently, it is assumed that $F : E \to V$ is Borel measurable, $Im(F) \subset Im(\Phi)$, for $G := \Phi^{-1}F$, $G : E \to V$, and

$$\|G(x)\| \leq \hat{k}\left(1 + \|x\|_E^{\rho}\right)$$

and

$$\|F(x)\|_E \leq \hat{k}\left(1 + \|x\|_E^{\rho}\right)$$

for each $x \in E$ and some $\rho \geq 1$. Furthermore, it is assumed that there is a constant $\bar{K}$ such that for each pair (x, y) in $Dom(A)$, there is a $z^* \in \partial \|z\|_E$ such that

$$\langle Ax - Ay + F(x) - F(y), z^* \rangle_{E,E^*} \leq \bar{K} \|x - y\|_E$$

where $\partial \|z\|_E$ is the subdifferential of the norm $\|z\|_E$ at the point $z = x - y$ and $\langle \cdot, \cdot \rangle_{E,E^*}$ is the pairing between E and E^*. The last inequality is a one-sided growth condition that ensures the absence of explosions of solutions of (1) in a finite time. Some illustrative examples should clarify its interpretation. The notion of a mild solution of (1) is given now.

A mild solution, $(X(t), t \geq 0)$ of the equation (1) is an E-valued process on a fixed probability space $(\Omega, \mathscr{F}, \mathbb{P})$ with a given standard cylindrical fractional Brownian motion satisfying

$$X(t) = S(t)X_0 + \int_0^t S(t-r)F(X(r))dr + \int_0^t S(t-r)\Phi dB(r). \quad (2)$$

A primary goal in this paper is to verify existence and uniqueness of a mild solution of (1). Since the cases $H \in (0, 1/2)$ and $H \in (1/2, 1)$ require different methods, they are treated separately.

The following three assumptions are made to construct a solution of (1):

(H1). The semigroup $(S(t), t \geq 0)$ generated by A is analytic on V and for each $t \geq 0$, $S(t)|_E \in \mathscr{L}(E)$ and $\|S(t)|_E\|_{\mathscr{L}(E)}$ is bounded on compact time intervals.

(H2). $\Phi \in \mathscr{L}(V)$ is injective and for $T > 0$, the stochastic convolution process

$$\left(\int_0^t S(t-r)\Phi dB(r), t \in [0, T]\right)$$

has a version with $C([0, T], E)$ sample paths.

The case $H \in (0, 1/2)$ is considered.

Theorem 1. *Let $H \in (0, 1/2)$ and (H1) and (H2) be satisfied. Let $\Phi \in \mathscr{L}(V)$ be injective, $\Phi^{-1} \in \mathscr{L}(E, V)$ and $(S(t)|_E, t \geq 0)$ be a strongly continuous semigroup on E such that*

$$|S(t)|_E|_{\mathscr{L}(E)} \leq e^{\tilde{w}t}$$

for $t \geq 0$ and some $\tilde{w} \in \mathbb{R}$. Let $F : E \to E$ be continuous and satisfy

$$\|F(x)\|_E \leq k_1\left(1 + \|x\|_E^{\rho}\right)$$

for $x \in E$ for some $k_1 \geq 0$ and $\rho \geq 1$ and for each pair $x, y \in E$, there is a $z^* \in \partial \|x - y\|_E$ where $\partial \|z\|_E$ is the subdifferential of the norm $\|\cdot\|_E$ at $z \in E$ such that

$$\langle F(x) - F(y), z^* \rangle_{E,E^*} \leq k_2 \|x - y\|_E$$

for some $k_2 \in \mathbb{R}$, that is, $F - k_2 I$ is dissipative on V. Then there is one and only one mild solution of (1) and its probability law on $\check{\Omega} = C([0, T], E)$ is mutually absolutely continuous with respect to the probability law of the fractional Ornstein-Uhlenbeck process.

The Theorem (2) will be formulated for the case $H \in (1/2, 1)$.

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Semilinear Stochastic Equations in a Hilbert Space with a Fractional Brownian Motion

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Keywords: Semilinear stochastic equations, fractional Brownian motion, stochastic partial differential equations, absolute continuity measures

1. Introduction

Fractional Brownian motion denotes a family of Gaussian processes with continuous sample paths that are indexed by the Hurst parameter $H \in (0,1)$ and that have properties that appear empirically in a wide variety of physical phenomena, such as hydrology, economic data, telecommunications, and medicine. Since some physical phenomena are naturally modeled by stochastic partial differential equations and the randomness can be described by a fractional Gaussian noise, it is important to study the problems of the solutions of stochastic differential equations in a Hilbert space with a fractional Brownian motion. A significant family of these stochastic equations is the set of semilinear equations, so it is important to investigate the existence and the uniqueness of the solutions of the equations and the sample path properties of the solutions. If primarily only some growth assumptions are made on the nonlinear terms in the semilinear equations then it is natural to investigate weak solutions, especially those that arise by an absolutely continuous transformation of the measure of the solution of the associated linear stochastic equation.

2. Main Topics

Existence and uniqueness for weak solutions are obtained for some semilinear equations in a Hilbert space with a fractional Brownian motion. The weak solution is obtained by a measure transformation where absolute continuity with respect to the measure for the solution of the associated linear equation is verified. Some examples of stochastic differential and partial equations are given that satisfy the assumptions for the solutions of the semilinear equations.

The following semilinear stochastic equation is considered:

$$dX(t) = (AX(t) + F(X(t)))\, dt + \Phi\, dB(t) \tag{2.1}$$

where $t \in \mathbb{R}_+$, $X(t)$, $X_0 \in V$, $(B(t), t \geq 0)$ is a standard cylindrical fractional Brownian motion with the Hurst parameter $H \in (0,1)$, $\Phi \in \mathcal{L}(V)$, $A : Dom(A) \to V$, $Dom(A) \subset V$, and A is the infinitesimal generator of a strongly continuous semigroup $(S(t), t \geq 0)$ on V. The function $F : V \to V$ is nonlinear and for the applications to stochastic partial differential equations it is more useful to assume that F is only defined on a (dense) subspace of V. So, let $(E, \|\cdot\|_E)$ be a separable Banach space that is continuously embedded in V and $F : E \to V$ with $X_0 \in E$. Subsequently, it is assumed that $F : E \to V$ is Borel measurable, $Im(F) \subset Im(\Phi)$, for $G := \Phi^{-1}F$, $G\colon E \to V$, and

$$\|G(x)\| \leq \hat{k}\left(1+\|x\|_E^{\rho}\right) \tag{2.2}$$

and

$$\|F(x)\|_E \leq \hat{k}\left(1+\|x\|_E^{\rho}\right) \tag{2.3}$$

for each $x \in E$ and some $\rho \geq 1$. Furthermore, it is assumed that there is a constant $\bar{K}$ such that for each pair (x,y) in $Dom(A)$, there is a $z^* \in \partial\|z\|_E$ such that

$$\langle Ax - Ay + F(x) - F(y), z^* \rangle_{E,E^*} \leq \bar{K}\|x-y\|_E \tag{2.4}$$

where $\partial\|z\|_E$ is the subdifferential of the norm $\|z\|_E$ at the point $z = x-y$ and $\langle \cdot,\cdot,\rangle_{E,E^*}$ is the pairing between E and E^*. The inequality (2.4) is a one-sided growth condition that ensures the absence of explosions of solutions of (2.1) in a finite time. Some subsequent examples should clarify its interpretation.

The notion of a weak solution of (2.1) is given now.

Definition 2.1. *A weak solution of the equation* (2.1) *is a triple* $(X(t), B(t), (\tilde{\Omega}, \tilde{\mathcal{F}}, \tilde{\mathbb{P}}), t \geq 0)$ *where* $(B(t), t \geq 0)$ *is a standard cylindrical fractional Brownian motion in* V *that is defined on the probability space* $(\tilde{\Omega}, \tilde{\mathcal{F}}, \tilde{\mathbb{P}})$ *and* $(X(t), t \geq 0)$ *is an* E*-valued process satisfying*

$$\begin{aligned} X(t) =& S(t)X_0 + \int_0^t S(t-r)F(X(r))\,dr \\ &+ \int_0^t S(t-r)\Phi\,dB(r)\ . \end{aligned} \tag{2.5}$$

The equation (2.5) *has a unique weak solution if for any two weak solutions* $(X(t), B(t), (\Omega, \mathcal{F}, \mathbb{P}), t \geq 0)$ *and* $(\tilde{X}(t), \tilde{B}(t), (\tilde{\Omega}, \tilde{\mathcal{F}}, \tilde{\mathbb{P}}), t \geq 0)$*, the processes* $(X(t), t \geq 0)$ *and* $(\tilde{X}(t), t \geq 0)$ *have the same probability law.*

The following three assumptions are made to construct a solution of (2.1):

(H1). The semigroup $(S(t), t \geq 0)$ generated by A is analytic on V and for each $t \geq 0$, $S(t)|_E \in \mathcal{L}(E)$ and $\| S(t)|_E \|_{\mathcal{L}(E)}$ is bounded on compact time intervals.

(H2). $\Phi \in \mathcal{L}(V)$ is injective and for $T > 0$, the stochastic convolution process

$$\left(\int_0^t S(t-r)\Phi\,dB(r), t \in [0,T]\right)$$

has a version with $C([0,T], E)$ sample paths.

(H3). The function $F\colon E \to V$ in (2.1) is Borel measurable, $Im(F) \subset Im(\Phi)$ and the function $G = \Phi^{-1}F\colon E \to V$ satisfies

$$\|G(x)\| \leq k\left(1+\|x\|_E\right)$$

for some $k > 0$ and all $x \in E$.

The following result verifies a weak solution for $H \in (0, 1/2)$.

Theorem 2.1. *If* $H \in (0, 1/2)$ *and conditions (H1)-(H3) are satisfied, then the equation* (2.1) *has a weak solution. If additionally* $F\colon E \to E$ *and*

$$\|F(x)\|_E \leq k_1\left(1+\|x\|_E\right)$$

for some $k_1 > 0$ *and all* $x \in E$*, then the weak solution is unique.*

A corresponding result can be verified for the case of $H \in (\frac{1}{2}, 1)$.

Toward real-time model-based temperature assimilation for Structural Health Monitoring

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Keywords: Optimal control, heat equation, inverse heat transfer, final time, duality

1. Introduction and main results

Temperature variations and their effects on structures act like perturbations for damage detection techniques based on vibration monitoring. The elimination of temperature effects appears as a bottleneck in this field. The work presented here deals with the reconstruction of the thermal field inside a structure when only some pointwise temperature measurements along a time interval $[0,T]$ are available. In view of real-time applications, we focus on the reconstructed temperature at time T. A model-based least-square data assimilation approach is proposed. The algorithm builds upon optimal control theory applied to the determination of both initial temperature and boundary heat fluxes. Because of a known and documented difficulty of the adjoint method, the temperature at final time fails to converge.

It is shown numerically that minimizing the performance index over a space of smooth enough initial temperatures and boundary fluxes (of H^1 type in time) eliminates this difficulty. Moreover, the proposed framework yields a both accurate and stable final temperature.

The temperature field at any time results from a standard postprocessing. This so-called adjoint method proves truely multi-dimensional and compatible with all existing finite element softwares.

In view of rapid inverse heat transfer for 3D problems, duality is put to work. The space over which to minimize the dual functional is of the type $(L^2([0,T]))^m$, where m denotes the number of sensors. This opens the way to a potential splitting that would distribute the computation over the sensor network.

2. Problem statement

Consider a solid in a multidimensional domain Ω with boundary $\partial\Omega$. Assuming absence of internal heat sources and an initial state denoted by $\theta^0(x)$, the temperature field inside the solid is given by the heat equation:

$$\left\{\begin{array}{ll} \rho c\dfrac{\partial\theta}{\partial t} - div(\mathbf{K}\, grad\,\theta) = 0 & \Omega\times[0,T] \\ (\mathbf{K}\, grad\,\theta)\cdot\vec{n} + \alpha\theta = \Phi & \partial\Omega\times[0,T] \\ \theta(x,0) = \theta^0(x) & \Omega \end{array}\right. \tag{1}$$

Here, $\Phi(x,t) = g(x,t) + \alpha\theta_{ext}$ where g denotes an inward heat flux when Fourier-Robin conditions are considered and θ_{ext} is the external temperature, $\vec{n}$ is the outwards normal vector on the boundary, $x\in\Omega$ is the space variable, $t\in[0,T]$ the time variable, ρ the mass density, c the heat capacity and $\mathbf{K}$ the conductivity tensor of the material.

Assume that m sensors are available inside the structure at locations x_k, $k = 1..m$. They deliver the data $\{\theta_k^d(t)\}_{k=1}^m, t\in[0,T]$. Based on these measurements, the aim is to reconstruct the temperature field over the time interval $[0,T]$, focusing on the accuracy of the reconstruction at the final time T. One way to achieve this is to try to determine the couple $\{\theta^0,\Phi\}$ of initial and boundary conditions responsible for the measurements.

The problem can be formulated in a least-squares framework. In this approach, an iterative procedure will be put to work to minimize the difference between the given measurements $\{\theta_k^d(t)\}_{k=1}^m$ and the value at sensor locations of a reconstructed field. The inverse problem being by itself mathematically ill-posed in the sense of Hadamard, some regularization technique is

needed in order to guarantee numerical stability of the computational procedure even with noisy input data. The problem thus consists in minimizing a functional of the form

$$J(\{\theta^0, \Phi\}) = \frac{1}{2}\sum_{k=1}^{m}\int_0^T \Big(\theta(x_k,t) - \theta_k^d(t)\Big)^2 dt + \tfrac{\epsilon}{2}\|\{\theta^0,\Phi\}\|_X^2 \tag{2}$$

Here, the last term in (2) stands for the so-called Tikhonov regularization, ϵ being a small regularizing coefficient that provides extra convexity to the functional J.

The functional space X guarantees the existence of a sufficiently smooth solution to (1). $\|\cdot\|_X^2$ denotes a suitable norm for X. The pair $\{\theta^0, \Phi\}$ is referred to as the control variable and X as the control space. It will be seen that the choice of X has a crucial influence on the results. In what follows, two different choices will be presented to illustrate this.

3. Numerical results

The results on figure 1 show the disadvantages of the adjoint method in L^2.

They concern a beam of length L to which a given flux is prescribed at each end. All material constants are set to 1. Some direct simulations with an arbitrary input flux give measurements on sensors located at $\frac{L}{5}$, $\frac{L}{2}$ and $\frac{4L}{5}$ respectively. These measurements are then used to simulate the reconstruction algorithm.

The temperature field reconstruction is of acceptable accuracy far from $t = T$, while the reconstruction of $\theta(x, T)$, which is the most interesting output in view of our application, is very unsatisfactory (figure 1). This phenomenon is due to the definition of the adjoint and is well known in the literature (Alifanov; Hua). It will be explained and an alternative definition of the adjoint field enabled by a new choice of space X and associated scalar product will be considered.

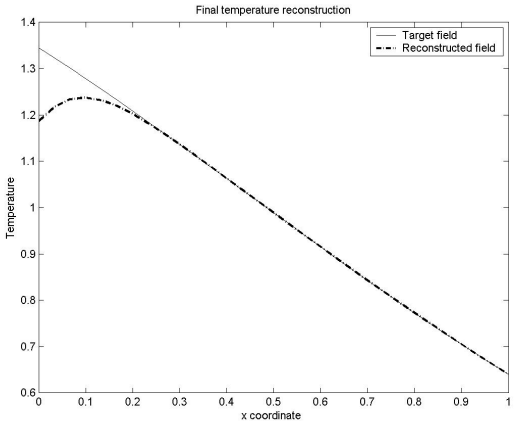

Fig. 1. Reconstruction in L^2: **final temperature**

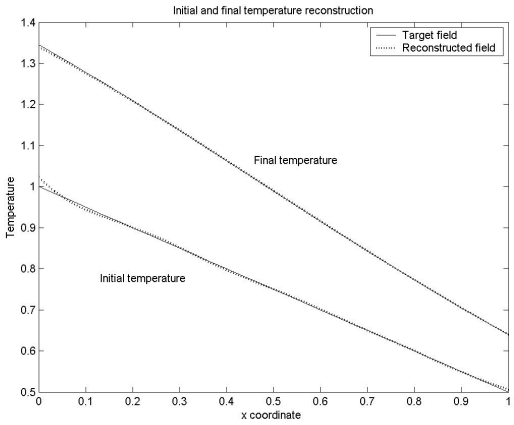

Fig. 2. Reconstruction in H^1: **intial** and **final** temperature

4. CONCLUSIONS

A three-dimensional extension of the computational framework will be presented for the dual formulation of the reconstruction problem. Numerical and experimental results obtained with a block of concrete in a climate chamber will be discussed.

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MESH INDEPENDENCE FOR LQR CONTROL OF CONVECTION DIFFUSION EQUATIONS

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Keywords: LQR-Control, Riccati Equation, Mesh Independence, Kleinman-Newton algorithm

The development of practical computational schemes for optimization and control of nonnormal distributed parameter systems requires that one builds certain computational efficiencies (such as mesh independence) into the approximation scheme. In this talk we consider the convergence as well as mesh independence of the infinite dimensional version of the Kleinman-Newton algorithm. The Kleinman-Newton algorithm is used to solve the algebraic Riccati operator equation that arises in the control of PDE systems. We consider some numerical issues concerning the application of the Kleinman-Newton algorithm to discretizations of infinite dimensional Riccati equations associated with the linear quadratic regulator (LQR) problem. We show that dual convergence and compactness play central roles in both convergence and mesh independence. We present numerical results using standard finite element and stabilizing Petrov-Galerkin approximations of convection diffusion equations to illustrate the theory.

A GENERALIZED EIGENPROBLEM FOR THE LAPLACIAN AND ITS APPLICATION TO THE LIGHTNING DISCHARGE

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Keywords: Laplacian, generalized eigenproblem, double layer potential, complete eigenbasis, lightning, electric potential, Ampere's law, Maxwell's equations

We consider the following evolution equation describing the electric potential in a domain Ω:

$$\begin{aligned} -\frac{\partial \Delta \phi}{\partial t} &= \nabla \cdot (\sigma \nabla \phi), \quad (\mathbf{x}, t) \in \Omega \times [0, \infty), \\ \phi(\mathbf{x}, t) &= 0, \quad (\mathbf{x}, t) \in \partial\Omega \times [0, \infty), \\ \phi(\mathbf{x}, 0) &= \phi_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{aligned}$$

where $\sigma \in L^\infty(\Omega)$. We determine the change in potential that results from letting the conductivity σ tend to ∞ in a subdomain $\mathcal{L} \subset \Omega$ at $t = 0^+$. This result is applicable to a lightning discharge and the resulting change in electric potential in the atmosphere. We show that in $\mathcal{L}$ the potential at $t = 0^+$ is the constant $\phi_L = \langle \nabla \phi_0, \nabla \Pi \rangle_\Omega / \langle \nabla \Pi, \nabla \Pi \rangle_\Omega$ where

$$\begin{aligned} \Pi &= 1 \text{ in } \mathcal{L}, \\ \Delta \Pi &= 0 \text{ in } \Omega \setminus \mathcal{L}, \\ \Pi &= 0 \text{ on } \partial\Omega, \end{aligned}$$

and $\langle \cdot, \cdot \rangle_\Omega$ is the $L^2(\Omega)$ inner product

$$\langle \nabla u, \nabla v \rangle_\Omega = \int_\Omega \nabla u \cdot \nabla v \, dx. \tag{1}$$

Outside of $\mathcal{L}$, the change in potential at $t = 0^+$ is the solution to the problem

$$\begin{aligned} \Delta \xi &= 0 \text{ in } \Omega \setminus \mathcal{L}, \\ \xi &= 0 \text{ on } \partial\Omega, \\ \xi &= \phi_L - \phi_0 \text{ on } \partial\mathcal{L}. \end{aligned}$$

The analysis hinges on recent results we have established for a generalized eigenproblem of the Laplacian: Find $u \in H_0^1(\Omega)$, $u \neq 0$, and $\lambda \in \mathbb{R}$ such that

$$\langle \nabla u, \nabla v \rangle_{\mathcal{L}} = \lambda \langle \nabla u, \nabla v \rangle_\Omega$$

for all $v \in H_0^1(\Omega)$. It is proved that any $f \in H_0^1(\Omega)$ can be expanded in terms of orthogonal eigenfunctions for the generalized eigenproblem. During the analysis, we present a new inner product on $H^{1/2}(\partial\mathcal{L})$ with the following properties: (a) the norm associated with the inner product is equivalent to the usual norm on $H^{1/2}(\partial\mathcal{L})$, and (b) the double layer potential operator is self adjoint with respect to the new inner product and compact as a mapping from $H^{1/2}(\partial\mathcal{L})$ into itself. The analysis identifies four classes of eigenfunctions for the generalized eigenproblem:

1. The function Π which is 1 on $\mathcal{L}$ and harmonic on $\Omega \setminus \mathcal{L}$; the eigenvalue is 0.
2. Functions in $H_0^1(\Omega)$ with support in $\Omega \setminus \mathcal{L}$; the eigenvalue is 0.
3. Functions in $H_0^1(\Omega)$ with support in $\mathcal{L}$; the eigenvalue is 1.
4. Excluding Π, the harmonic extension of the eigenfunctions of a double layer potential on $\partial\mathcal{L}$. The eigenvalues are contained in the open interval $(0, 1)$. The only possible accumulation point is $\lambda = 1/2$.

COMPARISON OF FULL- AND REDUCED-ORDER MODELS FOR FEEDBACK CONTROL OF FLUIDS

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Keywords: feedback control, fluids, model reduction

1. Abstract

The feedback control of fluid flows using model reduction techniques has been studied for the past decade. However, the challenge of computing feedback control laws for the full-order problem has limited the assessment of these control techniques to determine their effectiveness in representing the optimal feedback controller. However, the availability of the latest generation of high-performance computers has now made these comparisons possible. In this talk, we investigate the effectiveness of the model reduction approached based on proper orthogonal decomposition and Galerkin projection (POD/Galerkin) and a related controller reduction approach. Numerical results comparing these popular approaches with Riccati equation-based linear state feedback will be presented. One study will examine the effectiveness of the reduced-order modeling approach as the number of reduced-basis functions are increased. Case studies will include both linear and nonlinear PDE examples motivated by control of fluid flow.

Stabilization of Linked Structures of Differing Dimensions

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Keywords: stabilization, boundary control, elastic structures, coupled systems

1. Introduction

A tremendous challenge in the study of control and stabilization of dynamic elastic systems is the ability to rigorously address whether linked dynamic structures can be controlled using boundary feedback alone. Early work focusing on the question of boundary controllability considered the behavior of individual component, asking whether a string, a beam, or a plate could be stabilized via feedback control acting on all or a portion of the boundary. However, in spite of the availability of many results on control and stabilization for single components, comparatively limited results have been established for linked systems. When a structure is composed of a number of interconnected elastic elements or is modelled by a system of coupled partial differential equations, the behavior becomes much harder to both predict and to control. It cannot simply be considered as a single large flexible structure, as the effects of each element or each equation upon the next are critical in determining its motion.

2. Model Development

When it comes to linked dynamic structures, the question of control is often secondary to the issue of constructing a feasible mathematical model that is not only accessible to the mathematical tools, but is also consistent with engineering considerations and restrictions. While modeling of linked structures was extensively considered by Lagnese, Leugering and Schmidt (2), much work remains to be done. In their monograph, the authors primarily focused on linked structures composed of multiple elements of the same type, although plate-beam systems are considered in the final chapter.

Under appropriate assumptions, (2) derives a linear model for this configuration. In particular, when the beam is attached orthogonally to the edge of the plate, the model is comprised of the Reissner-Mindlin plate, the Timoshenko beam, and the linearized equation of torsion in a rod. All variables are coupled through geometric and dynamic boundary conditions.

Extensions to nonlinear plate-beam systems systems are motivated by issues arising from large-amplitude periodic oscillations in elastic systems. A classic example is the oscillation in suspension bridges. An interesting discussion of the explanations behind large oscillations and their inherent challenges can be found in (3). In the particular context of a suspension bridge, fundamental nonlinearities exist due to the behavior of the cables which support the bridge. As a first step in addressing nonlinear behavior of coupled systems, we consider a von Kármán plate coupled with a nonlinear beam equation.

In our work, we have constructed a model comprised of a nonlinear von Kármán plate coupled with a nonlinear beam equation, developed from first principles (1). To formulate the model, the plate and beam are assumed to obey the following basic kinematic hypotheses. Cross-sections of the beam move rigidly and linear filaments of the plate which are perpendicular in the reference configuration remain perpendicular to the midsurface

and do not contract or expand. Additionally, to obtain the nonlinear von Kármán plate model and the corresponding nonlinear beam, linear strain-displacement relations cannot be assumed. Instead, the strain relations from finite elasticity are imposed. While this is a "large deflection" model, the vertical displacement is nonetheless assumed to be small in comparison to the lateral dimensions of the plate. Therefore, we can use the linear displacement relations from Kirchhoff plate theory. Finally, in-plane accelerations are assumed to be negligible.

Under these assumptions, the model obtained is analogous to the linear model in (2), but retains some nonlinearities, including the von Kármán nonlinearity and a corresponding nonlinear term in the beam equation. However, at this stage, the model is still quite complex, including both vertical and in-plane displacements for the plate and vertical displacement, torsional rotation and vertical and lateral flexion of the beam. To simplify the model further, the shear moduli are allowed to approach infinity, yielding a limit model which depends only upon the vertical displacements of the plate and beam and the torsional rotation. At this point, the torsional rotation is assumed to be small and the beam is assumed to be thin, allowing any warping of the cross-section to be neglected.

Dynamic junction conditions are imposed at the interface. Wellposedness is established by first considering a corresponding linear problem, then applying a perturbation theorem for nonlinear semigroups. Proof of regularity takes advantage of elliptic theory, as well as the regularity of the Airy's stress function. The compatibility constraints at the junction give rise to mathematical challenges not seen in earlier work on the individual plate and beam models.

3. Controllability

A natural question that often arises is whether control must be imposed on the entire boundary or on every component in order to effect stabilization. Much work has been done to minimize the proportion of the boundary that must be controlled. In such cases, geometric constraints must be imposed on the uncontrolled portion of the boundary. Thus, for coupled systems, the logical extension is whether all components must be controlled or if the structure can be stabilized when control is not imposed on every component.

In linked dynamic systems, the use of boundary control becomes even more important. Within a multi-link structure, the natural locations to implement control are at the joints or edges of the structure. Because of the connections between the elements, the transfer of energy from one to the other creates effects which are frequently difficult to counteract. In many cases, the goal of exact controllability cannot be reached. Instead, either approximate controllability or optimization of the available controls with respect to an appropriate cost functional becomes the question under consideration.

Techniques used in the analysis include semigroup theory, energy methods, sharp trace estimates which rely upon microlocal analysis, and unique continuation properties of a corresponding overdetermined homogeneous system.

Joint work with Günter Leugering, Institut für Angewandte Mathematik, Universität Erlangen-Nürnberg, Germany.

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SUBOPTIMAL FEEDBACK CONTROL DESIGN OF CONSTRAINED PARABOLIC SYSTEMS IN UNCERTAINTY CONDITIONS

BORIS S. MORDUKHOVICH [1]

Abstract. The talk concerns minimax control problems for linear multidimensional parabolic systems with distributed uncertain perturbations and control functions acting in the Dirichlet boundary conditions. The underlying parabolic control system is functioning under hard/pointwise constraints on control and state variables. The main goal is to design a feedback control regulator that ensures the required state performance and robust stability under any feasible perturbations and minimize an energy-type functional under the worst perturbations from the given area. We develop an efficient approach to the minimax control design of constrained parabolic systems that is based on certain characteristic features of the parabolic dynamics including the transient monotonicity with respect to both controls and perturbations and the turnpike asymptotic behavior on the infinite horizon. In this way, solving a number of associated open-loop control and approximation problems, we justify an easily implemented suboptimal structure of the feedback boundary regulator and compute its optimal parameters ensuring the required state performance and robust stability of the closed-loop, highly nonlinear parabolic control system on the infinite horizon.

The primary motivation for this study came from certain environmental models, in particular, those developed within the Dynamical System and Environmental Projects of the International Institute of Applied System Analysis (IIASA), Laxenburg, Austria.

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CONTROL AND INVERSE PROBLEMS FOR THE WAVE AND HEAT EQUATIONS ON GRAPHS

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Keywords: controllability, inverse problems, wave equation, heat equation, graphs, trees

Boundary exact and spectral controllability and inverse problems on graphs are studied. We suppose that the wave equation is defined on each edge of the graph, and standard compatibility conditions are satisfied at the internal vertices. We prove that the system is exactly controllable if the graph is a tree and the control is applied to all (or to all but one) boundary vertices. Otherwise the system is generally not exactly controllable but may be spectrally controllable. The latter means that the space of reachable states contains all finite linear combinations of the eigenfunctions.

We discuss connections between controllability and inverse problems and show how to recover a tree (its connectivity and the lengths of the edges together with coefficients of the wave equation) by given response operator or Weyl matrix function.

We consider also null and spectral controllability and inverse problems for the heat equation on graphs.

The talk is based in part on joint work with P. Kurasov and V. Mikhaylov.

A VARIATIONAL APPROACH TO WELL-POSEDNESS FOR INITIAL VALUE PROBLEMS

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This talk will describe the analysis of certain variational principles for initial boundary value problems for parabolic-type equations. These variational principles are based on considerations of convex analysis and duality theory and extend earlier work of Brezis, Ekeland and the author.

Direct methods will then be used to prove well-posedness results for these problems under very weak assumptions on the data. Examples illustrating new applications of these principles to classical initial value problems of continuum mechanics will be described.

ON THE STABILITY OF EQUILIBRIA FOR THE STEFAN PROBLEM WITH SURFACE TENSION

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Keywords:

The Stefan problem is a model for phase transitions in solid-liquid systems. In this paper, we consider the two-phase Stefan problem with the modified Gibbs-Thomson law

$$u = \sigma H + \delta V \quad \text{on} \ \ \Gamma(t), \quad \sigma > 0, \ \delta \geq 0, \ (1)$$

and the kinetic condition

$$[d\partial_\nu u] = (\ell - [\kappa]u)V \quad \text{on} \quad \Gamma(t). \qquad (2)$$

Here $\Gamma(t)$ denotes the unknown moving hypersurface that separates the liquid from the solid phase, u is the temperature, H the mean curvature of $\Gamma(t)$, σ the surface tension coefficient, δ the coefficient of kinetic undercooling, V the normal velocity of $\Gamma(t)$, ℓ the latent heat, $[\kappa]$ the jump of the heat capacities across $\Gamma(t)$, and $[d\partial_\nu u]$ the jump of the heat fluxes across $\Gamma(t)$.

Under appropriate boundary conditions we will show that spheres (together with constant temperature distributions) are the only equilbrium states for this system, and we will characterize the stability of these equilibria in dependence of physical and geometric quantities.

INCOMPRESSIBLE IONIZED NON-NEWTONIAN FLUID MIXTURES

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Keywords: chemically reacting fluids, Eckart-Prigogine concept, Navier-Stokes equation, Nernst-Planck equation, Poisson equation, heat equation, diffusive fluxes, thermodynamics.

Chemically reacting mixtures represent a framework for modelling of various complicated processes in biology and chemistry. The model proposed in (Rou05a; Rou05b; Rou06; Rou07) uses incompressible framework with the barycentric impulse balance. This "barycentric" approach is called the Eckart-Prigogine's (Eck40; Pri47) concept, simplifying phenomenologically the description by considering only one temperature and one velocity of the whole mixture and having been awarded in the context of non-equilibrium thermodynamics of dissipative structures by Nobel prize in chemistry in 1977; in the compressible case, see also (ADM82; dGM62; Gio99). For a comparison with less phenomenological Truesdell model (TrTo60) see (Sam07). The incompressibility refers here both to each particular constituent and, through a volume-additivity hypothesis (i.e. Amagat's law) also to the overall mixture. To cover biological applications on a cellular or subcellular level where intensity of electric field on cell membranes is very high, the self-induced electrostatic field must be considered, too.

We consider a 3-dimensional incompressible flow of a mixture of L mutually reacting chemical ionic constituents; the $\ell^{\rm th}$-constitutent having a specific charge z_ℓ, $\ell = 1, ..., L$. Our model consists in a system of $4{+}L{+}1{+}1$ differential equations combining the *non-Newtonian* modification of the *Navier-Stokes equation* (balancing the barycentric momentum ϱv) with the incompressibility constraint $\mathrm{div}(v) = 0$, the *Nernst-Planck equation* modified for moving media (balancing the mass of particular constituents), the *heat equation* (balancing the heat part $c_{\rm v}\theta$ of the internal energy), and the quasistatic *Poisson equation* for the electrostatic field (balancing the electric induction $\varepsilon\nabla\phi$):

$$\varrho\frac{\partial v}{\partial t} - \mathrm{div}\big(\tau(\mathrm{D}v, c, \theta) - \varrho v{\otimes}v\big) + \nabla\pi = -q\nabla\phi, \tag{1}$$

$$\mathrm{div}(v) = 0, \tag{2}$$

$$q = c{\cdot}z, \tag{3}$$

$$\frac{\partial c}{\partial t} - \mathrm{div}\big(\mathcal{D}(c,\theta)\nabla c + \mathcal{M}(c,\theta)\otimes\nabla\phi - c{\otimes}v\big) = r(c,\theta)\,, \tag{4}$$

$$c_{\rm v}\frac{\partial\theta}{\partial t} - \mathrm{div}\big(\kappa\nabla\theta - c_{\rm v}v\,\theta\big) = \tau(\mathrm{D}v, c, \theta){:}\mathrm{D}v + \big(\mathcal{D}(c,\theta)\nabla c + \mathcal{M}(c,\theta)\otimes\nabla\phi\big) : {:}\,(z\otimes\nabla\phi) + h(c,\theta), \tag{5}$$

$$-\mathrm{div}(\varepsilon\nabla\phi) = q\ . \tag{6}$$

The variables v, π, c, θ, and ϕ have the following meaning:

$v = (v_1, v_2, v_3)$ barycenter velocity,
π pressure,
$c = (c_1, ..., c_L)$ concentrations,
ϕ electrostatic potential,
θ temperature,

where the concentration vector c is to satisfy the constraint

$$\forall\ell = 1, ..., L: \qquad c_\ell(t,x) \geq 0 \tag{7}$$

and

$$\textstyle\sum_{\ell-1}^{L} c_\ell(t,x) = 1 \qquad \text{for a.a. } (t,x). \tag{8}$$

The meaning of the data is:

$\tau = \tau(\mathrm{D}v, c, \theta)$ the stress tensor,
$\mathrm{D}v = \frac{(\nabla v)^\top + \nabla v}{2}$ symmetric velocity gradient,
$\varrho > 0$ mass density,
$z = (z_1, ..., z_L)$ charges of the constituents,

$q = c \cdot z$ the total charge,
$\varepsilon > 0$ permitivity,
$r = (r_1, ..., r_L)$ chemical production rates,
h heat production rate by chemical reactions,
$\mathcal{D} = [\mathcal{D}_{kl}]_{k,l=1}^{L}$ a diffusion matrix,
$\mathcal{M} = (\mathcal{M}_1, ..., \mathcal{M}_L)$ effective mobilities,
$\kappa > 0$ thermal conductivity, and
$c_{\rm v} > 0$ heat capacity.

In terms of phenomenological diffusive fluxes j_ℓ, (4) can be written as $\frac{\partial c}{\partial t} + \mathrm{div}(c \otimes v - j_\ell) = r(c, \theta)$. A standard "ansatz" for the these fluxes is

$$j_\ell := \sum_{k=1}^{L} \mathcal{M}_{k\ell}(c) \nabla \mu_k, \tag{9}$$

where

$$\mu_\ell := \rho \ln c_\ell + z_\ell \phi \tag{10}$$

is the electrochemical potential. These fluxes should satisfy a zero-sum condition, i.e. the mobility matrix $[\mathcal{M}_{k\ell}(c)]$ should satisfy

$$\forall k = 1, ..., L, \ \forall c, \ c_\ell \geq 0, \ \textstyle\sum_{\ell=1}^{L} c_\ell = 1 : \\ \textstyle\sum_{\ell=1}^{L} \mathcal{M}_{k\ell}(c) = 0 \tag{11}$$

because then obviously

$$\sum_{\ell=1}^{L} j_\ell = \sum_{\ell=1}^{L} \sum_{k=1}^{L} \mathcal{M}_{k\ell}(c) \nabla \mu_k \\ = \sum_{k=1}^{L} \underbrace{\sum_{\ell=1}^{L} \mathcal{M}_{k\ell}(c)}_{=0} \nabla \mu_k = 0. \tag{12}$$

This ensures the constraint (8) satisfied. Moreover, by the celebrated (Nobel-prize awarded) Onsager's principle (Ons31), the matrix $[\mathcal{M}_{k\ell}(c)]$ should be symmetric. An example (proposed already by de Gennes (dGe80), another Nobel prize winner) is

$$\mathcal{M}_{k\ell}(c) := m_\ell c_\ell \left(\delta_{k\ell} - \frac{m_k c_k}{\sum_{l=1}^{L} m_l c_l} \right) \tag{13}$$

with m_ℓ being "actual" mobilities of particular constituents (assumed to be) known from experiments. It yields

$$\mathcal{D}_{k\ell}(c) = \rho m_\ell \left(\delta_{k\ell} - \frac{m_k c_\ell}{\sum_{l=1}^{L} m_l c_l} \right), \tag{14}$$

$$\mathcal{M}_\ell(c) = m_\ell z_\ell c_\ell - m_\ell c_\ell \frac{\sum_{k=1}^{L} m_k c_k z_k}{\sum_{l=1}^{L} m_l c_l}. \tag{15}$$

Existence of a (very) weak solutions of the system (1)–(6) is proved for a non-Newtonian fluid with $\tau(\cdot, c, \theta)$ having a p-polynomial coercivity with $p > 11/5$. Positive definiteness of $\mathcal{D}(c)$ is employed. Unfortunately, in the case (14), it may fail if the mobilities m_ℓ vary too much but holds if they are not too much mutually different, as shown recently in (Hav07).

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THE NEUMANN PROBLEM FOR HIGHER ORDER ELLIPTIC OPERATORS ON C^1 DOMAINS

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In this talk we present well-posedness results for boundary value problems for the biharmonic equation with Whitney-Sobolev and Whitney-Besov data in VMO_1 domains. These results are obtained through establishing the invertibility of the associated multiple layer potential operators on the aforementioned function spaces.

CARLEMAN ESTIMATES AND THEIR APPLICATIONS TO ELASTICITY WITH RESIDUAL STRESS

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We derive Carleman type estimates for classical dynamical elasticity system with residual stress. The residual stress is described by general scalar second order operator which makes the system anisotropic. We derive Carleman estimates with second large parameter for general second order operators and use them to get estimates for systems. Applications include exact controllability and global uniqueness and stability of recovery of residual stress from one set of boundary measurements.

CARLEMAN ESTIMATES FOR SOME FIRST-ORDER SYSTEMS OF PARTIAL DIFFERENTIAL EQUATIONS

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Keywords: systems of partial differential equations, Carleman estimates

1. INTRODUCTION

Carleman estimates were developed in order to prove uniqueness for non-hyperbolic Cauchy problems for operators with non-analytic coefficients. More recently they have become powerful tools for many problems in the control of partial differential equations. The theory for scalar equations is rather complete, however concerning systems of equations the picture is less clear. The only general result pertaining Carleman estimates for systems of equations is due to Calderón (1).

In this talk we will establish Carleman estimates for certain first order systems. In contrast to previous works (see for example (2),(3) and the references therein) our result does not rely on pseudo-differential operators or diagonalization methods which allows for minimal smoothness assumptions on the coefficients. This is of some significance when considering nonlinear problems. Moreover, the explicit nature of the estimate makes the inclusion of boundary terms possible.

2. THE RESULT

Consider the 4×4 matrix partial differential operator

$$A(x,\partial)u = (\nabla \times u_1 + \nabla u_2, -\nabla \cdot u_1)$$

of first order where $u = (u_1, u_2)$ and u_1 a vector-valued function with three components and u_2 a scalar-valued function. Let $\Omega \subset \mathbf{R}^3$ be an open set and assume that $\psi \in C^2(\overline{\Omega})$ with $\nabla\psi \neq 0$ in $\overline{\Omega}$. Set $\phi = e^{s\psi} - 1$ where $s \geq s_0$.

By elementary methods we will prove the following Carleman estimate. There exist constants τ_0 and C such that for $\tau \geq \tau_0$

$$\tau \int_\Omega e^{2\tau\phi}|u|^2 dx \leq C \int_\Omega e^{2\tau\phi}|A(x,\partial)u|^2 dx$$

for all compactly supported functions $u \in C_0^\infty(\Omega)$.

We will also discuss the case of variable coefficients

$$A_\alpha(x,\partial)u = (\nabla \times u_1 + \alpha\nabla u_2, -\nabla \cdot (\alpha u_1))$$

where $\alpha \in C^1(\overline{\Omega})$ and the dynamic case, i.e. the operator

$$P(x,\partial) = \begin{pmatrix} \partial_t - A(x,\partial) \\ \partial_t + A(x,\partial) \end{pmatrix}$$

acting on a vector-valued function with eight components.

3. APPLICATIONS

We will show that our result for the first-order system can be used to obtain Carleman estimates for the stationary and dynamic system of elasticity. These Carleman estimates will not only bound the displacement vector but also its first-order derivatives.

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NONLINEAR BOUNDARY CONTROL FOR A CLASS OF 1-D NONLINEAR PARABOLIC PDES

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Keywords: boundary control, backstepping, parabolic PDEs

Abstract. *Certain classes of parabolic PDEs that arise in chemical process control include nonlinear Volterra series operators on the right hand sides of the PDEs, with the spatial coordinate as the integration variable. A stabilizing feedback law in the form of a Volterra series will be presented. The kernels of the series are given through a sequence of hyperbolic PDEs on spatial domains of increasing dimension and dependent on the Volterra kernels of the plant nonlinearity. We present a priori estimates for the control kernels, the convergence analysis of the Volterra nonlinear feedback operator, and numerical results for several benchmark nonlinear PDEs.*

1. Introduction

Boundary control of linear parabolic PDEs is a well established subject with extensive literature. On the other hand, boundary control of *nonlinear* parabolic PDEs is still an open problem as far as general classes of systems are concerned.

Our method is a direct infinite dimensional extension of the finite-dimensional feedback linearization/backstepping approaches and employs spatial Volterra series nonlinear operators. We only sketch our method here; a two-part paper [3] has been submitted presenting the method and its properties in full detail, with examples. This result solves open problem 5.1 in the *Unsolved Problems* volume [1].

2. Volterra Series

Volterra series represent general solutions for nonlinear equations and are widely studied in the literature [2]. A (spatial) Volterra series is defined as

$$F[u] = \sum_{n=1}^{\infty} \int_0^x \int_0^{\xi_1} \cdots \int_0^{\xi_{n-1}} f_n(x,\xi_1,\ldots,\xi_n) \left(\prod_{j=1}^{n} u(t,\xi_j) \right) \times d\xi_1 \ldots d\xi_n, \quad (1)$$

where f_n is known as the n-th (triangular) kernel of F.

3. Outline of the Method

We consider the stabilization problem for the plant

$$u_t = u_{xx} + \lambda(x)u + F[u] + uH[u], \quad (2)$$

$$u_x(0,t) = qu(0,t) \quad (3)$$

$$u(1,t) = U(t), \quad (4)$$

where $F[u]$ and $H[u]$ are Volterra series and $U(t)$ the actuation variable. In [3] we show how nonlinear plants found in applications can be written in the form (2)–(4).

We solve the problem by mapping u into a *target system* w which verifies

$$w_t = w_{xx} - cw, \quad (5)$$

$$w_x(0,t) = \bar{q}w(0,t)$$

$$w(1,t) = 0, \quad (6)$$

where $\bar{q} = \max\{0, q\}$. For mapping u into w we use a Volterra transformation

$$w = u - K[u]. \quad (7)$$

In [3] we derive the equations that the kernels k_n of K in (7) verify. It is a set of *linear* hyperbolic PDEs. For each k_n, we get a PDE evolving on a domain of dimension $n+1$ and

with a domain shape in the form of a "hyper-pyramid," $0 \leq \xi_n \leq \xi_{n-1} \ldots \leq \xi_1 \leq x \leq 1$. The equations can be solved recursively, i.e., first for k_1 (which verifies an autonomous equation), then for k_2 (which is coupled with k_1) using the solution for k_1, and so on. We also show in [3] that the Volterra series defined by the k_n's in (7) is always convergent and invertible (at least locally).

Once we have the k_n's, the stabilizing control law is determined by (7) at $x = 1$

$$\begin{aligned} U(t) &= \sum_{n=1}^{\infty} \int_0^1 \int_0^{\xi_1} \cdots \int_0^{\xi_{n-1}} \\ &\quad k_n(1, \xi_1, \ldots, \xi_n) \left(\prod_{j=1}^{n} u(t, \xi_j) \right) \\ &\quad \times d\xi_1 \ldots d\xi_n. \end{aligned} \tag{8}$$

In [3], using the invertibility properties of K and the exponential stability of (5)–(6), we show that the origin of the closed-loop system (2)–(4) with control law (8) is exponentially stable in the L^2 and H^1 norms (at least locally). We also illustrate this result with numerical simulations of several examples of interest.

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Convolution/Evolution Equations-Representation Theory

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Abstract. The convolution-evolution (semigroup) equation in a Hilbert space:

$$\dot{Y}(t) = AY(t) + \int_0^t L(t-\sigma)\dot{Y}(\sigma)d\sigma, \quad t \geq 0$$

abstracts the dynamics of a flexible structure under inviscid subsonic aerodynamic loading – the core of Aeroelasticity Theory. Our main result is to show that by enhancing the Hilbert space it is possible to construct a pure semigroup equation leading to the representation

$$\dot{Z}(t) = \mathcal{A}_C Z(t)$$
$$Y(t) = PZ(t)$$

where $\mathcal{A}_C$ is the generator of a C_0-semigroup over a Banach space, and P is a projection. In particular the aeroelastic modes can thus be identified as bonafide eigenvalues of the generator $\mathcal{A}_C$. We actually give a construction for the semigroup generated by $\mathcal{A}_C$ as well as for the resolvent.

REGULARIZING EFFECTS OF NONLINEAR DAMPING IN SUPERCRITICAL DEFOCUSING NONLINEAR WAVE EQUATIONS

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There are many results on global well-posedness and regularity for the equation $u_{tt}-\Delta u+u^5=0$ in R^3 (the so-called critical case). In contrast, the global existence of smooth solutions in the supercritical case $p>1+\frac{4}{n-2}$ appears to be an open problem, even for the space dimension $n=3$. We show that semi-linear wave equations with a conveniently chosen nonlinear damping $g(u_t)$ and with defocusing smooth nonlinearlities $|u|^{p-1}u$ in the supercritical case $p>5$ are globally well-posed in radially symmetric Sobolev spaces $H^k_{rad}(R^3)\times H^{k-1}_{rad}(R^3)$ for all integers $k\geq 3$. The results apply to the case $k=2$ without the requirement of radial data. We emphasize that the damping is not stronger than the nonlinearity and does not depend on the supercritical growth of the nonlinearity. The results also extend to certain exponential nonlinearities. Finally, we obtain scattering results for radial initial data in Sobolev spaces with $k\geq 2$.

UNIFORM STABILIZATION OF THE WAVE EQUATION ON COMPACT SURFACES AND LOCALLY DISTRIBUTED DAMPING

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Abstract. This work is concerned with the study of the wave equation on compact surfaces and locally distributed damping, described by

$$u_{tt} - \Delta_{\mathcal{M}} u + a(x)\, g(u_t) = 0 \quad \text{on } \mathcal{M} \times]0, \infty[\,,$$

where $\mathcal{M} \subset \mathbb{R}^3$ is an oriented embedded compact surface without boundary, such that $\mathcal{M} = \mathcal{M}_0 \cup \mathcal{M}_1$, where

$$\mathcal{M}_1 := \{x \in \mathcal{M}; m(x) \cdot \nu(x) > 0\} \text{ and } \mathcal{M}_0 = \mathcal{M} \backslash \mathcal{M}_1.$$

Here, $m(x) := x - x^0$, ($x^0 \in \mathbb{R}^3$ fixed) and ν is the exterior unit normal vector field of $\mathcal{M}$.

For $i = 1, \ldots, k$, assume that there exist open subsets $\mathcal{M}_{0i} \subset \mathcal{M}_0$ of $\mathcal{M}$ such that they are umbilical, or more generally, that the principal curvatures k_1 and k_2 satisfy $|k_1(x) - k_2(x)| < \varepsilon_i$ (ε_i considered small enough) for all $x \in \mathcal{M}_{0i}$. Moreover suppose that the *mean curvature* H of each $\mathcal{M}_{0i}$ is *non-positive* (i.e. $H \leq 0$ on $\mathcal{M}_{0i}$ for every $i = 1, \ldots, k$). If $a(x) \geq a_0 > 0$ on an open subset $\mathcal{M}_* \subset \mathcal{M}$ that contains $\mathcal{M} \backslash \cup_{i=1}^{k} \mathcal{M}_{0i}$ and if g is a monotonic increasing function such that $k|s| \leq |g(s)| \leq K|s|$ for all $|s| \geq 1$, then uniform decay rates of the energy holds.

SYSTEMS OF NONLINEAR WAVE EQUATIONS WITH DAMPING AND SOURCE TERMS

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Keywords: wave equations, damping and source terms, weak solutions, blow-up of solutions

In this talk we consider systems of wave equations where one of the nonlinearities act as a dissipative term (which can be degenerate) and the other acts as a strong source. Under some conditions on the parameters in the system we obtain several results on the existence of local and global solutions, uniqueness, and blow up of solutions.

ON EXISTENCE, UNIFORM DECAY RATES AND BLOW UP FOR SOLUTIONS OF THE 2-D WAVE EQUATION WITH EXPONENTIAL SOURCE

MARCELO M. CAVALCANTI

Abstract. This work is concerned with the study of the nonlinear damped wave equation

$$u_{tt} - \Delta u + h(u_t) = g(u) \qquad \text{in } \Omega \times]0, \infty[\,,$$

where Ω is a bounded domain of $\mathbb{R}^2$ having a smooth boundary $\partial\Omega = \Gamma$.

Assuming that g is a function which admits *exponential growth at the infinity* and, in addition, that h is a monotonic continuous increasing function with polynomial growth at the infinity, we prove both: global existence as well as blow up of solutions in finite time, by taking the initial data inside the potential well. Moreover, optimal and uniform decay rates of the energy are proved for global solutions.

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Verification theorem and construction of ϵ-optimal controls for control of abstract evolution equations

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Keywords: optimal control of PDE, verification theorem, dynamic programming, ϵ-optimal controls, Hamilton-Jacobi-Bellman equations

1. Introduction

We are concerned with an optimal control problem for abstract evolution equations, including a class of semilinear partial differential equations. More precisely our control problem has the state equation

$$\begin{cases} \dfrac{dx(t)}{dt} = Ax(t) + b(t, x(t), u(t)), \\ x(0) = x, \end{cases}$$

where A is a linear, densely defined maximal dissipative operator in a real separable Hilbert space H, and we want to minimize a cost functional of the form

$$J(y; u(\cdot)) = \int_0^T L(t, x(t), u(t))\, dt + h(x(T))$$

over all controls $u(\cdot) : [0, T] \to U$, where U is a metric space. We will discuss two aspects of the dynamic programming approach to the above optimal control problem. One is a viscosity solution based verification theorem which provides sufficient conditions for optimality. The other is sub- and superoptimality principles of dynamic programming whose proofs give an explicit construction of ϵ-optimal controls.

2. Verification theorem

The verification theorem we present is an infinite dimensional version of such a result for finite dimensional problems obtained in [5]. It gives a sufficient conditions for optimality stated in an integral form. The theorem is based on the notion of viscosity solution, the Hamilton-Jacobi-Bellman equation associated with the problem, and an appropriate notion of superdifferential which is linked to the test functions used in the definition of viscosity solution. Other related results in this direction have been obtained before in [1,2].

3. Construction of ϵ-optimal controls

The construction of ϵ-optimal controls is a fairly explicit procedure which relies on the proof of superoptimality inequality of dynamic programming for viscosity supersolutions of the corresponding Hamilton-Jacobi-Bellman equation. It is a delicate generalization of such a method for the finite dimensional case from [4]. Similar method has been used in [3] to construct stabilizing feedbacks for nonlinear systems. The main idea of the method is to approximate the value function by its appropriate inf-convolution which is more regular and satisfies a slightly perturbed HJB inequality pointwise. One can then use this inequality to construct ϵ-optimal piecewise constant controls. This procedure in fact gives the superoptimality inequality of dynamic programming and the suboptimality inequality can be proved similarly.

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A Coupled Parabolic-Hyperbolic PDE system Arising in Fluid-Structure Interaction

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Abstract

This presentation will deal with several problems: (i) semigroup well-posedness in the natural energy space with explicit generator; (ii) spectral properties of the generator; (iii) strong stability; (iv) uniform stabilization under dissipation at the interface. This is joint work with George Avalos.

HEAT AND SCHRÖDINGER EQUATIONS: BOUNDARY CONTROL IN ONE SHOT

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Keywords: null boundary control,Ovcyannikov Theorem, Schrödinger equation

We discuss the null boundary controllability of the heat and Schrödinger equations with a potential. The unified approach applies not just to both of these PDEs, but also to a one-parameter family of PDEs that they belong to.

We consider:

$$e^{i\zeta}\frac{\partial u}{\partial t}(x,t) = \frac{1}{2}\Delta u(x,t) - V(x)u(x,t) \quad (1)$$

$$u(x,0) = u_0(x),\ x \in \Omega, \quad (2)$$

$$u(x,t) = g(x,t),\ x \in \partial\Omega, \quad (3)$$

where $\zeta \in [-\pi/2, 0]$ is a constant, $\Omega \subset \mathbb{R}^N$ is a bounded domain, and g is a boundary control function. We are interested in the null boundary controllability of the heat and Schrödinger equations, which are obtained with $\zeta = 0, -\pi/2$ respectively, but our analysis applies for all $\zeta \in [-\pi/2, 0]$.

Of course the heat and Schrödinger equations are important in their own right, but to some extent (1) is a model system in the sense that the method we use should apply to an equation obtained by replacing the right-hand-side of (1) by an elliptic operator with variable coefficients. The main assumption that we require on the coefficients is that they be analytic in $\mathbb{R}^N$, and that is what we assume about the potential $V(x)$. As this is the first time that we have applied this particular method to a problem in more than one space dimension, it seemed to us that the PDE (1) is a good place to start; it illustrates the method without the burden of some tedious estimates that the general case would require and yet the problem is rich enough to show how the method may be applied in the general case.

As an example of the kind of controllability result that may be obtained by the use of this method, we state the following theorem, which we prove.

Theorem *Suppose that the potential V satisfies an analyticity assumption. Let $T > 0$. Then, given $u_0 \in L^2(\Omega)$, we can find a boundary control function g such that $u(x,T) = 0$. Furthermore, for all $\epsilon > 0$,*

$$g \in \begin{cases} C([0,T]);\ H^{1/2-\epsilon}(\partial\Omega), & \zeta = -\frac{\pi}{2}, \\ C([0,T]);\ H^{3/2-\epsilon}(\partial\Omega), & \zeta \in \left(-\frac{\pi}{2}, 0\right]. \end{cases}$$

The proof of the Theorem involves taking a trace on the boundary of Ω and for this some regularity must be assumed for Ω. It is sufficient that $\partial\Omega$ be C^2 (C^1 for the $\zeta = -\frac{\pi}{2}$ Schrödinger case). It is also sufficient that $\overline{\Omega}$ be the C^2 (C^1 for the $\zeta = -\frac{\pi}{2}$ Schrödinger case) diffeomorphic image of a polyhedron P; the diffeomorphism being defined in an open set containing P. In the latter case, the above description of g holds for the deformed faces of the polyhedron. In contrast to the mainstream approach for the Schrödinger equation based on duality, in the present paper we use a method based on a smoothing property to calculate the control functions directly.

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ON A STRUCTURAL ACOUSTIC MODEL WHICH INCORPORATES SHEAR AND THERMAL EFFECTS IN THE STRUCTURAL COMPONENT

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Keywords: structural acoustic model, Reissner-Mindlin plate, thermal effects, shear effects, uniform stabilization, feedback boundary controls

1. STATEMENT OF THE PROBLEM

There is an extensive literature on structural acoustic models. Pioneering contributions are due to Avalos, Lasiecka and Lebiedzik (see e.g. [1],[4][5],[6]). These models in which the interaction between an acoustic medium, e.g. a gas and an elastic medium, which may be a plate which coincides with one flat wall (the interface) of the surface of the chamber containing the gas, is analyzed, are challenging from a mathematical point of view due to their interactive nature which manifests in the coupling of the variables which come into play in the problem. The focus in the mathematical investigations of these models is on the question of stabilizability as well as exact controllability.

Until recently the deflections of the structural component of the structural acoustic model were described by the Euler-Bernoulli equations or the Kirchoff equation to provide for rotational inertia effects in addition to deformation effects, or the Von Karman equations to provide for larger deflections while thermal effects have also been incorporated. The inclusion of these effects is important not only from a physical point of view, but due to the parabolic nature of the uncoupled heat equation, such effects also play a vital role in the stabilization of the energy associated with the models.

Recently a new model was formulated by M. Grobbelaar [2,3] in which the equations for the plate are modified to take account of shear effects over and above displacement and rotational inertia effects in the interface. Thus in the three-dimensional case, i.e. when the acoustic chamber is three-dimensional and the plate two-dimensional, the deflections of the plate are modelled by the Reissner-Mindlin plate equations. This not only yields a model which is more accurate over the whole frequency range, but appropriate when high frequencies of the structural vibrations occur, i.e., when the wave phase length becomes comparable to the thickness parameter, in which case the Euler-Bernoulli equation ceases to be valid. The three-dimensional model is analyzed from the point of view of existence and uniqueness while for the two-dimensional model in which the structural component is a one-dimensional Timoshenko beam, existence and uniqueness as well as uniform stabilization is obtained by incorporating linear feedback boundary controls at the rigid and the flexible walls of the acoustic chamber and at the free end of the beam and using carefully chosen multipliers. Both in the linear and nonlinear cases restrictions on the physical parameters in the problem emanate which turn out to be feasible from a physical point of view.

Further reflection on the problem gives rise to the following question: *Can one, over and above the recently introduced shear variables in the model, introduce another degree of freedom by allowing for temperature variations in the plate, i.e. introducing thermal effects in the Reissner-Mindlin equations for the structural component of the model? Would this also result in a reduction of mechanical damping devices as in*

the case of the classical Kirchoff equation or the Von Karman equations when one wishes to establish uniform stability of the energy associated with the model?

In this talk we propose a model for a three-dimensional structural acoustic model in which the plate is subject to transversal displacement, shear effects and temperature variations and establish conditions for the uniform stabilizability of the structure.

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An Intrinsic Model for Thermoelastic Thin Shells

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Keywords: Shells, Modeling, Thermoelasticity, Stabilization

In view of the control of the thermoelastic thin shells, we consider the problem of modeling a dynamic thin shell with thermal effects, using the coordinate-free intrinsic model introduced by Michel Delfour and Jean-Paul Zolésio (5; 4). The aim of this method is to produce a coordinate free version of the shell equations, in contrast to the classical equations which require explicit representation of the nonconstant coefficients. With the intrinsic approach, one can exploit the underlying geometry of the shell to derive equations in which the nonconstant coefficients are written in the form of tangential operators. This enables us to better modify and apply known techniques that were developed for use in the constant-coefficient case (flat plate models).

In previous work (2; 3; 1) we have developed a linear dynamic model of the thin shell and shown several stability/controllability results. However, as thermal effects are very important in many applications of engineering, we wish to include them in our shell model. We proceed in the development of a (linear) thermoelastic shell model based essentially on similar assumptions to those which are used in the derivation of classical linear thermoelastic plate models (see, e.g. (6)).

As such, we subject the elastically and thermally isotropic shell to an unknown temperature distribution. Eventually this yields a fully-coupled system of four linear equations whose variables are the displacement of the shell midsurface and the thermal stress resultants.

This work continues the development of the model introduced in (7). We will present an improved modeling which improved the way the curvature is taken into account. Wellposdeness will be established.

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Morrey Regularity and Continuity of Minimizers for Asymptotically Convex Integrals

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Keywords: Morrey regularity, asymptotically convex, obstacle problems

1. Introduction

I will present some Morrey regularity results for minimizers of functionals with the general form

$$\mathbf{u} \mapsto \int_{\Omega} g(\mathbf{x}, \mathbf{u}(\mathbf{x}), \boldsymbol{\nabla}\mathbf{u}(\mathbf{x}))\, d\mathbf{x}, \tag{1}$$

where Ω is an open, bounded subset of $\mathbb{R}^n$ and $\mathbf{u} \in W^{1,1}(\Omega;\mathbb{R}^N)$, with $n, N \geq 1$. The primary property that I assume g possesses is that there is a $p \in (1,\infty)$ such that for each $\mathbf{x} \in \mathbb{R}^n$ and each $\mathbf{u} \in \mathbb{R}^N$, the function $\mathbf{F} \mapsto g(\mathbf{x},\mathbf{u},\mathbf{F})$ behaves like $\mathbf{F} \mapsto \|\mathbf{F}\|^p$ whenever $\|\mathbf{F}\|$ is sufficiently large. Integrands with this property are called asymptotically convex.

To make things more precise, let us say that a function $g : \Omega \times \mathbb{R}^N \times \mathbb{R}^{N\times n} \to \mathbb{R}$ is $\mathcal{C}^0$-asymptotically convex if for each $\varepsilon > 0$ and each $(\mathbf{x},\mathbf{u}) \in \Omega \times \mathbb{R}^N$, there exists a $\sigma_\varepsilon(\mathbf{x},\mathbf{u}) < +\infty$ such that

$$\left| g(\mathbf{x},\mathbf{u},\mathbf{F}) - \left(1 + \|\mathbf{F}\|^2\right)^{\frac{p}{2}} \right| < \varepsilon \|\mathbf{F}\|^p, \quad (\mathcal{C}^0\text{-A})$$

whenever $\|\mathbf{F}\| > \sigma_\varepsilon(\mathbf{x},\mathbf{u})$. If $g : \mathbb{R} \to \mathbb{R}$ is given by $g(F) := \left(1 + |F|^2\right)^{\frac{p}{2}} - |F|\chi_{\mathbb{Q}}$, where $\chi_{\mathbb{Q}}$ is the characteristic function for the set of rational numbers, then we see that g is $\mathcal{C}^0$-asymptotically convex with $\sigma_\varepsilon = \varepsilon^{-\frac{1}{p-1}}$, yet g is nowhere convex. Nevertheless, one can show that a $\mathcal{C}^0$-asymptotically convex function does, in some sense, behave like a convex function at infinity. Our regularity results apply to a minimizer, provided one exists, for functionals of the general form (1), provided that g is $\mathcal{C}^0$-asymptotically convex and the function $(\mathbf{x},\mathbf{u}) \mapsto \sigma_\varepsilon(\mathbf{x},\mathbf{u})$ satisfies some growth and regularity conditions.

2. Statement of Result

The statements for the main results are given in terms of a generalized notion of an almost minimizer and are fairly technical, so I present an application which conveys an idea of the content of the main results while reducing the technicalities. In the following, I use $L^{p,\kappa}$ to denote a Morrey space and $\mathscr{L}^{p,\kappa}$ to denote a Companato space.

Theorem 1 *Let $0 \leq \kappa < n$, $0 \leq s < r < +\infty$ and $1 < q < +\infty$ be given. Let $\alpha \in L^{1,\kappa}(\Omega)$ be given. Suppose that there is a $\lambda \geq 0$ such that $h : \Omega \times \mathbb{R}^N \times \mathbb{R}^{N\times n} \to \mathbb{R}$ satisfies*

$$|h(\mathbf{x},\mathbf{u},\mathbf{F})| \leq \alpha(\mathbf{x}) + \lambda\|\mathbf{u}\|^r + \|\mathbf{F}\|^q,$$

for each $(\mathbf{x},\mathbf{u},\mathbf{F}) \in \Omega \times \mathbb{R}^N \times \mathbb{R}^{N\times n}$. Let $\delta > 0$ and $p > \max\left\{q, \frac{nr}{n+r}\right\}$ be given. Define the functional $J : W^{1,1}(\Omega;\mathbb{R}^N) \to \overline{\mathbb{R}}$ by

$$J[\mathbf{u}] := \int_{\Omega} \left\{ \delta \left(1 + \|\boldsymbol{\nabla}\mathbf{u}(\mathbf{x})\|^2\right)^{\frac{p}{2}} + h(\mathbf{x},\mathbf{u}(\mathbf{x}),\boldsymbol{\nabla}\mathbf{u}(\mathbf{x})) \right\} d\mathbf{x}.$$

We have the following: If $\mathbf{u} \in W^{1,p}_{\text{loc}}(\Omega;\mathbb{R}^N)$ is a local minimizer for J; i.e. $J[\mathbf{u}] \leq J[\mathbf{u}+\boldsymbol{\varphi}]$, for each $\boldsymbol{\varphi} \in W^{1,p}(\Omega;\mathbb{R}^N)$ with $\operatorname{supp}(\boldsymbol{\varphi}) \subset\subset \Omega$; then $\boldsymbol{\nabla}\mathbf{u} \in L^{p,\kappa}_{\text{loc}}(\Omega;\mathbb{R}^{N\times n})$ and $\mathbf{u} \in \mathscr{L}^{p,p+\kappa}_{\text{loc}}(\Omega;\mathbb{R}^N)$.

This result actually holds up to the boundary provided that $\partial\Omega$ and the boundary conditions are sufficiently smooth. It also holds for certain variational problems with sufficiently smooth obstacles. It is also possible to allow the coefficient δ to be a continuous function that is uniformly positive in Ω.

3. Conclusion

To conclude, I make a few comments about the implications of the above result to the broader endeavor of establishing a lower-order regularity theory for variational problems. Until recently, results for such a theory have been for the most part unavailable (see (2) for a discussion). As demonstrated by V. Šverák & X. Yan (3), even if an integrand $h \in \mathcal{C}^\infty(\mathbb{R}^{N\times n})$ is strictly convex and has a uniformly bounded Hessian, a minimizer for the functional $\mathbf{u} \mapsto \int_\Omega h(\boldsymbol{\nabla}\mathbf{u}(\mathbf{x}))\, d\mathbf{x}$ can be unbounded at an interior point in Ω. Thus without additional assumptions on h, one can not expect everywhere regularity for a minimizer. In (1), M. Foss & G. Mingione showed that if $h \in \mathcal{C}^0(\Omega \times \mathbb{R}^N \times \mathbb{R}^{N\times n})$ is quasiconvex and possesses some additional growth and continuity properties with respect to its third argument, then a minimizer for the functional

$$\mathbf{u} \mapsto \int\limits_\Omega h(\mathbf{x}, \mathbf{u}, \boldsymbol{\nabla}\mathbf{u}(\mathbf{x}))\, d\mathbf{x} \tag{2}$$

is partially continuous; i.e. continuous on an open subset of Ω with full measure. Since $\mathscr{L}^{p,p+\kappa} \subset \mathcal{C}^{0,1-\frac{n-\kappa}{p}}$ whenever $p+\kappa > n$, Theorem 1 shows that for each $\delta > 0$ minimizers for the functional

$$\mathbf{u} \mapsto \int\limits_\Omega \Big\{ \delta \left(1 + \|\boldsymbol{\nabla}\mathbf{u}(\mathbf{x})\|^2\right)^{\frac{p}{2}} + h(\mathbf{x}, \mathbf{u}(\mathbf{x}), \boldsymbol{\nabla}\mathbf{u}(\mathbf{x})) \Big\}\, d\mathbf{x} \tag{3}$$

must be everywhere continuous, provided that $p > \max\left\{q, \frac{nr}{n+r}, n-\kappa\right\}$. This result only requires h to satisfy some very mild growth conditions. Thus $\delta \left(1 + \|\boldsymbol{\nabla}\mathbf{u}(\mathbf{x})\|^2\right)^{\frac{p}{2}}$ serves as a rather robust regularizing term. It would be interesting to discover if it is possible to obtain information about the lower-order regularity of a minimizer for the functional in (2) by approximating it using minimizers for functionals of the form (3) and the regularity provided by Theorem 1.

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FINITE DIMENSIONAL AND SMOOTH ATTRACTORS ARISING IN WAVE DYNAMICS WITH BOUNDARY DISSIPATION AND SOURCES OF CRITICAL EXPONENTS

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Recent developments in the area of long time behavior of nonlinear hyperbolic flows will be presented. These include issues such as existence of global attractors, their smoothness and dimensionality. One of the difficulties arising in the analysis of attractors for hyperbolic flows is the lack of smoothing mechanism generated by the free dynamics (unlike parabolic flows). In addition, instability in the hyperbolic dynamics is intrinsincly an infinite-dimensional phenomenon. This, in particular, implies that the dissipation needed to ensure an existence of bounded absorbing sets can not be compact. Consequently, hyperbolic models with nonlinear dissipation require rather subtle analysis that is necessary in order to determine long time behavior of the underlying dynamics. One of the canonical example is classical wave equation with nonlinear dissipation and source of critical exponent. Non-compactness of the source, along with nonlinearity of the dissipation, renders the known techniques no longer applicable.

The goal of this talk is to present an intrinsic theory of long time behavior corresponding to hyperbolic-like flows with critical sources and nonlinear (critical) dissipation. This will be largely based on recent results presented in [1] below.

We shall first formulate several theorems stating abstract PDE inequalities that need to be established for proving results on attractors. These conditions will be shown much weaker than conditions resulting from up-to-date theories on dissipative systems. We shall show next how the above referred conditions relate to "inverse-observability" type of inequalities that have been recently studied in the context of control theory. However, the needed inverse inequalities must be established not for a single trajectory (as in the case of controllability or stabilization), but for a family of trajectories trajectories. This leads to additional and substantial technicalities which are dealt with by resorting to Carleman's estimates.

The general theory will be applied to semilinear wave equation with a nonlinear boundary damping and source of critical exponent. The ultimate results (see [2]) provide existence of finite-dimensional attractors which are, in addition, "smooth". Thus, the results obtained demonstrate finite dimensional and ultimately smooth long time behavior of a hyperbolic flow with geometrically constrained damping and critical nonlinearity.

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Decay Rates for Wave Equations with Linear Damping and Variable Coefficients

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Keywords: wave equation with variable coefficients, weak dissipation, decay rates, multiplier method

1. THE CAUCHY PROBLEM

The authors establish decay rates for the energy associated with the Cauchy problem

$$\begin{cases} u_{tt} - \text{div}(b(x)\nabla u) + a(x)u_t = 0, \\ u(0,x) = u_0(x), \quad u_t(0,x) = u_1(x), \end{cases} \tag{1}$$

where $x \in \mathbf{R}^n$, $t > 0$ and a and b are positive C^1 functions. For simplicity we work with compactly supported initial data $u_0 \in H^1(\mathbf{R}^n)$, $u_1 \in L^2(\mathbf{R}^n)$

$$u_0(x) \text{ and } u_1(x) = 0 \text{ for } |x| > R.$$

It is well known that (1) admits a unique weak solution u with the regularity

$$u \in C((0,\infty), H^1(\mathbf{R}^n)), \quad u_t \in C((0,\infty), L^2(\mathbf{R}^n)).$$

The main quantities of interest are the L^2 norm and energy associated with u :

$$\int u^2 dx \quad \text{and} \quad \int (u_t^2 + b(x)|\nabla u|^2)\, dx,$$

respectively. Hence the energy is a non-increasing function of t. It is a natural question whether the energy decays to zero as t goes to infinity and if so, how fast it decays.

Although there is a vast literature on the study of decay rates for damped wave equations, very little work has been done in the case when the Laplacian is replaced by an elliptic operator with variable coefficients. In (1) Ikehata analyzes the wave equation with variable coefficients in the exterior of a star-shaped domain in the more restrictive setting where $a \equiv 0$ and b behaves like a constant at infinity.

Our results employ a multiplier method first developed by Todorova and Yordanov in (2).

2. THE MULTIPLIER METHOD

Fourier analysis is a powerful tool when the potential $a = a(t)$ is a function of time and has been used by many authors (see [W1], [W2], [R]). When $a = a(x)$ Fourier techniques become cumbersome as they involve localizations in both frequency space and extended phase space $(0,\infty) \times \mathbf{R}^n$. A simple alternative is the multiplier method. In general multiplier techniques yield weaker decay estimates than Fourier techniques whenever the latter can be applied to (1). We can strengthen the multiplier method for (1) by factoring out an asymptotic profile ϕ for u and working with $\phi^{-1}u$. This quotient will admit more precise estimates since it will vary relatively slowly. Unexpectedly ϕ is allowed to be an approximate solution of

$$a(x)\phi_t - \text{div}(b(x)\nabla\phi) = 0, \quad x \in \mathbf{R}^n, \quad t > 0.$$

The decay rate of u will be expressed in terms of ϕ and, implicitly, in terms of a and b.

The construction of the multipliers uses subsolutions of the equation

$$\text{div}(b(x)\nabla A(x)) = a(x), \quad x \in \mathbf{R}^n. \tag{2}$$

Assuming that a behaves like $|x|^{-\alpha}$ and b behaves like $|x|^{\beta}$ as $|x| \to \infty$, we require that A

should also satisfy with the following properties:

$$(a1) \qquad A(x) \geq 0 \ \text{ for all } \ x,$$
$$(a2) \qquad A(x) = O(|x|^{2-\alpha-\beta}) \ \text{ for large } \ |x|,$$
$$(a3) \qquad m(a) = \liminf_{x\to\infty} \frac{a(x)A(x)}{b(x)|\nabla A(x)|^2} \ > \ 0.$$

We show that such subsolutions $A(x)$ can be explicitly constructed in many cases, including for radial coefficients $a(x)$ and $b(x)$.

3. THE MAIN RESULT

Theorem 1 *Assume that* $0 \leq \alpha < n, 0 \leq \beta < 2$ *and (a1)–(a3) hold. Then for every* $\delta > 0$ *the solution of (1) satisfies*

$$\int e^{(m(a)-\delta)\frac{A(x)}{t}} a(x)u^2 \, dx$$
$$\leq C_\delta(\|\sqrt{b(x)}\nabla u_0\|_{L^2}^2 + \|u_1\|_{L^2}^2)t^{\delta-m(a)},$$
$$\int e^{(m(a)-\delta)\frac{A(x)}{t}} (u_t^2 + b(x)|\nabla u|^2) \, dx$$
$$\leq C_\delta(\|\sqrt{b(x)}\nabla u_0\|_{L^2}^2 + \|u_1\|_{L^2}^2)t^{\delta-m(a)-1}$$

for all $t \geq 1$. *The constant* C_δ *depends also on* R, a, *and* n.

Hence $m(a)$ determines the decay rate and $A(x)$ determines the actual support of solutions. (Solutions decay exponentially in the region $A(x) > t$.) Moreover, $m(a)$ is invariant under scaling $a \mapsto Ca$. Definition $(a3)$ shows that $m(a)$ is determined by the behavior of $a(x)$ as $|x| \to \infty$.

4. CONCLUSIONS

The multiplier method remains a powerful tool in establishing estimates for equations with variable coefficients. This has been successfully used even for nonlinear wave equations (see (3)) since the multipliers are determined by expected asymptotic profile of solutions rather than the invariance of the wave operator. We believe that this method could be successfully applied even for wave equations with time dependent coefficients a and b.

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EXACT GLOBAL CONTROLLABILITY OF SEMILINEAR THERMOELASTIC SYSTEMS

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Results of exact controllability will be reported for a semilinear thermoelastic system, with control placed in either the mechanical or thermal equation. The controlled partial differential equation (PDE) model will be considered in two cases: (i) rotational forces are present in the PDE, in which case, the underlying dynamics evince hyperbolic behavior; (ii) the rotational inertia parameter is absent, in which case the PDE is of parabolic-like (analytic) character.

Shape Derivative in Maxwell System by Hidden Regularity

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Keywords: Shape derivative, Hiden regularity, Saddle point

1. Introduction

The shape sensitivity analysis for hyperbolic problems yields some specific complications due to the hyperbolic regularity, or the lack thereof.

In previous works we investigated the wave equation and came up with some shape sensitivity results. In this paper we investigate sensitivity of the solutions to the Maxwell equation with respect to the shape of the domain. We explicit a derivative with respect to a deformation parameter. The transport of the free divergence property requires a specific shape different quotient that is not necessary in the scalar case. The hyperbolic situation needs a sharp analysis due to the specific complications related to the solutions regularity at the boundary.

In (1) and (2) we announced some results concerning the case with right hand side in L^2 and Dirichlet boundary condition when the data is the restriction of a function defined on the entire space. This important case of the wave equation with the right hand side in L^2 and Dirichlet boundary which is part of the control theory framework, yields a solution that does not have a *material derivative*, while the formal calculus leads to a wave problem for the *shape derivative* which "survives" (*i.e.* has a solution) due to the so call hidden regularity described in (3)

We prove that the shape derivative exists in a weak sense while the material one does not, and this is a new situation which captures the boundary hidden regularity as a profit for the shape derivative which mainly depends on the solution at the boundary. We present an exhaustive analysis of the scalar wave equation with general coefficients being time depending. In order to recover sharp quantifications in the hidden regularity properties we extend the *extractor* technique introduced in (4).

2. Maxwell System

We consider a bounded domain D in R^3 and a family O_k of open connected domains Ω in D whose boundary $\Gamma = \partial\Omega$ is a C^k manifold oriented by the unitary normal field n outgoing to Ω. Throughout this paper we assume $k \geq 2$.

We suppose that Ω is occupied by an electromagnetic medium of constant electric permittivity ε and constant magnetic permeability μ. We suppose the electrical charge density and the current density in Ω are zero.

Let T be a non negative real and $I = [0, T]$ be the *time interval*. We note

$$Q =]0; T[\times\Omega$$

the *cylindrical evolution domain* and

$$\Sigma =]0, T[\times\Gamma$$

the *lateral boundary* associated to any element Ω of the family O_k.

Let $E(t, x)$ and $H(t, x)$ denote the electric field and magnetic fields, respectively, at a point $x \in \Omega$ and a time $t \geq 0$. They satisfy the Maxwell's equations

$$\varepsilon\partial_t E - curl H = 0 \quad \text{on} \quad Q \tag{1}$$

$$\mu\partial_t H + curl E = 0 \quad \text{on} \quad Q \tag{2}$$

$$div(E) = div(H) = 0 \quad \text{on} \quad Q \tag{3}$$

$$H \times n = 0 \quad \text{on} \quad \Sigma \tag{4}$$

$$E(0) = E_0 \quad \text{on} \quad \Omega \tag{5}$$

$$H(0) = H_0 \quad \text{on} \quad \Omega \tag{6}$$

3. Shape Differentiation

Let S be a non-negative real number and E_k be the set of $V \in C([0, S]; C^k(D, R^3))$ with $V \cdot n_{\partial D} = 0$. For any $V \in \mathcal{E}_k$ we consider the flow

mapping $T_s(V)$. At the point x, V has the form as follows:

$$V(s)(x) = \left(\frac{\partial}{\partial s} T_s\right) \circ T_s^{-1}(x)$$

Such transformations were studied in (5) and (6) where a full analysis of the situation was given.

The family $\mathcal{O}_k$ is stable under the perturbations We denote by $Q_s =]0;T[\times\Omega_s(V)$ the *perturbed cylinder*, $\Gamma_s = \partial\Omega_s$ and $\Sigma_s =]0,T[\times\Gamma_s$ the *perturbed lateral boundary*. We consider a map defined on the family $\mathcal{O}_k$

$$\mathcal{O}_k \to \bigcup_{\Omega\in\mathcal{O}_k} (\mathcal{L}^2(Q)\times\mathcal{L}^2(Q))$$

To each element $\Omega \in \mathcal{O}_k$ we associate the solution $(E,H) = (E(\Omega), H(\Omega))$ of the Maxwell's equations described above. For any $V \in \mathcal{E}_k$ and $s \in [0;S]$ we set $E_s = E(\Omega_s) \in \mathcal{L}^2(Q_s)$ and $H_s = H(\Omega_s) \in \mathcal{L}^2(Q_s)$. The mapping $\Omega \mapsto E(\Omega)$ is said to be *shape differentiable in* $L^2(I, H^m(D))$

$$\exists \bar{E} \in C^1([0;S], L^2(I, \mathcal{H}^m(D)))$$

$$\bar{E}(s,\cdot,\cdot)\big|_{Q_s} = E(\Omega_s)$$

then $\partial_s \bar{E}(0,\cdot,\cdot)\big|_Q$ which is the restriction to Q of the derivative with respect to the perturbation parameter s at $s=0$ is independent of the choice of $\bar{E}$. The *shape derivative* is this unique element

$$E'(\Omega;V) = \left(\frac{\partial}{\partial s}\bar{E}\right)\Big|_{s=0\ (t,x)\in Q} \in L^2(I,\mathcal{L}^2(\Omega))$$

The element $\dot{E}(\Omega;V)$ is the *material derivative* of E in $L^2(I,\mathcal{H}^m(D))$ if it is the limit in $L^2(I,\mathcal{H}^m(D))$ of

$$\frac{1}{s}\left(E(\Omega_s)\circ T_s - E(\Omega)\right)$$

when s tends to 0

4. Main Results

We assume $E_0 \in J_n^*(\Omega)$ and $H_0 \in J_t^*(\Omega)$. The solution to the Maxwell's equations is weakly shape differentiable in $H(curl,\Omega)$, furthermore the shape derivative is solution to

$$\varepsilon\partial_t E' - curl H' = 0 \quad \text{on} \quad Q \qquad (7)$$

$$\mu\partial_t H' + curl E' = 0 \quad \text{on} \quad Q \qquad (8)$$

$$div(E') = 0 \quad \text{on} \quad Q \qquad (9)$$

$$div(H') = 0 \quad \text{on} \quad Q \qquad (10)$$

$$H'\times n = [V(0),H]\times n \quad \text{on} \quad \Sigma \qquad (11)$$

$$E'(0) = 0 \quad \text{on} \quad \Omega \qquad (12)$$

$$H'(0) = 0 \quad \text{on} \quad \Omega \qquad (13)$$

where $[\cdot,\cdot]$ stands for the Lie brackets. Let

$$W(s) = \frac{1}{2} K_s n\cdot n \| {}^*DT_s^{-1} n\|^{-1} DT_s^{-1} V(s)\circ T_s$$

then

$$\bar{h}(s) = \int_Q f_s'\circ T_s \Lambda^s \, dx\, dt$$

$$+\int_\Sigma \left(\left[\frac{\partial(y^s+\Lambda^s)}{\partial n}\right]^2 - \left[\frac{\partial y^s}{\partial n}\right]^2 - \left[\frac{\partial \Lambda^s}{\partial n}\right]^2\right)$$

$$W(s)\cdot n d\Gamma\, dt$$

Each of these positive three terms are treated via the extractor technique in the Maxwell system.

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Tubes and Saddle Point Analysis

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Keywords: Uniqueness, transport equation, saddle point, density

1. Eulerian Tubes Analysis

For any smooth vector field $\in {}^1(0\ \tau\ {}^{1,\infty}(\ {}^N))$, verifying a " - bilateral viability" condition, say $\ = 0$ on , the flow mapping ${}_t(\ )$ maps smoothly the set onto itself. Let be given two real numbers $(\ )$, $1\ \ \leq \infty$, $1 \leq\ \ \infty$, and the linear space for speed vector fields:

$$\mathcal{E}^{p,q} = \{\ \ \in\ {}^p(0\ \tau\ {}^q(\ \ {}^N))$$
$$:\ \ \ \in\ {}^p(0\ \tau\ {}^q(\ \ ))$$
$$= 0 \text{ in } {}^{-1,1}(\ \ )\ \}$$

$$\phi(0) = \phi_0\ \ -\phi + \nabla\phi\ \ = \qquad (1)$$

$$\psi(0) = \psi_0\ \ -\psi +\ \ (\psi\ \ ) = \qquad (2)$$

Proposition 1.1 *(Galerkine method, (5) (8)). Assume*

$$\in \mathcal{E}^{2,2}\ (\ \ )^+ \in\ {}^1(0\ \tau\ {}^\infty(\ \ ))$$

then (1) has solutions

$$\phi \in\ {}^\infty(0\ \tau\ {}^2(\ \ )) \cap\ {}^1(0\ \tau\ {}^{-1}(\ \ ))$$

If $(\ \ )^- \in {}^1(0\ \tau\ {}^\infty(\ \ ))$ *then (2) has solutions*

$$\psi \in\ {}^\infty(0\ \tau\ {}^2(\ \ )) \cap\ {}^1(0\ \tau\ {}^{-1}(\ \ ))$$

The first idea would be to consider $\ \in {}^1(0\ \tau\ {}^\infty(\ \ ))$. Then both problems have solutions. They are, formerly, adjoints problems one an other then we could be tempted to conclude for uniqueness to both problems. That argument does not apply as one of the two solutions ϕ or ψ should be smooth in order to be "put in duality". Then under previous poor regularity on we will not get existence nor uniquiness for shape convection problem 3:

$$\ (0) = \ {}_{\Omega_0}\ \ -\ \ + \nabla\ \ \ = 0\ \ \ = {}^2 \qquad (3)$$

1.1. Saddle point

we consider a vector fields in $\mathcal{E}^{2,2}$ and any function $\in {}^\infty(\ \ )$. We consider the Lagrangian "Tube Energy" functional in the form

$$\mathcal{L}_V(\ \ \phi) = \int_0^\tau \int_D \{\ 1\ 2\ \ {}^2$$
$$+\ \ (-\phi +\ \ (\phi\ \ ))\} \qquad - \int_{\Omega_0} \phi(0)$$
$$\mathcal{H}_V\ = \{\ \phi \in\ {}^2(0\ \tau\ {}^2(\ \ ))$$
$$-\phi +\ \ (\phi\ \ ) \in\ {}^2(\ \times\ \ )\ \ \phi(\tau) = 0\}$$

$\mathcal{U}_V\ =\ {}^2(\ \times\ \ )$. The Lagrangian $\mathcal{L}_V$ is concave-convex on $\mathcal{U}_V \times \mathcal{H}_V$ Saddle points $(\xi\ \lambda)$ are solution to the system composed of equation 1 (with $\Phi_0 = \chi_{\Omega_0}\ \ = 0$) and the following backward "adjoint equation"

$$-\lambda +\ \ (\lambda\ \ ) =\ -\xi_V \qquad \lambda(\tau) = 0 \quad (4)$$

The converse is true when we have an extra density condition on and .

Assumption on V:

$$\{\phi \in\ \ {}^\infty(\ \times\ \ ) \cap \mathcal{E}^{2,2}\ \} \text{ is dense in } \mathcal{H}_V \quad (5)$$

That weakly coupled system 1, 4 posesses solutions when $(\ \ )^+ \in {}^1(\ \ {}^\infty(\ \ ))$. We derive the following uniquiness results for the convection problem 1:

Proposition 1.2 *Assume* $\in \mathcal{E}^{2,2}$*, verifying (5) and* $(\ \ )^+ \in {}^1(\ \ {}^\infty(\ \ ))$*. Then, with* $= 0$ *and* $\Phi_0 = \chi_{\Omega_0}$ *(convection problem), or more generally* $\Phi_0 \in {}^\infty(\ \ )$*, the problem 1 posesses a unique solution* ${}_V$ *verifying*

$$0 \leq\ {}_V \leq 1 \qquad (\ \ ) \in\ \times$$

or (in the more general setting)

$$\ \ \ \Phi_0 \leq\ {}_V \leq\ \ \ \Phi_0$$

We have the monotony : $\Omega_0^1 \subset \Omega_0^2$ *(or, in the more general setting* $\Phi_0^1 \leq \Phi_0^2$ *) implies* $_V^1 \leq {}_V^2$.

Proof : from the strong assumption 5 the set of saddlepoints is not empty and is completely characterized by the system 1-4. let us denote by $\mathcal{S}_V$ the set of saddle points. We know that it can be written as $\mathcal{S}_V = {}_V \times {}_V$, which means that if $({}^i \lambda^i)$ $= 1\ 2$ are saddle points then ${}^1 \lambda^2$ and ${}^2 \lambda^1$ are also saddle points. We derive that equation 4 with right hand side ^{i} has solutions and we derive uniquiness of ${}_V$ (from the fact that 0), single element in ${}_V$ (in other words ${}_V$ is reduced to a single element ${}_V$). From uniquiness we know that $0 \leq \leq 1$. From (6) the density assumption is true when verifies some regularity ($\in {}^2($ $($ ${}^N)$... see (11)). Using the rank one theorem of Alberti for the jacobian of BV vector field Ambrosio builts a mollifier sequence ρ_n such that te "commutator term"

$$_n := (\rho_n * \nabla\phi) \quad -\rho_n * (\nabla\phi \quad) \rightarrow 0 \rightarrow 0 \text{in} \quad {}^2$$

an then the density (5) is classiquely derived. (Indeed P.L. Lions and Di Perna (7) obtained this results 14 years before with more regularity on the field $\in {}^2(0\ \tau \quad {}^{1,1}($ ${}^N))$). It is interesting that this result was associated with ^{1,1} vector field smoothness and recentely (6) droped to smoothness. It seems that this smoothness is yet not the "bottom" assumption as it can very easily seen that in the previous saddle point existence the previous density assumption can be weakned by the following one:

It is just enough (to derive the previous uniquiness proof) that has the following property:

$$\forall \in {}^2(\times) \quad \forall \phi \in \mathcal{H}_V$$

$$\exists \text{ a mollifier sequence}$$

$$\rho_n(\quad) \in {}^\infty([0\ \tau] \times {}^-) \text{ with :}$$

$$_n := \int_0 \int_D [(\rho_n * \nabla\phi) \quad -\rho_n * (\nabla\phi \quad)] \qquad \rightarrow 0$$

Indeed the "delicate" point in the proof is to get from the equations to the saddle point. Then when writting the derivative of the Lagrangian functional $\mathcal{L}$ in the direction $\rho_n * \phi \quad \phi \in \mathcal{H}_V$ we can pass to the limit with the additional term ${}_n$ which goes to zero and the element appears as being the partial minimum of $\mathcal{L}$. The uniqueness for the solution to (1) is necessary for the analysis of the derivative of the mapping $\rightarrow$ which is used in several applications in (2), (9),...(11). and also concerning more general convection equation for level set solution and oriented distance function evolution.

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Minimal smoothness of the midsurface in the asymptotic theory of shells

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Keywords: thin shell, asymptotic shell, midsurface, smoothness, representation of a surface, oriented distance function, bilipschitz mapping, tubular neighborhood

Many surfaces ω in $\mathbf{R}^3$ can be viewed as a subset of the boundary Γ of an open subset Ω of $\mathbf{R}^3$ and the associated *oriented distance function* b_Ω to the underlying set Ω completely describes the surface ω: its (outward) normal is the gradient ∇b_Ω and its first, second, and third fundamental forms are $\nabla b_\Omega \otimes \nabla b_\Omega$, its Hessian $D^2 b_\Omega$, and $(D^2 b_\Omega)^2$ restricted to the boundary Γ (10; 15). In addition, a fairly complete intrinsic theory of Sobolev spaces on $C^{1,1}$-surfaces is available in (7).

In the theory of shells, the asymptotic model, only depends on the choice of the *constitutive law*, the *midsurface*, and the appropriate subspace of the space of solution that properly handles the loading applied to the shell. So, a central question is how rough this midsurface can be to make sense of asymptotic *membrane shell* and *bending equations* without ad hoc mechanical or mathematical assumptions. It turns out that this is possible for a general $C^{1,1}$-midsurface with or without boundary such as a sphere, a donut, or a closed reservoir. Moreover, it can be done without local maps, local bases, and Christoffel symbols via the purely intrinsic methods developed starting in 1992 with (11) and in a number of subsequent papers (12; 13; 14; 4; 5; 6; 8; 9; 3).

In recent work on the representation of a surface, (2) have introduced a class of bi-lipschitzian representations subject to a strong Lipschitz condition on the normal field. This work was also used by (16) to study the G_1-junction of such patches, called K-regular patches. It was already known that $C^{1,1}$-surfaces have a Lipschitzian normal field, but it was not, a priori, clear that the midsurfaces generated in this parametrized set-up would be strictly rougher than $C^{1,1}$.

In this paper, we show that the bilipschitzian surfaces with a Lipschizian normal field introduced in (2) are $C^{1,1}$-surfaces with a bounded measurable second fundamental form on $\overline{\omega}$. So $C^{1,1}$ is still the currently available minimum smoothness to make sense of asymptotic *membrane shell* and *bending equations*. The results are given for an hypersurface in $\mathbf{R}^N$, $N \geq 2$, since the proofs are independent of the dimension. As a consequence, the G_1-junctions of K-regular patches along a join δ_{12} developed in (16) are in fact $C^{1,1}$-junctions at points of the joint δ_{12} where the surface has a local G_1 join. Finally, for the family of surfaces ω in (2), we adapt an example from (1) to show that the *tubular neighborhood* or *sandwich* of thichness $2h$ around the surface ω is not a Lipschitzian domain in $\mathbf{R}^3$ because, for all $h > 0$, its lateral boundary is not Lipschitzian. This means that classical results from three-dimensional linear elasticity over Lipschitzian domains cannot be readily applied to the class of thin shells studied in (2).

To complete and update the references in (2) on the theory of shells and to provide a broader perspective to the reader, we briefly recall a few results starting with the key paper (4) on intrinsic methods in the asymptotic analysis of three models of thin shells for an arbitrary linear 3D constitutive law. They all converge to asymptotic shell models that consist of a coupled system of two variational equations. They only differ in their resulting effective constitutive laws. The first equation yields the generally accepted classical *membrane shell equation* and the Love-Kirchhoff terms. The second is a generalized *bending equation*. It explains why convergence results for the 3D models were only established for plates and in the bending dominated case for shells. The

most pertinent of the three is the $P(2,1)$-model, since it converges to the right asymptotic model with the right effective constitutive law. We also show in (5) that models of the Naghdi's type can be obtained directly from the $P(2,1)$-model by a simple elimination of variables without introducing the a priori assumption on the stress tensor $\sigma_{33} = 0$. Bridges are thrown with classical models using local coordinates. Those results are completed in (5) with the characterization of the space of solution for the $P(2,1)$ thin shell model and the space of solutions of the asymptotic membrane shell equation in (6). This characterization was only known in the case of the plate and the uniformly elliptic shell.

In (8), a new choice of the projection achieves the complete decoupling of the membrane and bending equations without the classical plate or bending dominated assumptions, after reduction of the number of variables. In the second part of (8) we present a dynamical thin shell model for small vibrations and investigate the corresponding dynamical asymptotic model. Those papers complete (4) and make the connection with most existing results in the literature thus confirming the pertinence and the interest of the methods we have developed. Extensions of the $P(2,1)$-model have also been developed for piezoelectric shells (9; 3) where a complete decoupling of the membrane and bending equations is also obtained.

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SHAPE APPROXIMATION. GALERKIN STRATEGY FOR LEVEL SET SHAPE ANALYSIS

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Keywords: Level set, Galerkin method, Connecting Tubes

1. GALERKIN METHOD

We address the approximation of geometries by finite dimensional process with no restriction on the topologies. In view of possible topological changes in the approximation process, we consider a level set modeling (see (3) and (2)). Let $\Phi(t,.)$ be a continuous function defined over a domain D with $\Phi : D \times R_+^* \to R$. In order to build the domain Ω_t through a finite dimensional process, we consider a Galerkin extension by expanding the function Φ in a vector space of finite dimension in the basis $\mathcal{B} = \{e_1, \ldots, e_M\}$ as follows $\Phi(t,x) = \sum_{k=1}^{M} \alpha_k(t) e_k(x)$, where the functions e_k are given smooth functions defined over D. Thus the coefficients α_k of Φ will be the solution to a differential equations system. The approximation process is now to find the coefficients $\alpha \in R^M$ in oder to *minimize* the distance between a given domain $\Omega_o \subset D$ and the moving domain Ω_t. At that point this method should be completed on the following two points: the choice of the Galerkin basis e_k and the topology that we consider in the minimization process.

2. DIFFERENTIABLE SHAPE TOPOLOGIES

We consider the metric associated with the characteristic function defined by : $\chi_\Omega(x) = 1$ if $x \in \Omega$ and 0 if $x \in D \backslash \Omega$. We know that for smooth domains we have : $\chi_\Omega \in H^s(R^N),\ \ s < 1/2$. The idea is to consider metric associated to that regularity : $0 < s < 1/2$

$$d_s(\Omega_1, \Omega_2) = ||\chi_{\Omega_1} - \chi_{\Omega_2}||_{L^2(R^N)} + ||\chi_{\Omega_1} - \chi_{\Omega_2}||_{H^s(R^N)}$$

So that

$$||\chi_\Omega||_{H^s(R^N)} = 2 \int_\Omega \int_{D\backslash\bar{\Omega}} G(x,y)\ dxdy$$

Where the kernel $G(x,y) = ||x-y||^{-(N+2s)}$ is singular on the diagonal

$$\Delta = \{(x,x) \subset D \times D,\ x \in D\ \}.$$

When the domain boundary $\partial\Omega$ is smooth we consider the two inner and outer tubular neighborhood of the boundary

$$\mathcal{U}_h(\partial\Omega) = \{x \in D,\ 0 < b_\Omega(x) < h\ \},$$

$$\mathcal{U}_{-h}(\partial\Omega) = \{x \in D,\ -h < b_\Omega(x) < 0\ \}$$

Then

$$||\chi_\Omega||_{H^s(R^N)} = a_h + b_h$$

$$b_h = \int_{\mathcal{U}_h(\partial\Omega)} \int_{\mathcal{U}_{-h}(\partial\Omega)} g(x,y)\ dxdy$$

$$= \int_0^h \int_{\partial\Omega} \int_{-h}^0 \int_{\partial\Omega} G(x+z\nabla b_\Omega(x),\ y+r\nabla b_\Omega(y))\ j_z(x) j_r(y)\ d\Gamma(x) dz d\Gamma(y) dr$$

Where $j_s(w) = 1 + sH(w) + s^2\,K(w)$ (in the specific case $N = 3$ with $H(w) = \Delta b_\Omega(w), w \in \partial\Omega$, is the mean curvature of the manifold $\Gamma = \partial\Omega$, while $K(w)$ is the Gauss curvature).

2.1. Level set method

The specific parameterization for moving domains is : $\Omega_t = \{\ x \in D\ s.t.\ \ \Phi(t,x) > 0\ \}$, with $\Phi \in C^1([0,T], H_0^1(D))$. Then we consider the following vector field

$$V = -\frac{\partial}{\partial t}\Phi\ \frac{\nabla_x \Phi}{||\nabla_x \Phi||^2},$$

We know that $\Omega_t = T_t(V)(\Omega_0)$, that is to say that the domain Ω_t can be equivalentely considered as the image by the flow mapping $T_t(V)$ of the initial domain Ω_0 associated with the function $\Phi(0,x)$. At the boundary the normal component of the vector field turns into

$$v = \langle V(t,.), n_t(.)\rangle = -\frac{\partial}{\partial t}\Phi / ||\nabla_x \Phi||.$$

2.2. Galerkin Expansion

We consider the evolution of a level set generated by the expansion of the function Φ in a vector space of finite dimension

$$\Phi(t,x) = \sum_{k=1}^{M} \alpha_k(t)\ e_k(x)$$

where e_k is a family of given functions: Wavelets, Polynomials or finite elements basis. Thus according to this formulation, moving domains parameterization turns into

$$\Omega_t := \{\, x \in D \ \ s.t. \ \ \sum_{k=1}^{M} \alpha_k(t)\, e_k(x) \ > \ 0 \ \ \}$$

where the normal component of the flow vector field is defined as follows

$$v \ := \ -\sum_{k=1}^{M} \frac{\partial \alpha_k(t)}{\partial t}\ e_k(x)\ ||\sum_{m=1}^{M} \alpha_m(t)\, \nabla_x e_m(x)||^{-1}$$

3. LEVEL SET h-SCALING FORMULATION

We are dealing with shape gradient as referred to in (3) and (2), which (from the structure theorem) are boundary integrals in the following form :

$$\int_{\partial\Omega_t} F\, \langle V(t), n_t \rangle\, d\Gamma_t,$$

Using Federer measure decomposition theorem and assuming the mapping :

$$z \in (-h,\, +h) \rightarrow \ (\int_{\Phi^{-1}(z)} \ \frac{F}{||\nabla_x \Phi||}\ d\Gamma\ )$$

to be continuous, we obtain for $h \rightarrow 0$

$$\int_{\Gamma} \frac{F(x)}{||\nabla_x \Phi(x)||}\, d\Gamma(x) = \frac{1}{2h} \int_{\mathbf{U}_h^{\Phi}(\Gamma)} F(x)\, dx \ + \ o(1)$$

where $\mathbf{U}_h^{\Phi}(\Gamma) = \{\, x \in D \ \mid \ |\Phi(x)| \ < \ h \,\}$. Consequently, the shape gradient is approximate through the choise of the parameter $h \rightarrow 0$ by :

$$\int_{\partial\Omega_t} \langle V(t), n_t \rangle\, d\Gamma_t = -\frac{1}{2h} \int_{\mathbf{U}_h^{\Phi}(\Gamma)} |\frac{\partial}{\partial t}\Phi(t,x)|\, dx$$

The point being that, in this approximation, the denominator $||\nabla_x \Phi(t)||$ has been eliminated.

4. NUMERICAL EXPERIMENT

Concerning 3D active contour, we consider the graph of $\Phi(t,.)$ in R^4 and the example bellow of the domain Γ_0 (4 cubes boundaries). We start with a random initialization for parameter α so that, the boundary $\Gamma_{t=0}$ is a "terrific" shape in 3D (figure 1). The figure 2 shows the optimal evolution of boundary Γ_t with topological changes. Finally, we discuss accuracy following the choice of different basis and also possible hierarchical algoritms.

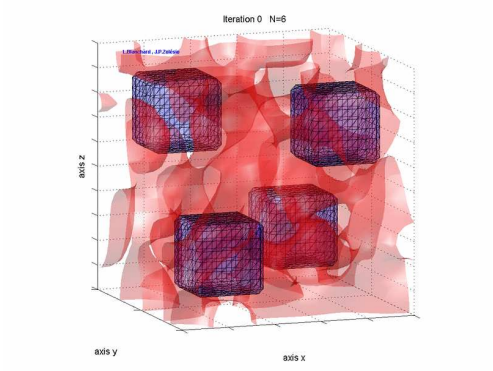

Fig. 1. given domain Γ_0 and initial domain $\Gamma_{t=0}$

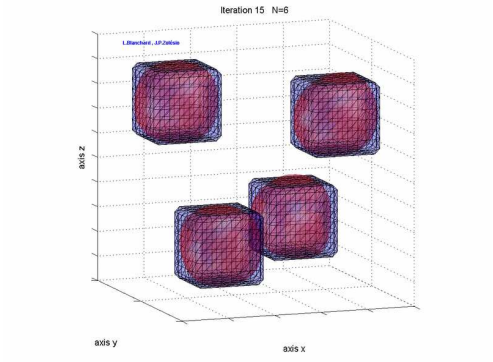

Fig. 2. given domain Γ_0 and optimal domain Γ_t

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Stability of discrete approximations for optimal control of one-sided Lipschitzian Differential Inclusions

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Keywords: differential inclusions, stability theory

* This talk is devoted to the study of *differential inclusions* given in the form

$$\dot{x}(t) \in F\big(t, x(t)\big) \ \text{ for a.e.}$$
$$t \in T := [0,1], x(0) = x_0 \in H,$$

where H is a *Hilbert space*, and where $F\colon T \times H \rightrightarrows H$ is a set-valued mapping with nonempty *compact* values (some results hold also with no compactness assumption). It is well known that the differential inclusion description under consideration is important for its own sake and covers many other conventional and nonconventional models involving dynamical systems in finite and infinite dimensions. In particular, differential inclusions extend control systems

$$\dot{x}(t) = f(t, x, u), \quad u \in U(t, x),$$

where the control region $U(t, x)$ can depend on the state variable x, which is a challenging issue in control theory and applications.

The primary purpose of this talk is to present new results on *stability theory* for *discrete approximations* of differential inclusions and of certain *dynamic optimization/optimal control* problems associated with them. These topics have been addressed in many publications, mostly in finite-dimensional spaces. The vast majority of publications in these directions impose the classical *Lipschitz continuity* of the mapping F in x, which seems to be restrictive for a number of applications.

In this study we systematically replace the Lipschitz continuity by a certain *modified one-sided Lipschitzian* (*MOSL*) *property* of F in x, which is an essentially weaker assumption; see more discussions below.

The scope and results of this talk are fully different from the previous developments in these directions. Our main efforts are to establish the *strong approximation/stability* (in the $W^{1,p}$-norm as $p \geq 1$) of feasible trajectories for MOSL differential inclusions by those for their discrete approximations and also to justify the *strong $W^{1,p}$-convergence* of optimal solutions to the associated problems of *dynamic optimization/optimal control* under discrete approximations. The results obtained extend, to the case of MOSL differential inclusions in finite-dimensional and Hilbert spaces, the corresponding developments of the third

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author (2) for differential inclusions satisfying the classical Lipschitz condition.

Another achievement of this study, motivated by applications to the convergence of discrete approximations in optimal control while certainly significant for its own sake, is establishing a Bogolyubov-type *relaxation/density* theorem for differential inclusions satisfying the MOSL condition. The latter result is known to *hold* for Lipschitzian differential inclusions and to *fail* for OSL ones. All the results presented in this talk seem to be *new* in both *finite-dimensional* and *infinite-dimensional* settings.

The *major results* of this talk concern *discrete approximations* of *dynamic optimization* Bolza-type problems for nonconvex MOSL differential inclusions. We justify the *strong* $W^{1,p}$*-convergence* of optimal solutions for the discrete approximation problems to the given optimal solution (actually an arbitrary *local minimizer* of the "relaxed intermediate" and strong types) for the continuous-time generalized Bolza problem under consideration. We also establish general conditions (both *necessary* and *sufficient*) for the *value convergence* of discrete approximations of the generalized Bolza problem for MOSL differential inclusions. The results obtained significantly improve known results in this direction by weakening assumptions on the initial data dependence with respect to both the state and time variables. The proofs are essentially based on strong approximation and relaxation stability for MOSL differential inclusions discussed above.

The main results of this talk correspond to the forthcoming paper (1) of the authors.

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A Collocation Method for Quadratic Control Problems Governed by Ordinary Elliptic Differential Equations

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Keywords: Linear quadratic optimal control problems, elliptic equations, collocation method, error estimates

1. INTRODUCTION

We consider the one-dimensional elliptic optimal control problem

$$\text{(CP)} \quad \min \frac{1}{2} \int_0^T |z(t) - z_d(t)|^2 + \nu \, |u(t)|^2 \, dt$$

s.t.

$$-\ddot{z}(t) + Az(t) = Bu(t) + e(t) \text{ for a.a. } t \in [0,T]\,,$$
$$z(0) = z(T) = 0\,,$$
$$a \le u(t) \le b \quad \text{for a.a. } t \in [0,T]\,,$$

where $u \in L_2(0,T;\mathbb{R}^m)$, $z, z_d \in W_2^2(0,T;\mathbb{R}^n)$, $\dot{e} \in BV(0,T;\mathbb{R}^n)$, $A \in \mathbb{R}^{n\times n}$ is symmetric and positive semidefinite, $B \in \mathbb{R}^{n\times m}$ and $a, b \in \mathbb{R}^m$, $a < b$.

2. DISCRETIZATION OF THE STATE EQUATION

For the discretization of the state equation

$$\begin{aligned} &-\ddot{z}(t) + Az(t) = y(t) \text{ for a.a. } t \in [0,T]\,, \\ &z(0) = z(T) = 0\,, \end{aligned} \tag{1}$$

we use a uniform grid

$$G = \{t_i = ih \mid i = 0, \dots, N\} \tag{2}$$

with mesh size $h = T/N$, $N \ge 2$. By $S_h = S_h(y)$ we denote the quadratic spline with knots t_i, $i = 0, \dots, N$, defined by the collocation and boundary conditions

$$\begin{aligned} &-\ddot{S}_h(t_i) + AS_h(t_i) = y(t_i),\ i = 0, \dots, N\,, \\ &S_h(0) = S_h(T) = 0\,. \end{aligned}$$

If z ist the solution of the state equation (1) and $\dot{y} \in BV(0,T;\mathbb{R}^n)$, then

$$\|z - S_h\|_\infty \le c\, h^2$$

with a constant c independent of h (see Sendov (5), Theorem 7.3).

3. DISCRETIZATION OF THE CONTROL PROBLEM

We define $U_{\text{ad}} = \{u \in L_2(0,T;\mathbb{R}^m) \mid a \le u(t) \le b \text{ for a.a. } t \in [0,T]\}$. For a function f continuous on $[0,T]$ we define

$$\|f\|_h = \sqrt{h \sum_{i=0}^{N} |f(t_i)|^2}\,.$$

Let $V_h(0,T;\mathbb{R}^m)$ be the space of continuous, piecewise linear functions on the grid (2). Using the operator $\mathcal{S}_h$ we discretize problem (CP) in the following way:

$$\text{(CP)}_h \ \min \frac{1}{2} \|\mathcal{S}_h(Bu_h + e) - z_d\|_h^2 + \nu \, \|u_h\|_h^2$$
$$\text{s.t. } u_h \in U_h^{ad} = U_{\text{ad}} \cap V_h(0,T;\mathbb{R}^m).$$

Problem $(\text{CP})_h$ has a unique solution $\bar{u}_h$.

4. ERROR ESTIMATES

First we derive a result on discrete quadratic convergence for the solutions $\bar{u}_h \in V_h(0,T;\mathbb{R}^m)$ of the problems $(\text{CP})_h$.

Theorem 1. *Let $\bar{u}$ be the solution of* (CP2) *with $\dot{\bar{u}} \in BV(0,T;\mathbb{R}^m)$ and $\bar{u}_h \in V_h(0,T;\mathbb{R}^m)$ the solution of the discrete problem* $(\text{CP})_h$. *Then*

$$\|\bar{u} - \bar{u}_h\|_h \le c\, h^2, \tag{3}$$

holds true with a constant c independent of h.

The *continuous* error $\|\bar{u} - \bar{u}_h\|_\infty$ is only of order $3/2$. Therefore, we adopt the idea of Meyer/Rösch (4) (see also (1), (2)) to construct a new feasible control by

$$\tilde{u}_h = \Pi_{[a,b]}\left(-\frac{1}{\nu} B^{\mathsf{T}} p_h(\bar{u}_h)\right), \tag{4}$$

for which we can prove continuous convergence of order 2.

Theorem 2. *Let $\bar{u}$ be the solution of problem* (CP2) *with $\dot{\bar{u}} \in BV(0,T;\mathbb{R}^m)$ and $\bar{u}_h \in V_h(0,T;\mathbb{R}^m)$ the solution of the discrete problem* $(\mathrm{CP})_h$. *Then for the control $\tilde{u}_h$ defined by* (4) *we have the continuous error estimate*

$$\|\bar{u} - \tilde{u}_h\|_\infty \leq c\, h^2$$

with a constant c independent of h.

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Update Strategies for Perturbed Nonsmooth Equations

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Keywords: variational inequality, nonsmooth equation, Bouligand derivative, optimal control, Taylor expansion

1. Introduction

In this talk we consider nonsmooth operator equations of the form

$$u = \Pi_{[a,b]}(g(\theta) - G(\theta)\, u), \tag{1}$$

where the unknown $u \in L^2(D)$ is defined on some bounded domain $D \subset R^N$, and $\Pi_{[a,b]}$ denotes the pointwise projection onto the set

$$U_{ad} = \{u \in L^2(D) : a(x) \le u(x) \le b(x) \text{ a.e.}\}.$$

Such nonsmooth equations appear as a reformulation of the variational inequality

$$\begin{aligned} &\text{Find } u \in U_{ad} \text{ s.t. for all } v \in U_{ad}, \\ &\langle u + G(\theta)\, u - g(\theta), v - u\rangle \ge 0. \end{aligned} \tag{2}$$

Applications of (2) abound, and we mention control-constrained optimal control problems as a particular one.

Throughout, $G(\theta)$ is a bounded and monotone linear operator with smoothing properties, such as the solution operator to a differential equation, and $g(\theta) \in L^\infty(D)$. Both G and g may depend nonlinearly and also in a nonsmooth way on a perturbation parameter θ from some normed linear space Θ.

2. Update Strategies

Under appropriate assumptions, (1) has a unique solution $u[\theta]$ for any given θ. We are concerned with update strategies which allow to approximately recover the solution $u[\theta]$ from a reference solution $u[\theta_0]$ in its vicinity. In particular, we consider the strategies

$$\begin{aligned} \mathcal{C}_1(\theta) &:= u[\theta_0] + u'[\theta_0](\theta - \theta_0) \\ \mathcal{C}_2(\theta) &:= \Pi_{[a,b]}\big(u[\theta_0] + u'[\theta_0](\theta - \theta_0)\big) \\ \mathcal{C}_3(\theta) &:= \Pi_{[a,b]}\big(\phi[\theta_0] + \phi'[\theta_0](\theta - \theta_0)\big). \end{aligned}$$

The latter involves the solution $\phi[\theta]$ of an adjoint problem

$$\phi = g(\theta) - G(\theta)\Pi_{[a,b]}\phi.$$

3. Main Result

We prove that under appropriate assumptions, these strategies admit the error estimates

$$\frac{\|\mathcal{C}_i(\theta) - u[\theta]\|_p}{\|\theta - \theta_0\|_\Theta} \to 0 \text{ as } \|\theta - \theta_0\|_\Theta \to 0,$$

where $\|\cdot\|_p$ denotes the $L^p(D)$ norm and $p \in [2,\infty]$ for $i = 3$ but only $p \in [2,\infty)$ for $i = 1, 2$. That is, the strategy $\mathcal{C}_3$ involving the adjoint quantities allows a uniform error estimate on D, while the other two do not. To prove this result, we verify the Bouligand differentiability of the maps $u[\theta]$ and $\phi[\theta]$, which amounts to Fréchet differentiability without the requirement that the derivative depend linearly on the direction.

4. Numerical Results

As an application, we consider an optimal boundary control problem for an elliptic partial differential equation with pointwise control constraints. The solution $u[\theta_0]$ and its directional derivative $u'[\theta_0]\,\delta\theta$ are obtained using a semismooth Newton (active set) iteration. The adjoint quantities $\phi[\theta_0]$ and $\phi'[\theta_0]\,\delta\theta$ are computed simultaneously at no additional cost.

A comparison verifies the superiority of the update strategy $\mathcal{C}_3$.

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CONVERGENCE ANALYSIS OF SQP METHOD FOR SEMILINEAR ELLIPTIC OPTIMAL CONTROL PROBLEMS WITH MIXED CONTROL-STATE CONSTRAINTS

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Keywords: optimal control problem, Lipschitz stability, semilinear elliptic equation, mixed control constraints, generalized equation, strong regularity, sequential quadratic programming method

1. INTRODUCTION

We are interested in optimal control of elliptic partial differential equations with *mixed* pointwise inequality constraints:

$$\text{minimize} \int_\Omega \varphi(y,u,x)\,dx + \int_{\partial\Omega} \psi(y,s)\,ds$$

subject to

$$\begin{cases} -\Delta y + f(y) = u & \text{in } \Omega, \\ y = 0 & \text{on } \partial\Omega, \\ u \geq 0 & \text{in } \Omega, \\ \varepsilon u + y \geq y_c & \text{in } \Omega. \end{cases} \tag{1}$$

In (1), y and u denote the state and control variables, respectively. Problems with mixed control-state constraints are important as Lavrientiev-type regularizations of pointwise state-constrained problems [3, 4, 5], but they are also interesting in their own right.

2. CONVERGENCE OF SQP METHOD

Optimal problems involving semilinear PDEs can be efficiently solved using the sequential quadratic programming (SQP) method. The theory of local convergence of SQP methods is already developed for finite dimensional and infinite-dimensional optimization problems with nonlinear equality and inequality constraints [1]. Its convergence analysis is based on a relation between the SQP method and a generalized Newton method, i.e., one considers first-order necessary optimality conditions of (1) as a so-called generalized equation

$$0 \in F(w) + N(w), \tag{2}$$

where the mapping $F(w) := F(y,u,p,\mu_1,\mu_2)$ reflects the differentiable part of the system described by the necessary optimality conditions of (1) and the multivalued mapping $N(w)$ corresponds to that part of necessary optimality conditions which are connected to the inequality constraints of (1). It contains with $N_1(u)$ and $N_2(y,u)$ so-called dual cones. Next, one applies to (2) the Newton method, which gives a locally convergent sequence computed from the linearized equation

$$0 \in F(w^k) + F'(w^k)(w - w^k) + N(w). \tag{3}$$

This interplay between the Newton method and the SQP method is a specific feature, which cannot be derived from general results in Banach spaces [1], since we have to discuss pointwise relations. Until now, such convergence results for optimal control problems governed by PDEs are only known for control-constrained problems.

3. LIPSCHITZ STABILITY

The local convergence behavior of SQP method relies essentially on the strong regularity [6] of a generalized equation (2), which means Lipschitz continuous dependence of the solution of the linearized generalized equation (3) on a perturbation parameter. In the context of PDE-constrained optimization, the linearized generalized equation represents necessary and sufficient optimality conditions of an auxiliary linear-quadratic optimization problem, the form of which arises from (1). The proof of this core step has recently been achieved in [2]. We considered a family of linear-quadratic optimal control

problems with pointwise mixed state-control constaints governed by a linear elliptic partial differential equation in which all data depend on a vector parameter of perturbations δ. The presence of simultaneous control and mixed constraints complicates our analysis. The multipliers associated to these constraints are present in every equation involving the adjoint state. Therefore, the direct estimation of the norm of the adjoint state is not possible in this situation. The new Lipschitz stability result [2] for linear quadratic optimal problem paves the way for the subsequent convergence proof of the SQP method applied to the nonlinear problem (1).

4. NUMERICAL EXAMPLE

The quadratical convergence of SQP method applied to the nonlinear problem of type (1) will be illustrate by a numerical example.

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A posteriori error estimates for elliptic optimal control problems with inequality constraints

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Keywords: optimal control, a posteriori error estimates, mesh refinement, pointwise inequality constraints

In this talk we will discuss a posteriori error estimation for elliptic optimal control problems with inequality constraints on the control and the state variable. The derived error estimates have the goal to guide an adaptive mesh refinement algorithm for finding economical meshes for the optimization problem under consideration.

The use of adaptive techniques based on a posteriori error estimation is well accepted in the context of finite element discretization of partial differential equations, see e.g. [3, 6, 13]. To our knowledge, there are only few published results on adaptive finite elements for optimization problems, see [1, 2, 4, 5, 12] and [7, 8, 9, 10, 11].

In articles [7, 8, 9, 10, 11], the authors provide a posteriori error estimates for elliptic optimal control problems with distributed or Neumann control subject to box constraints for the control variable. These estimates access the error in the control, state and the adjoint variable with respect to the natural norms of the corresponding spaces. In [1] another approach for the estimating of the error with respect to the norm of the control space is presented. In [7] convergence of an adaptive algorithm for a control constrained optimal control problem is shown.

However, in many applications, the error in global norms does not provide a useful error bound for the error in the quantity of physical interest. In this talk, we discuss error estimates with respect to a given functional.

In [2], the authors present a general concept for a posteriori estimation of the discretization error with respect to the cost functional in the context of optimal control problems. In papers [4, 5], the authors have extended this approach to the estimation of the discretization error with respect to an arbitrary functional (quantity of interest) depending on both the control and the state variable. However, in all these publications, optimal control problems without any inequality constraints are considered.

Recently, in [14] a posteriori error estimators for elliptic problems with pointwise inequality constraints on the control variable have been derived, which assess the discretization error with respect to a given quantity of interest. In this talk, we will discuss some extensions of these techniques for the case optimal control problems involving state constrains.

To this end we consider a model problem

$$\min\ J(q,u) = \frac{1}{2}\|u-u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2_{L^2(\Omega)}$$

subject to $q \in Q = L^2(\Omega)$, $u \in V_{ad}$, with

$$V_{ad} = \left\{u \in H^1_0(\Omega)\ :\ u_a \le u \le u_b\right\},$$

and

$$\begin{cases} -\Delta u = f + q \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega. \end{cases}$$

We discuss a finite element discretization of this problem leading to the discrete solution (q_h, u_h) and derive an error estimator for the error with respect to the cost functional, i.e.

$$J(q, u) - J(q_h, u_h).$$

The behavior of the adaptive algorithm based on our error estimator is demonstrated on numerical examples.

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Semidiscretizaton for semilinear elliptic optimal control problems with control constraints

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Keywords: optimal control, semilinear equations, semidiscretization, control constraints

1. INTRODUCTION

We apply the semidiscrete approach developed in (1) to control constrained semilinear elliptic optimal control problems of the form

$$(P) \min_{U\in U_{ad}} \hat{J}(u) = \int_\Omega L(x,y(u))dx + \frac{\alpha}{2}\|u\|_U$$

where the state $y = y(u)$ is coupled to the control u through the semilinear elliptic PDE

$$\begin{aligned} Ay &= f(x,y) + Bu \text{ in } \Omega \\ y &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

Here $\Omega \subset \mathbb{R}^2$ denotes a sufficiently smooth, bounded domain, U the Hilbert space of controls, $U_{ad} \subset U$ a closed and convex subset, A an elliptic differential operator, $B : U \to L^2(\Omega)$ the control operator and $\alpha > 0$ a constant.

2. DISCRETE APPROACH

In the semidiscrete approach problem P is replaced by problem

$$(P_h) \min_{U\in U_{ad}} \hat{J}_h(u) = \int_\Omega L(x,y_h(u))dx + \frac{\alpha}{2}\|u\|_U$$

where of given $u \in U$ the function $y_h(u)$ is a continuous, piecewise polynomial finite-element approximation to $y(u)$. We emphasize that the set of admissible controls is not dicretized in our approach.

3. RESULTS

Although problem (P_h) remains infinite-dimensional, it is possible to solve it numerical by fixed-point iterations or semi-smooth Newton methods applied to the first-order necessary optimality conditions. The latter can be specified in terms of a semi-smooth operator equation in the control space U. Under suitable conditions on L and f we prove existence of solutions to (P) and (P_h), respectively. We further prove convergence of solutions u_h of (P_h) to a solution u of (P) and provide optimal error estimates for $\|u - u_h\|_U$, provided that the limit u satisfies a second order sufficient condition. Optimal in this context means that

$$\begin{aligned} \|u-u_h\|_U \sim \|y(u)-y_h(u)\|_{L^2} + \\ + \|p(y(u))-p_h(y(u))\|_{L^2}, \end{aligned}$$

i.e. the error in the controls admits the same quality as the errors of the state and the adjoint state, respectively. Here $p(y(u))$ denotes the adjoint state, and $y_h(u)$ and $p_h(y(u))$ denote finite-element approximations to $y(u)$ and $p(y(u))$ respectively. In the case of H^2-regular state equations we thus obtain

$$\|u - u_h\|_U = O(h^2)\,(h \to 0).$$

4. NUMERICAL EXAMPLE

In Fig. 1 we present numerical results for $\Omega = [0,1]^2$, $L(x,y) = \frac{1}{2}\int_\Omega (y-z)^2$ and $f(x,y) = y^3$ with $A = -\Delta$, $B = Id$, $\alpha = 1$, $U = L^2(\Omega)$, $U_{ad} = \{v \in U; v \le 20\}$, and $z = 10^4 x_1 x_2(1 - x_1)(1-x_2)$. The numerical solution is computed using a fixed point iteration which takes about 25 to 30 iterations to converge. As can be seen, the discrete active set is resolved independently of the finite element edges an delivers a very well approximation of the active set of the continuous solution already on rather coarse meshes. For a comparison also the active set obtained by the conventional approach with piecewise linear, continuous controls is presented.

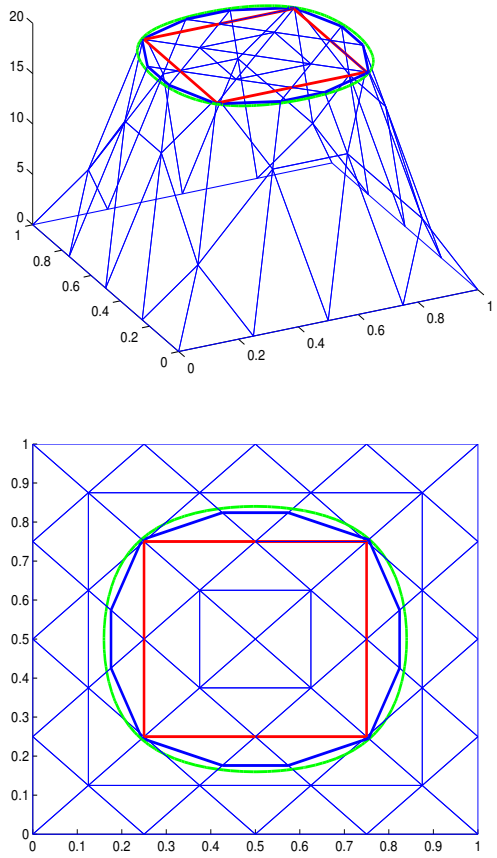

Fig. 1. control with semidiscretization
Optimal control (top) and active sets (bottom) of the continuous solution (green), of the discrete solution (blue) and of the conventional approach (red).

5. CONCLUSIONS

The semidiscrete approach of (1) ist extended to semilinear elliptic control problems. The numerical behaviour of the approach compares to that of the linear quadratic approach case investigated in (1). Details are given in (2).

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Discretization of Elliptic Control Problems with Time Dependent Parameters

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Keywords: Linear quadratic optimal control problems, elliptic equations, finite differences approximations, error estimates

1. Motivation

Problems of optimal control take an extended place in applied mathematics. The treatise of nonlinear cost functionals and nonlinear constraints is often reduced by SQP-methods. This approach leads us to the problem of finding a solution of a linear-quadratic control problem. We consider such problems with an elliptic state equation and control constraints. The coefficients are time dependent and we investigate systems of controls and states, so the coefficients are matrix functions.

The analytical solution of such problems is rather complicated or impossible. To find a reasonable numerical alternative we have to discretize the problem getting an approximation of the exact solution, the optimal state and adjoint state. Besides the obstacles of calculation such a numerical solution we seek to determine the occuring error. Together with the properties of the exact trajectories deduced from the continuous problem we develop upper bounds by means of the mesh size.

2. Treatise of the problem

Our problem is to find a solution of the following control problem with an elliptic constraint and pointwise control constraints. The cost functional is given by

$$J(z,u) = \frac{1}{2}\int_0^T |z(t)-z_d(t)|^2+u(t)^{\mathsf{T}}R(t)u(t)\,dt$$

while the state z is determined by

$$-(P(t)z(t)')' + A(t)z(t) = B(t)u(t) + e(t)$$

for almost all $t \in [0,T]$ and the boundary values $z(0) = z(T) = 0$. The values of the control u are restricted to $a \le u(t) \le b$ for almost all $t \in [0,T]$, where $a, b \in \mathbb{R}^m$ with $a < b$ and the relations hold for each component. The matrix functions P and R are supposed to be positive definite and A positive semidefinit.

The control problem has a unique solution $\bar{u} \in C^{0,1}(0,T,\mathbb{R}^m)$ and with the adjoint state $\bar{p}$, the solution of the adjoint equation, the necessary and sufficient optimality condition

$$(B^{\mathsf{T}}\bar{p} + \nu\,\bar{u}, u - \bar{u}) \ge 0 \quad \forall u \in U_{\mathrm{ad}}$$

holds pointwisely for almost all $t \in [0,T]$.

3. DISCRETIZATION

Applying suitable discretization methods for the equality constraint we estimate the error of the numerical solution and compare the assumptions. Building a bridge to a discretization of the control problem it is possible to develop error estimates for the discrete optimal control by using the discrete optimality conditions. The discrete concepts like the analogue of the continuous differential operator are useful because they mirror the main aspects of the continuous case, e.g. the selfadjointness is kept. The discretization of the control problem itself gives the circumstances which are necessary to use the properties of the discretization method.

The methods we used help us to find a numerical solution of the elliptic constraint. The error measured by powers of the mesh size is of order two. Afterwards we see that this property is transmitted on the control but only in the

nodes. To construct an continuous control we have to use the values at the nodes, but the error is now dominated by this last step. At the end we get for piecewise constant controls linear convergence and for piecewise linear controls $h^{\frac{3}{2}}$. A post-processing step finalize the computation and improve the order in both case to a quadratic behaviour.

In Figure 1 the continuous and the discrete control is shown. One can see clearly the most interesting points are the switching points where the control constraints become active or inactive.

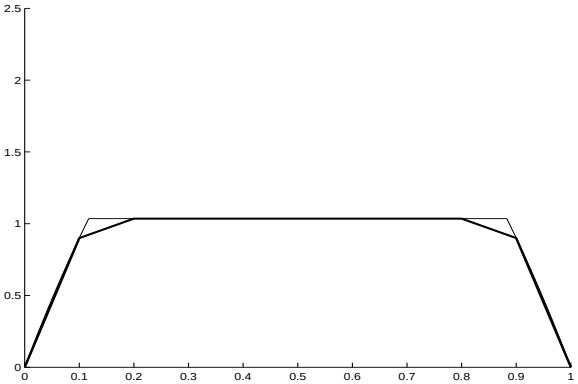

Fig. 1. Optimal control (thin line) and numerical solution (thick line).

In Figure 2 the error is sketched again the mesh size.

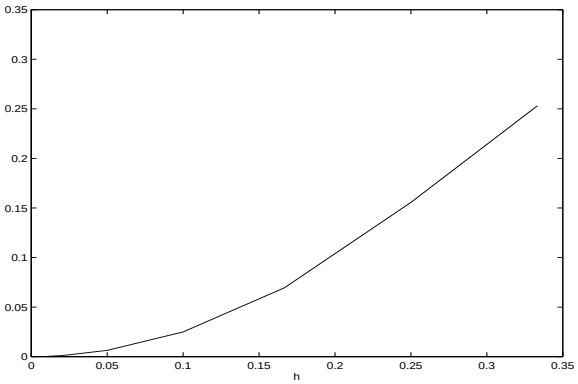

Fig. 2. Error between optimal control and post-processed discrete control.

4. CONCLUSIONS

The different methods of discretization of the given control problem cause different obstacles by finding a numerical solution. We develop error estimates and show connections between them and maintain the different assumptions to be made. In all cases the numerical solution has an order of convergence like the interpolate in the particular discrete space, measured in powers of the mesh size. Further it is possible the improve this by a post-processing which is explained afterwards.

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REFINED QUADRATIC ORDER OPTIMALITY CONDITIONS FOR SINGULAR EXTREMALS

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Keywords: weak minimum, Pontryagin minimum, order of minimum, second variation

We consider the optimal control problem on a fixed time interval $[t_0, t_1]$:

$$\begin{cases} \dot{x} = f(t,x) + F(t,x)\,u, \quad u \in U(t), \\ \eta_j(p) = 0, \quad j = 1,\dots,\mu, \\ \varphi_i(p) \le 0, \quad i = 1,\dots,\nu, \\ J = \varphi_0(p) \to \min, \end{cases}$$

where $x \in \mathbb{R}^n$, $u \in \mathbb{R}^r$, $p = (x(t_0), x(t_1))$, and analyze a process (x^0, u^0) with $u^0(t)$ going strictly inside $U(t)$. Assume that Maximum Principle holds with the Pontryagin function $H = \psi\,(f(t,x) + F(t,x)\,u)$ and the terminal Lagrange function $l(p) = \sum_{i=0}^{\nu} \alpha_i\,\varphi_i(p) + \sum_{j=1}^{q} \beta_j\,\eta_j(p)$, where $\alpha_0,\dots,\alpha_\nu \ge 0$, β not all zero, are unique up to the normalization.

Since the second variation $\Omega(\bar{x},\bar{u})$ of Lagrange function does not contain "the main" Legendre term with $\bar{u}^2$, we have a totally singular extremal. The previous results by the author and others give necessary and sufficient conditions for optimality (in the sense of weak minimum) of the given process (x^0, u^0), which consist in the sign definiteness of Ω on the cone of critical variations with respect to the following estimating quadratic functional, that we regard as a quadratic order of minimum:

$$\gamma(\bar{x},\bar{u}) = |\bar{x}(t_0)|^2 + |\bar{y}(t_1)|^2 + \int_{t_0}^{t_1} |\bar{y}(t)|^2\,dt,$$

$$\text{where} \qquad \dot{\bar{y}} = \bar{u}\,, \qquad \bar{y}(t_0) = 0.$$

In the case of so-called Pontryagin minimum some equality type conditions on coefficients of the third variation should be added.

The most "unpleasant" term in γ is $|\bar{y}(t_1)|^2$. Here we consider the reduced quadratic order

$$\gamma'(\bar{x},\bar{u}) = |\bar{x}(t_0)|^2 + \int_{t_0}^{t_1} |\bar{y}(t)|^2\,dt,$$

and specify the cases where the positive definiteness of Ω with respect to γ' ensures the weak or Pontryagin minimum at (x^0, u^0).

Theorem. Suppose that the Pontryagin and terminal Lagrange functions for the reference process satisfy the conditions

$$H''_{xu}(t_1) = 0,\ l''_{x_0\,x_1}(p^0) = 0,\ l''_{x_1\,x_1}(p^0) = 0,$$

while the cost functional and terminal constraints satisfy the conditions

$$\varphi''_{i\,x_1\,x_1}(p^0) = 0,\ \ \eta''_{j\,x_1\,x_1}(p^0) = 0,\ \ \forall\, i,j.$$

In this case, if $\exists\, a > 0$ such that

$$\Omega(\bar{w}) \ge a\,\gamma'(\bar{w}) \quad \text{for all } \ \bar{w} \in K,$$

then w^0 provides a strict weak minimum. If, in addition $H_{uxx}(t_1) = 0$, then w^0 provides a strict Pontryagin minimum. $\diamond$

If F does not depend on x, then the positive definiteness of Ω with respect to γ guarantees the strong minimum at (x^0, u^0), and we specify some cases when γ can be reduced to γ'.

We also consider the case where the time interval $[t_0, t_1]$ is variable, and give similar optimality conditions.

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A CHARACTERIZATION OF STABILITY AND SENSITIVITY PROPERTIES FOR STATE – CONSTRAINED OPTIMAL CONTROL

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Keywords: Optimal control, nonlinear ODEs, state constraints, parametric problems, stability and sensitivity analysis.

The paper concerns parameter dependent optimal control problems, governed by nonlinear ODEs and subject to state constraints of the first order. In recent papers of the author (see (1; 2; 3; 4)), weakened conditions are derived, under which the solutions and Lagrange multipliers of the problems are locally Lipschitz continuous and directionally differentiable functions of the parameter. The conditions consist of standard constraint qualifications and weakened second order sufficient optimality conditions, which should be satisfied at the reference point. The second order conditions are weakened by taking into account the strongly active state constraints.

In the present paper, it is shown that, in the case of the so called canonical perturbations, those conditions are not only sufficient, but also necessary, for Lipschitz stability and directional differentiability of the solutions and Lagrange multipliers. Thus, they constitute a characterization of those properties.

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Stability and Sensitivity Analysis for Optimal Control Problems with a First-Order State Constraint and Application to Continuation Methods

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Keywords: Optimal Control, First-order State Constraint, Strong Regularity, Homotopy method

This talk deals with stability and sensitivity analysis for optimal control problems of an ordinary differential equation with a first-order state constraint. We consider the case when the Hamiltonian and the state constraint are regular. Malanowski (2) obtained Lipschitz continuity and directional differentiability of solutions in L^2, using generalized implicit functions theorems in infinite dimensional spaces, and without any assumptions on the structure of the trajectory. Malanowski and Maurer (3) proved that the solution and multipliers are C^1 with respect to the parameter by application of the implicit function theorem to the shooting mapping, when there are finitely many junction times and strict complementarity holds. Under those assumptions the structure of the perturbed solutions is stable.

The shooting algorithm, known to provide the solution of optimal control problems with a very high precision and low cost, requires in return a careful initialization of all parameters, as well as a knowledge a priori of the structure of the optimal trajectory (number and order of boundary arcs and touch points). In practice, the latter is not known and even though, it remains difficult to initialize the shooting parameters. A method to make up for this difficulty is to combine the shooting algorithm with an homotopy (or continuation) method. Starting from an "easier" problem (e.g. the problem without the state constraint), one solves a sequence of problems depending continuously from a parameter. The more information we have on the continuity/differentiability of solutions and shooting parameters with respect to the homotopy parameter, the easier it is to follow the homotopy path, for example using a predictor-corrector algorithm if the homotopy path is C^1. It is well known that for first-order state constraints, touch points (locally unique times when the constraint becomes active) are nonessential, i.e., strict complementarity never holds, and hence the structure of solutions is not stable. Among the different possibilities, a touch point can become inactive on the perturbed problem, remain a nonessential touch point, or it may give rise to a boundary arc.

Our main result is that, under natural hypotheses, these are the only three possibilities. We provide first-order expansions of the solution, multipliers and of all the shooting parameters. The main idea of the proof is to introduce touch points as boundary arcs of zero measure in the shooting formulation, and apply Robinson's strong regularity theory to a system of equalities and inequalities, whose Jacobian corresponds to the optimality conditions of the tangent linear quadratic problem involved in the no-gap second-order optimality conditions (see (1)).

We present an application of those results to an homotopy method, whose novelty is to handle automatically changes in the structure (apparition/disparition of a boundary arc). Preliminary numerical results are given.

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ON LIPSCHITZ STABLE SWITCHING BEHAVIOR OF BANG-BANG EXTREMALS IN PARAMETRIC CONTROL

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Keywords: bang-bang control, stability in optimal control, nonsmooth optimization, shooting method

In the paper, we consider ODE driven optimal control problems with bang-bang type extremals. The specific nature of bang-bang controls causes some difficulties in optimality and stability analysis. Usual convexity arguments like (strong) Legendre-Clebsch condition fail to hold, and the control discontinuity has to be taken into account. In recent years, substantial results on second-order optimality conditions have been obtained in [8], also [6], [1], or [7]. The solution stability under parameter perturbation was investigated e.g. in [5] and [2], [3].

Optimality and stability conditions therein are:
(i) bang-bang regularity assumptions (finite number of switches, excluding e.g. endpoints),
(ii) strict bang-bang properties (nonvanishing time derivatives of switching functions at switching points e.g.),
(iii) assumption of simple switches (switch of no more than one control component at each time),
(iv) appropriate second-order conditions (positive definiteness of related quadratic forms e.g.).

Stability properties for the switching points localization had been obtained from the so-called deduced finite-dimensional problem using standard sensitivity results from nonlinear programming, or from a shooting type approach applied to the first-order system of conditions in Pontryagin's maximum principle e.g. [2], [4]).

Consider the parametric problem

$$\begin{aligned}
\textbf{(P}_h\textbf{)}\quad & \min\ k(x(T),h)\\
\text{s.t.}\quad & \dot{x}(t) = f(x(t),h) + g(x(t),h)\,u(t)\ \ (\forall)\,t,\\
& x(0) = x_0(h),\quad h \in R\ -\ \text{parameter},\\
& |u_i(t)| \le 1,\ \ i=1,\dots,m,\ (\forall)\,t,
\end{aligned}$$

Stability investigations have shown

1. the differentiability of switching points w.r.t. parameters under conditions (i), (ii) for linear state systems ($f = Ax, g = B$), cf. [2],

2. differentiable behavior and local uniqueness of structure of extremals for semilinear systems ($f = f(x), g = B$) under (i), (ii), (iv), cf. [4],

3. Lipschitz behavior (and possible lack of differentiability) for (P) in case of simultaneous switches of two control components.

Up to our knowledge, the latter result is new. The proofs are based on certain backward shooting approach for characterizing broken extremals and make use of nonsmooth Implicit Function Theorems. For illustration, an example will be provided.

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About nonuniform grids in control constrained optimal control problems

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Keywords: Optimal control, control constraints, finite elements, discretization error

1. Introduction

In the last years a lot of papers were published discussing the discretization error of a problem

$$\frac{1}{2}\|y - y_d\|^2 + \frac{\nu}{2}\|u\|^2 = \min!$$

subject to

$$y = Su$$

and

$$u_a \le u \le u_b.$$

Here S denotes the solution operator of an elliptic boundary value problem. We are interested in the case where the domain is polygonal (polyhedral).

Among these papers there are only a few which recommend the usage of nonuniform grids, see (1), (5). The common opinion is that nonuniform meshes are only needed for problems in nonconvex domains or for problems with singularities.

In this talk, we discuss several situations where nonuniform grids can improve the approximation rate.

2. Distributed control

For control constrained problems are at least two approaches known which can ensure approximation rate h^2 for the optimal control. The variational approach of Hinze (3) yields this rate for convex domains in 2-d and 3-d. For the superconvergence approach introduced by Meyer and Rösch (4) the rate h^2 is guaranteed only with an additional angle condition in the 3-d case see (6). Apel and Winkler obtain the same condition in their studies. However, the condition is only needed if the boundary between the active and inactive set hits exactly the corner of the polyhedral.

The situation changes if one is interested in optimal rates also in the L^∞-norm. Then, nonuniform refinements are necessary for all corners with angle larger the $\pi/2$.

3. Boundary control

The situation is much more difficult for boundary control problems. Let us focus first on Neumann control problems. Here, two saturation effects occur: First, an approximation rate of order $h^{2-\varepsilon}$ for linear finite elements can only guaranteed if the largest angle is smaller than $\pi/2$. In general, a convergence rate of $h^{3/2}$ is obtained for convex domains.

The approximation rate is better for higher order finite elements. The order h^2 can be guaranteed if the largest angle is less than $2\pi/3$. Numerical studies of Mateos and Rösch observed these approximation rates also numerically. Consequently, nonuniform grids lead to better approximation results even for 2-d convex domains with a largest angle greater than $2\pi/3$.

Of course, the situation changes again for Dirichlet boundary control. Casas and Raymond (2) determine the approximation rate dependent on smoothness properties of the solution operator. These properties depend on the size of the largest angle of the polygon. Their error estimates indicate that nonuniform grids increases the approximation rate for 2-d convex domains with a largest angle greater than $\pi/2$. Again, nonuniform grids are needed in general if one is interested in optimal rates in the L^∞-norm.

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Optimal Control of the Convection-Diffusion Equation using Stabilized Finite Element Methods

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Keywords: optimal control, convection-diffusion equations, stabilized finite elments, error estimates, pointwise inequality constraints

The talk is concerned with the discretization of optimal control problems using stabilized finite element methods, see [2].

We consider an optimal control problem governed by a linear convection diffusion reaction equation with the convection dominated behavior. It is well known that for convection dominated problems standard finite element discretizations lead to strongly oscillatory solutions unless the mesh size h is sufficiently small. Several stabilization methods are known to improve the approximation properties of the pure Galerkin discretization and to reduce the oscillatory behavior.

In [3] the authors apply the SUPG method (streamline upwind Petrov Galerkin method, see e.g. [5]) to the optimal control problem governed by a convection dominated equation. They discuss two different approaches to the discretization of the optimal control problem: "optimize-then-discretize" and "discretize-then-optimize". In the "optimize-then-discretize" approach first the necessary optimality conditions are established on the continuous level consisting of the state, adjoint and the optimality equations, and then these equations are discretized using a stabilized finite element scheme, e.g. SUPG. In the "discretize-then-optimize" approach the state equation is discretized and then the optimality system for the finite dimensional optimization problem is derived. It is well known that these two approaches lead to the same discretization scheme provided a pure Galerkin discretization is used. However, in the presence of stabilization terms these approaches may differ. In [3] it is shown by numerical computations that for the SUPG discretization the "optimize-then-discretize" approach leads to better asymptotic convergence properties. However, the "discretize-then-optimize" approach has the important advantage of consistency of the state and the adjoint equations on the discrete level which is reflected in the fact that the corresponding optimality system is symmetric.

In the paper [2] we analyze a stabilization method, which leads to symmetric optimality systems and has optimal order of convergence. For the resulting discretization scheme the approaches "optimize-then-discretize" and "discretize-then-optimize" coincide. The presented method uses standard finite element discretization with stabilization based on local projections (called LPS-method), see [4] for convection diffusion reaction equations and for the Stokes equations see e.g. [1]. The control space is likewise discretized by first-order finite elements.

Our main contribution is the a priori error analysis of the discretization of the optimal control problem governed by a convection dominated equation. We obtain the estimate of order $\mathcal{O}(h^{3/2})$ for the L^2-error in

the control, state and the adjoint state in the case without control constraints as well as in the case with pointwise inequality control constraints.

Our results are optimal for the following two reasons: First, it is well known that stabilized finite elements leads to optimal order of convergence of $\mathcal{O}(h^{3/2})$ in $L^2(\Omega)$-norm for the convection diffusion reaction equations on general quasi-uniform meshes. Second, the presence of control constraints leads to the fact that the optimal control $\bar{q}$ is in general not in $H^2(\Omega)$ and only $\mathcal{O}(h^{3/2})$ convergence can be expected for the piecewise (bi)linear discretization of the control space, see e.g. [6].

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OPTIMAL CONTROL OF THE THERMISTOR PROBLEM

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Keywords: Optimal control, thermistor problem, pointwise state constraints, coupled systems

1. THE APPLICATION PROBLEM

The presented talk deals with the optimal control of the thermistor problem that models the conductive heat transfer in a conductor produced by an electric current. This leads to the following quasi-linear system of partial differential equations (PDEs):

$$\partial_t \theta - \operatorname{div}(\kappa \nabla \theta) = (\sigma(\theta)\nabla\varphi)\cdot\nabla\varphi \quad \text{in Q} \tag{1}$$

$$\nu \cdot \kappa \nabla\theta + \alpha\theta = \alpha\theta_l \quad \text{onΣ} \tag{2}$$

$$\theta(0) = \theta_0 \quad \text{in } \Omega \tag{3}$$

$$-\operatorname{div}(\sigma(\theta)\nabla\varphi) = 0 \quad \text{in } Q \tag{4}$$

$$\nu \cdot \sigma(\theta)\nabla\varphi = u \quad \text{on } \Sigma_0 \tag{5}$$

$$\varphi = 0 \quad \text{on } \Sigma\backslash\Sigma_0, \tag{6}$$

with a Lipschitz domain $\Omega \subset \mathbf{R}^2$, $Q = \Omega\times]0,T[$, $\Sigma = \partial\Omega\times]0,T[$, and $\Sigma_0 = \Gamma_0\times]0,T[$, where Γ_0 denotes a fixed part of $\partial\Omega$. Moreover, θ represents the temperature, while φ is the electric potential. Furthermore, θ_l and θ_0 are given functions, and u is the control that can be interpreted as a current induced on Γ_0. A possible application for this coupled system of PDEs is the resistance stud welding, where two work pieces are welded together by means of the Joule effect (cf. Figure 1).

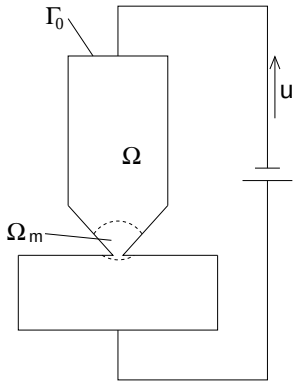

Fig. 1. Resistance stud welding

Our aim is to adjust the control u such that

$$J(\theta,u) := \frac{1}{2}\,\|\theta(T)-\theta_d\|^2_{L^2(\Omega_m)} + \frac{\beta}{2}\,\|u\|^2_{L^2(\Sigma_0)}$$

is minimized subject to (1)–(6) and the following inequality constraints

$$u_a \leq u(t,x) \leq u_b \quad \text{a.e. on } \Sigma_0 \tag{7}$$

$$\theta_a(t,x) \leq \theta(t,x) \leq \theta_b(t,x) \quad \text{a.e. in } Q. \tag{8}$$

Notice that (8) represents a pointwise state constraint that is known to be numerically and theoretically challenging to handle.

2. DISCUSSION OF THE NONLINEAR STATE SYSTEM

Based on maximal parabolic and elliptic regularity results in the spirit of Gröger (3; 4), one can employ Banach's contraction principle to show existence and uniqueness of solutions in

$$(\varphi,\theta) \in L^\infty(]0,T[;W^{1,q}(\Omega)) \times W^{1,r}(]0,T[;W^{1,q'}(\Omega)^*) \cap L^r(]0,T[;W^{1,q}(\Omega))$$

provided that $u \in L^\infty(]0,T[;L^2(\Gamma_0))$ and that θ_0 and θ_l are sufficiently smooth. Here, q is a fixed number in $]2,4[$ and r satisfies $r > 2q/(q-2)$ such that

$$W^{1,r}(]0,T[;W^{1,q'}(\Omega)^*) \cap L^r(]0,T[;W^{1,q}(\Omega)) \hookrightarrow C([0,T];C(\bar{\Omega})),$$

which is needed for the derivation of first-order necessary optimality conditions by means of the Karush-Kuhn-Tucker theory (cf. (2)). Notice that the required regularity of the optimal control is ensured by (7).

3. FIRST-ORDER NECESSARY CONDITIONS

Similarly to the discussion of the state system, the existence and uniqueness of solutions for the linearized state system can be shown. Based on that, in a standard way, the implicit function theorem gives the continuous Fréchet-differentiability of the control-to-state mapping and the objective functional J, respectively. It is well known that the Lagrange multipliers w.r.t. the pointwise state constraints are in general regular Borel measures and appear as inhomogeneity in the adjoint equation. Using a duality argument according to Amann (1), the unique existence of solutions of this equation in $L^{r'}(]0,T[;W^{1,q'}(\Omega))^2$ is established, where r' and q' denote the conjugate exponents of r and q. Corresponding to the first-order conditions, a gradient method has been implemented to solve the optimal control problem. The associated results will be presented.

4. CONCLUSION AND OUTLOOK

Up to now, in (5), we derived the first-order analysis for the optimal control problem subject to (1)–(6), (7), and (8). In the near future, second-order sufficient conditions have to be established. Furthermore, according to this, higher-order optimization methods, as e.g. SQP-methods, have to be implemented.

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REGULARITY OF LAGRANGE MULTIPLIERS FOR OPTIMAL CONTROL PROBLEMS WITH PDEs AND MIXED CONTROL STATE CONSTRAINTS

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1. INTRODUCTION

Lagrange multipliers for distributed parameter systems with mixed control-state constraints may exhibit better regularity properties than those for problems with pure pointwise state constraints, (1), (2), (4). Under natural assumptions, they are functions of certain L^p-spaces, while Lagrange multpliers for pointwise state constraints are, in general, measures. Following an approach suggested in (3) for ODEs, a new and simplified technique is applied to prove L^1-regularity in the case of elliptic PDEs. Moreover, an idea of (5) is extended to derive L^∞-estimates for the Lagrange multipliers, along with the proof of Lipschitz regularity of optimal controls.

2. OPTIMAL CONTROL PROBLEM

We consider first the following elliptic optimal control problem:

$$\min J(y,u) = \int_\Omega \varphi(x,y,u)\,dx + \int_\Gamma \psi(x,y)\,ds \tag{1}$$

subject to

$$\begin{aligned} A\,y + d(x,y) &= u \quad \text{in } \Omega \\ \frac{\partial y}{\partial \nu_A} + b(x,y) &= 0 \quad \text{on } \Gamma \end{aligned} \tag{2}$$

and to

$$g_i(x,y(x),u(x)) \le 0 \quad \text{a.e. on } \Omega,\ i = 1,..,k. \tag{3}$$

The inequalities (3) are the mixed control-state constraints.

In this setting, $\Omega \subset \mathbf{R}^N$, $N \in \mathbf{N}$, is a bounded Lipschitz domain and A is a uniformly elliptic differential operator of the form

$$Ay = -\sum_{i,j=1}^{N} \frac{\partial}{\partial x_i}\left(a_{ij}\frac{\partial}{\partial x_j}y\right) + c_0\,y$$

with coefficients $a_{ij} \in C^{0,1}(\bar\Omega)$, $i,j = 1,..,N$, where $c_0 \ge 0$ belongs to $L^\infty(\Omega)$ and satisfies $c_0(x) > 0$ on a set of positive measure.
The functions $\varphi = \varphi(x,y,u) : \Omega \times \mathbf{R}^2 \to \mathbf{R}$, $g_i = g_i(x,y,u) : \Omega \times \mathbf{R}^2 \to \mathbf{R}$, $\psi = \psi(x,y) : \Gamma \times \mathbf{R} \to \mathbf{R}$, $d = d(x,y) : \Omega \times \mathbf{R} \to \mathbf{R}$, and $b = b(x,y) : \Gamma \times \mathbf{R} \to \mathbf{R}$, are assumed to enjoy the following properties (consider all functions formally as depending on (x,y,u)):

For all fixed (y,u), they are measurable with respect to $x \in \Omega$ or $x \in \Gamma$, respectively. They are partially differentiable with respect to (y,u) for all fixed $x \in \Omega$ or $x \in \Gamma$. These functions and their derivatives are locally Lipschitz with respect to (y,u) in the sense that the associated Lipschitz constant depends only on $|y| + |u|$ but not on x.

Moreover, we require that these functions and their partial derivatives are essentially bounded with respect to x in Ω or $x \in \Gamma$, respectively, at $(y,u) = (0,0)$. The derivatives $\frac{\partial d}{\partial y}(x,y)$ and $\frac{\partial b}{\partial y}(x,y)$ are assumed to be nonnegative for almost all $x \in \Omega$ or $x \in \Gamma$ to guarantee existence and uniqueness of the solution y to (2).

3. REGULARITY OF LAGRANGE MULTIPLIERS

The existence of Lagrange multipliers is obtained first in $(L^\infty(\Omega))^*$, the dual space to $L^\infty(\Omega)$. The elements of $(L^\infty(\Omega))^*$ can be represented

by finitely additive set functions on $\bar{\Omega}$ that are also called *finitely additive measures*.

To derive necessary optimality conditions, a standard *linearized Slater condition* is assumed as constraint qualification: There exist $\hat{u} \in L^\infty(\Omega)$ and $\sigma > 0$ such that

$$g_i(x,\bar{y}(x),\bar{u}(x)) + \frac{\partial g_i}{\partial y}(x,\bar{y}(x),\bar{u}(x))\hat{y}(x) + \frac{\partial g_i}{\partial u}(x,\bar{y}(x),\bar{u}(x))\hat{u}(x) \le -\sigma \quad \text{a.e. in } \Omega, \tag{4}$$

where $\hat{y} = G'(\bar{u})\hat{u}$ is the directional derivative of the control-to-state mapping $G : u \to y$, $G : L^\infty(\Omega) \to H^1(\Omega) \cap C(\bar{\Omega})$.

Theorem 1: *Suppose that $\bar{u}$ with associated state $\bar{y}$ is locally optimal for (1)–(3) and the condition (4) is satisfied at $(\bar{y},\bar{u})$. Then there exist non-negative finitely additive measures $\mu_i \in L^\infty(\Omega)^*$, $i = 1,..,k$, and an adjoint state $p \in W^{1,s}(\Omega)$ for all $1 \le s < \frac{N}{N-1}$, such that the conditions*

$$\int_\Omega \left(\frac{\partial \varphi}{\partial u} + p\right) h\, dx + \int_\Omega \sum_{i=1}^k \frac{\partial g_i}{\partial u} h\, d\mu_i = 0 \quad \forall h \in L^\infty(\Omega),$$

$$\int_\Omega g_i(\cdot,\bar{y},\bar{u})\, d\mu_i = 0, \quad i = 1,..,k,$$

and the adjoint equation

$$A^* p + \frac{\partial d}{\partial y} p = \frac{\partial \varphi}{\partial y} + \sum_{i=1}^k \left(\frac{\partial g_i}{\partial y}\right)^* \mu_i)|_\Omega,$$

$$\frac{\partial p}{\partial \nu_{A^*}} + \frac{\partial b}{\partial y} p = \frac{\partial \psi}{\partial y} + \sum_{i=1}^k \left(\frac{\partial g_i}{\partial y}\right)^* \mu_i)|_\Gamma$$

are satisfied, if the derivatives of φ, ψ, g_i, d, b in the expressions above are taken at $(x,\bar{y},\bar{u})$.

As linear continuous functionals on $L^\infty(\Omega)$, the finitely additive measures μ_i must vanish on sets of Lebesgue measure zero. Thanks to a theorem by Yosida and Hewitt (6), each $\mu \in L^\infty(\Omega)^*$ can be uniquely written in the form $\mu = \mu_c + \mu_p$, where μ_c is countably additive and μ_p is purely finitely additive. Moreover, if $\mu \ge 0$, then μ_c and μ_p are non-negative, too.

For higher regularity of multipliers, the following assumption is needed: Define, for $\delta > 0$, the δ-active sets

$$M_i^\delta := \{x \in \Omega :\ g_i(x,\bar{y}(x),\bar{u}(x)) \ge -\delta\}.$$

Assume that there exist $\delta > 0$ and $\tilde{u} \in L^\infty(\Omega)$ such that

$$\frac{\partial g_i}{\partial u}(x,\bar{y}(x),\bar{u}(x))\tilde{u}(x) \ge 1 \quad \text{a.e. on } M_i^\delta \tag{5}$$

holds for all $i \in \{1,..,k\}$.

This requirement is equivalent to a "uniformly positive linear independency condition", cf. Dmitruk (3). For some types of constraints, this assumption is automatically satisfied. In other cases, the optimal solution must fulfill a certain separation condition.

Theorem 2: *If $\bar{u} \in U$, $\bar{y} \in Y$ and $\mu_i \in L^\infty(\Omega)^*$, $\mu_i \ge 0$, $i \in \{1,..,k\}$, satisfy the first-order optimality conditions of Theorem 1 and (5) is satisfied, then the purely finitely additive parts of all μ_i are vanishing so that all μ_i, $i = 1,..,k$, can be represented by densities in $L^1(\Omega)$.*

The proof follows the one given by Dmitruk (3) for the case of ordinary differential equations.

If the functions φ and g_i, $i = 1,..,k$, are assumed to be Lipschitz with respect to (x,y,u), then locally optimal controls enjoy Lipschitz continuity, too. In associated parabolic control problems, Hölder continuity of the optimal controls can be derived.

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REGULARIZATION AND DISCRETIZATION OF CONSTRAINED OPTIMAL CONTROL PROBLEMS

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1. INTRODUCTION

We are interested in error estimates for elliptic optimal control problems with pointwise state constraints or mixed constaints. In particular, the main difficulties occur for cases with pure state constraints. To overcome these difficulties we use here a Lavrentiev type of regularization. Mixed pointwise control-state constraints typically have better theoretical and numerical properties than state constrained problems. Moreover, the existence of bounded and measurable Lagrange multipliers was proven in [4]. The optimal control problem with regularized state and control constraints is given by

$$\min_{(y,u)} \quad \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)}, \tag{1}$$

$$\text{subject to} \qquad \begin{aligned} Ay &= u && \text{in } \Omega \\ y &= 0 && \text{on } \Gamma, \end{aligned} \tag{2}$$

$$0 \le u \le b \qquad \text{a.e. in } \Omega, \tag{3}$$

$$y \ge y_c + \varepsilon u \qquad \text{a.e. in } \Omega', \tag{4}$$

where $\Omega \subset \mathbb{R}^2$ is a convex polygonal domain. Assume $\Omega' \subset \Omega$ with $dist(\Omega', \partial\Omega) > 0$, $\nu > 0$. Consider functions y_c in $L^\infty(\Omega)$, y_d in $L^q(\Omega)$ for $q > 2$, and the control u in $L^\infty(\Omega)$. By S we denote a linear continuous solution operator of $Ay = u$ such that $y = Su$. We reformulate (1)-(4) in the following form

$$\begin{aligned} \min_{u} \quad & \frac{1}{2}\|Su - y_d\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)} \\ & u \in U^\varepsilon_{ad}, \end{aligned} \tag{P_ε}$$

where $U^\varepsilon_{ad} := \{u \in L^\infty(\Omega) \mid 0 \le u \le b,\ Su \ge y_c + \varepsilon u \quad \text{a.e. in } \Omega\}$ is a set of admissible controls. The problem with regularized parameter $\varepsilon = 0$ is denoted by (P).

In the next sections we discuss regularization and discretization errors. Our main aim is to find a reasonable balance between regularization and discretization parameters for the considered problems.

2. REGULARIZATION ERROR

We are interested in the convergence rate with respect to the regularized parameter ε. For analysis we assume existence of Slater points and prove error estimates by means of constucted feasible controls

$$\|\bar{y} - \bar{y}_\varepsilon\|_{L^2(\Omega)} + \|\bar{u} - \bar{u}_\varepsilon\|_{L^2(\Omega)} \le c\varepsilon^{\frac{1}{2}}.$$

We have proven the stability properties of the regularized problem with respect to noisy data as well, see [1].

3. DISCRETIZATION ERROR

3.1. Discretization

We introduce a finite element based approximation of the regularized problem (P_ε) and define a discrete solution operator S_h. Now we are interested in error estimates with respect to the grid size h. The discrete regularized problem is denoted by $(P_{\varepsilon h})$. For analysis we use standard theory for finite elements, moreover we recall some results concerning the approximation of the discrete solution operator for more smooth boundaries from [2]. Further, we introduce the L_2- projection, which maps from L_2 to a discrete space and refer to results of [3] for error estimation with the projection operator.

3.2. Discrete Approximation for the Regularized Problem

Consider the continuous problem (P_ε) and discrete problem $(P_{\varepsilon h})$. Again, we assume the exis-

tence of an inner point with respect to constraints of $(P_{\varepsilon h})$, where ε is an arbitrary but fixed value. Therefore, for optimal controls $\bar{u}_\varepsilon$ and $\bar{u}_{\varepsilon h}$ to the problems (P) and $(P_{\varepsilon h})$, respectively, the following inequality holds

$$\|\bar{u}_\varepsilon - \bar{u}_{\varepsilon h}\|_{L^2(\Omega)} \leq ch^{\frac{1}{2}},$$

where c is a positive constant independent of h and ε.

3.3. Discrete Approximation for the Unregularized Problem

To improve the error estimate we consider the unregularized continuous problem (P), and in the problem $(P_{\varepsilon h})$ we now fix the regularization parameter ε be a fixed value of order h^2. However, it turns out that this tuning of the parameters increases the theoretically obtained approximation. We are able to show that for optimal controls $\bar{u}$ and $\bar{u}_{\varepsilon h}$ to the problems (P) and $(P_{\varepsilon h})$, respectively, the following error estimate holds true

$$\|\bar{u} - \bar{u}_{\varepsilon h}\|_{L^2(\Omega)} \leq ch^{1-\beta},$$

where β is arbitrary small and c is a positive constant independent of h and ε.

4. CONCLUSIONS

The Lavrentiev type of regularization overcomes analytical and numerical difficulties. We have estimated the discrete error for regularized problem with respect to (P_ε) and with respect to (P) analytically. Theoretical analysis shows convergence of order $h^{\frac{1}{2}}$ between the discrete regularized problem and (P_ε). The discrete approximation for (P) consists of two errors: regularization error and discretization error, where for the relation $\varepsilon \sim h^2$ we have estimated the convergence of order $h^{1-\beta}$. In both results analytical investigations were illustrated by numerical experiments.

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A virtual control concept for state constrained optimal control problems

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Keywords: Optimal control, state constraints, boundary control, regularization, virtual control

1. Introduction

A linear quadratic optimal control problem with pointwise state constraints and control constraints is considered. Furthermore, the control acts at the boundary:

$$\begin{array}{lcl} \min & J(y,u) := \dfrac{1}{2}\|y-y_d\|^2_{L^2(\Omega)} + \dfrac{\nu}{2}\|u\|^2_{L^2(\Gamma)} & \\ \text{s. t.} & -\triangle y + y = 0 & \text{in } \Omega \\ & \partial_n y = u & \text{on } \Gamma \\ \text{(P)} & u_a \le u(x) \le u_b & \text{a.e. on } \Gamma \\ & y(x) \ge y_c(x) & \text{a.e. in } \Omega, \end{array}$$

where $\Omega \subset \mathbb{R}^N$, $N = 2, 3$ is a bounded domain with $C^{0,1}$-boundary, $\nu > 0$ is a fixed number, y_d and y_c are given functions from $L^2(\Omega)$. Furthermore, u_a and u_b are given real numbers with $u_a < u_b$.

The difficulty of low regularity of solutions of problems with pointwise state constraints is pointed out in (1). Therefore, different regularization concepts are developed, see e.g. (2), (3), (4) and (5). However, a direct extension of the Lavrentiev regularization concept ((2), (4), (5)) is not possible since the control acts at the boundary. In a recent paper of Tröltzsch and Yousept (6) a source representation was used to overcome this problem.

We consider a modified optimal control problem with regularized state constraints by introducing a virtual control v:

$$\begin{array}{lcl} \min J_\varepsilon(y,u,v) := \dfrac{1}{2}\|y-y_d\|^2_{L^2(\Omega)} + & & \\ \qquad \dfrac{\nu}{2}\|u\|^2_{L^2(\Gamma)} + \dfrac{f(\varepsilon)}{2}\|v\|^2_{L^2(\Omega)} & & \\ \text{s. t.} & -\triangle y + y = g(\varepsilon)v & \text{in } \Omega \\ & \partial_n y = u & \text{on } \Gamma \\ (\mathrm{P}_\varepsilon) & u_a \le u(x) \le u_b & \text{a.e. on } \Gamma \\ & y(x) \ge y_c(x) - h(\varepsilon)v(x) & \text{a.e. in } \Omega \\ & 0 \le v(x) \le v_b & \text{a.e. in } \Omega, \end{array}$$

with a regularization parameter $\varepsilon > 0$. The real valued and positive parameter function $f(\varepsilon)$, $g(\varepsilon)$, and $h(\varepsilon)$ can be chosen in general arbitrarily.

2. Regularization error estimate

First we assume the existence of a feasible inner point concerning the pointwise state constraints:

There exists a function $\hat{u}(x)$ with $u_a \le \hat{u}(x) \le u_b$ a.e. on Γ, such that the corresponding state $\hat{y}$ fulfills $\hat{y}(x) \ge y_c + \tau$ a.e. in Ω for some $\tau > 0$.

This assumption yields the existence and uniqueness of the optimal solutions of both problems. Next, we derive an error estimate for the error between the solution of the unregularized problem (P) and the modified problem (P_ε). Therefore, we construct feasible solutions of the problems based on the optimal solution of the other one respectively.

It is very easy to show the feasibility of the optimal solution $\bar{u}$ of problem (P) for the regularized one, where the virtual control $\bar{v}$ is equal zero. On the other hand, the optimal solution $\bar{u}_\varepsilon$ of the problem (P_ε) is in general not feasible for problem (P). We construct for every $\varepsilon > 0$ the control

$$u_\delta := (1-\delta)\bar{u}_\varepsilon + \delta\hat{u},$$

which is feasible for (P) for every $\delta \in [\delta_\varepsilon, 1]$, where we define

$$\delta_\varepsilon := \frac{\kappa(\varepsilon)}{\kappa(\varepsilon)+\tau}, \quad \kappa(\varepsilon) := h(\varepsilon)v_b + \frac{Cg(\varepsilon)}{\sqrt{f(\varepsilon)}}.$$

With the help of the feasible solutions, we derive the following regularization error estimate:

$$\nu\|\bar{u}-\bar{u}_\varepsilon\|^2_{L^2(\Gamma)} + \|\bar{y}-\bar{y}_\varepsilon\|^2_{L^2(\Omega)} \le C_1\frac{\kappa(\varepsilon)}{\kappa(\varepsilon)+\tau} + C_2\frac{(g(\varepsilon))^2}{f(\varepsilon)}.$$

Furthermore, under the following assumptions

$$\lim_{\varepsilon\to 0} h(\varepsilon) = 0, \quad \lim_{\varepsilon\to 0} \frac{g(\varepsilon)}{\sqrt{f(\varepsilon)}} = 0$$

on the parameter functions, we ensure the strong convergence of the regularized optimal solution $\bar{u}_\varepsilon$ to the optimal solution $\bar{u}$ of problem (P). Moreover, we obtain certain convergence rates for the regularization error. For instance, the choice

$$f(\varepsilon) \equiv 1, \quad g(\varepsilon) = \varepsilon, \quad h(\varepsilon) = \varepsilon$$

yields the approximation rate

$$\|\bar{u} - \bar{u}_\varepsilon\|_{L^2(\Gamma)} = \mathcal{O}(\sqrt{\varepsilon}).$$

3. Numerical tests

We consider several numerical examples illustrating the influence of the parameter functions. To this end, we construct analytical solutions of the problem (P). Furthermore, we investigated the behaviour of the error between the regularized solutions and the optimal solution for $\varepsilon \downarrow 0$ for different settings of the parameter functions $f(\varepsilon)$, $g(\varepsilon)$ and $h(\varepsilon)$.

The numerical tests justify the validity of the regularization error estimate for different choices of the parameter functions. Moreover, we observed, that the calculated approximation rates are better than the expected ones.

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An interior point method for a parabolic optimal control problem with regularized pointwise state constraints

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Keywords: Parabolic optimal control, pointwise state constraints, Lavrentiev type regularization, interior point method

1. Introduction

In this talk, we extend our investigations on interior point methods for elliptic state-constrained optimal control problems in [4] and [2] to the parabolic case.

The main difficulty of the numerical analysis of interior point methods for such problems is the lack of regularity of Lagrange multipliers associated with the state constraints. Therefore, it is helpful to improve the properties of the multipliers have to be improved by suitable regularization techniques.

To consider the interior point algorithm in function space, we suggested in [4], [2] a Lavrentiev type regularization. The Lavrentiev regularization of elliptic problems was introduced in [3]. This method ensures regular Lagrange multipliers and preserves, in some sense, the structure of a state-constrained control problem. Moreover, compared with a direct application of interior point methods to state-constrained problems, the regularization improves the performance of the algorithm, [2].

Here we prove the convergence of a conceptual primal interior point method in function space. We confine ourselves to a problem with linear equation and an objective functional with observation at the final time. This seems to be more challenging in the analysis than functionals of tracking type.

2. Problem Setting

We consider the optimal control problem

$$\min J(y,u) = \frac{1}{2}\|y(T) - y_d\|_\Omega^2 + \frac{\kappa}{2}\|u\|_Q^2 \quad (1)$$

subject to the parabolic initial boundary value problem

$$\begin{aligned} y_t - \nabla\cdot(A\,\nabla y) + c_0 y &= u \quad \text{in } Q, \\ \partial_n y + \alpha y &= 0 \quad \text{in } \Sigma, \\ y(0) &= 0 \quad \text{in } \Omega, \end{aligned} \quad (2)$$

and to the pointwise state constraints

$$y_a(x,t) \le y(x,t) \le y_b(x,t) \quad \text{for all } (x,t) \in Q. \quad (3)$$

In this setting, $\Omega \subset \mathbb{R}^N$, $N \ge 1$ is a bounded domain with $C^{1,1}$-boundary Γ, and $(0,T)$ is a fixed time interval. We define $Q := \Omega \times (0,T)$ and $\Sigma := \Gamma \times (0,T)$.

A is a symmetric matrix with $a_{ij} \in C^{1,\gamma}(\Omega)$, $\gamma \in (0,1)$. It is assumed to satisfy the condition of uniform ellipticity. Moreover, functions $c_0 \in L^\infty(Q)$, $y_d \in L^\infty(\Omega)$ and y_a, y_b from $C(\bar{Q})$ are given that satisfy $y_a(x,t) < y_b(x,t)$ for all $(x,t) \in \bar{Q}$.

3. Interior Point Method

By the interior point method, the constrained problem is transformed into a formally unconstrained problem by adding a logarithmic penalty term to the objective functional J.

First, we intoduce the control-to-state operator G, the observation operator S and the Lavretiev-regularization operator $D := G + \lambda I$. Let $w := D^{-1}u$ the new control.

Now we are able to (re)define the problem:

$$\min F_\mu(w) = \frac{1}{2}\|SDw - y_d\|_\Omega^2 + \frac{\kappa}{2}\|Dw\|^2 \qquad \text{(Q)}$$
$$-\mu \iint_Q \ln(w - y_a) + \ln(y_b - w)\, dx\, dt,$$

where $\mu > 0$ is a path parameter that will tend to zero. To prove the existence of a solution of problem (Q), we apply a method that has been introduced in [4]. It considers the minimization of F_μ in a closed subset and, at the same time, finally permits to show that the solution w_μ has some positive distance to the bounds: We have $y_a + \tau \le w_\mu \le y_b - \tau$ for some sufficiently small $\tau > 0$ that depends on μ. We show that the transformed problems are solvable and that the associated *central path*, i.e. the mapping $\mu \mapsto w(\mu)$ exists.

A conceptual interior point algorithm in function space can be described by the following steps.

Algorithm *Choose* $0 < \sigma < 1$, $0 < eps$, *and an initial function* $w^0 \in L^\infty$ *such that* $y_a + \tau \le w^0 \le y_b - \tau$ *holds for some* $\tau > 0$ *and take* $\mu^0 > 0$.
$k = 0$.
while $\mu^k > eps$ do {
$\mu^{k+1} = \sigma\mu^k$,
$d^{k+1} = -\partial H_w(w^k; \mu^{k+1})^{-1} H(w^k; \mu^{k+1})$
$w^{k+1} = w^k + d^{k+1}$
$k = k + 1$
}

The code-sequence in the while-loop performs one classical Newton step for solving the equation $H(w^{k+1}; \mu^{k+1}) = 0$ for fixed μ_{k+1}. We proof the convergence of this algirithm in function space by using the refined Newton-Mysovskikh theorem provided in [1].

At the end, the theoretical properties of the algorithm are confirmed by numerical examples.

4. Conclusions

We have showed that by a Lavrentiev type regularization, the state constraints are transformed to mixed control-state constraints which, after a simple transformation, can be handled as control constraints. Existence and convergence of the central path are shown. Moreover, the convergence of a short step interior point algorithm is proven in a function space setting.

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EVOLUTION EQUATIONS DETERMINED BY VECTOR AND OPERATOR VALUED MEASURES AND OPTIMAL CONTROL

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1. ABSTRACT

In a previous paper, ref. (1) we considered control problems for differential inclusions of the form

$$dx \in Axdt + B(dt)x + F(t,x)dt + g(t,x)\nu(dt), x(0) = x_0, t \geq o \quad (1)$$

where A is the generator of a C_0-semigroup on a Banach space E and B is an operator valued measure countably additive in the uniform operator topology and ν is a countably additive vector measure having bounded variation and $\{F, g\}$ are respectively multivalued and single valued maps. The control is the vector measure ν. Here we presented several results on the questions of existence of optimal controls and also necessary conditions of optimality for control problems of the form

$$J(\nu) = \int_I \ell(t,x)dt + \Phi(\nu) \longrightarrow \inf, \quad (2)$$

$\nu \in \mathcal{V}_{ad}$ where $\mathcal{V}_{ad}$ is a class of admissible vector measures. We present a brief review of these results.

In a recent paper ref. (2) , we consider the class of evolution equations given by

$$dx = Axdt + B(dt)x + f(t,x)dt + g(t,x)\nu(dt), x(0) = x_0, t \geq o \quad (3)$$

where $\{A, B, \nu\}$ are as described above. Here we consider problems of structural control where the operator valued measure B is treated as control. The objective functional is given by

$$J(B) = \int_I \ell(t,x)dt + \Phi(B) \longrightarrow \inf, \quad (4)$$

$B \in \mathcal{L}_{ad}$, where $\mathcal{L}_{ad}$ is an admissible class of operator valued measures contained in $\mathcal{M}_c(\Sigma, \mathcal{L}(E))$ the space of operator valued measures countably additive in the uniform operator topology having bounded total variation.

Existence of optimal controls for linear and semilinear problems are presented. Some results on necessary conditions of optimality are also presented. The basic results are illustrated by several examples from systems governed by partial differential equations of parabolic and hyperbolic types containing coefficients which are vector measures.

In the study of optimal controls involving operator valued measures as controls many interesting problems related to topology and functional analysis are encountered not seen in the study of regular control problems in infinite dimensional spaces. In refs.(1; 2) we assumed that the operator valued measures are countably additive in the uniform operator topology. Recently we have obtained similar results under weaker assumptions that require countable additivity in the strong or weak operator topologies. For example, parabolic and hyperbolic systems of the forms

$$dx + A(dt)x = f(t,x)\alpha(dt), t \geq 0 \quad (5)$$

$$d\dot{x} + A_o x dt + B(dt)\dot{x} + C(dt)x = f(t)\nu(dt), t \geq 0, \quad (6)$$

generalize the typical models considered by J.L.Lions. Here $\{\alpha, \nu\}$ are countably additive nonnegative measures related to the operator valued measures $\{A, B\}$ respectively.

These results have wider application in systems governed by partial differential equations with coefficients which are measures. This includes systems that may experience continuous

as well as abrupt structural changes. Recently we have been able to extend our previous results on parabolic problems of the type given by (5) to strongly nonlinear problems, see ref (3).

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LYAPUNOV PAIRS AND APPLICATIONS

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Keywords: Lyapunov pair, m-accretive operator, semigroup, global solution, control system

Let X be a real Banach space, let $A : D(A) \subseteq X \to 2^X$ be a multivalued m-accretive operator and let $F : \overline{D(A)} \to X$ be a locally Lipschitz mapping. Given $\xi \in \overline{D(A)}$, we consider the initial value problem

$$\begin{cases} y'(t) + Ay(t) \ni F(y(t)) \\ y(0) = \xi\,. \end{cases}$$

The functions $V, g : \overline{D(A)} \to (-\infty, +\infty]$ form a Lyapunov pair for our problem if for every $\xi \in \mathrm{dom}(V)$ there exist $T > 0$ and a solution $y : [0,T] \to \overline{D(A)}$ such that $t \mapsto g(y(t))$ is integrable on $[0,T]$ and we have

$$V(y(t)) + \int_0^t g(y(s))ds \leq V(\xi) \quad \text{for all } t \in [0,\, T].$$

If $g = 0$, the classical definition of a Lyapunov function V is recovered.

Kokan and Soravia (5, Theorem 1.2) characterized the Lyapunov pairs in terms of viscosity solutions of a related differential inequality.

We provide a different and more explicit characterization of Lyapunov pairs (V, g) without making use of viscosity solutions, namely, V and g form a Lyapunov pair if and only if

$$\underline{D}^A V(x)F(x) + g(x) \leq 0 \quad \text{for all } x \in \mathrm{dom}(V)\,,$$

where $\underline{D}^A V$ is the contingent derivative associated to the operator A. Some requirements needed in (5) are weakened in our treatment.

The characterization of a Lyapunov pair (V, g) given above was already obtained in (4) in the case where X is a Hilbert space, A is a maximal monotone linear operator, F is Lipschitz continuous and V is lower semicontinuous. The approach in (4) is based on the representation formula of the mild solution for a linear operator A. This does not apply in our nonlinear framework.

The abstract result is used to discuss two significant applications. The first one points out the existence of global solutions, i.e., defined on $[0, +\infty)$, of an initial value problem with a multivalued ω-m-accretive operator and a locally Lipschitz term satisfying a unilateral growth condition. This is the consequence of certain a priori estimates which extend those proved by Fattorini (6, Theorem 5.2) in the case where the operator is linear.

The second application sets forth a new method in the study of controllability for a general control system involving a multivalued ω-m-accretive operator and an additional nonlinear term. Specifically, we provide a verifiable criterion of null-controllability with an explicit estimate of the time taken by a state to be steered to the origin. Our controllability results are more general and use a different approach in comparison to the corresponding results in (1; 2; 3).

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Discrete and Continuous Optimization of Asset Replacement in Economics and OR

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Keywords: integer programming; optimal control; technological change; vintage capital models

Vintage capital models of the economic growth theory describe optimal capital replacement under various restrictions on technological change, available resources, and natural environment. Such models are represented by non-linear Volterra integral equations with unknowns in the integration limits [1, 2]. In Operations Research and management science, similar processes of asset (machine, equipment) replacement are usually modeled in discrete time as *integer programming* (*IP*) problems. These two alternative techniques describe the same controlled dynamic process and possess their own theories. A rigorous comparative analysis of these theories is beneficial for both OR and economics.

The paper analyzes continuous and discrete replacement models and explores connections between them. It develops a new innovative methodology to analyze the replacement dynamics under technological change. Such issues as the dynamics of variable optimal lifetime, the impact of technological change, optimal capital accumulation, finite and infinite-horizon optimization, single- and multi-machine replacement, multi-factor production functions with energy and resource factors, nonlinear utility, discontinuous technical progress, and technological breakthroughs are discussed. In particular, it is proven that both continuous and discrete replacement models lead to the same nonlinear integral equations of a new type for optimal asset lifetime. This greatly simplifies the original control problem. The following two sections illustrate the general idea of the talk.

1. A basic discrete replacement model. Let a production shop keep P_j machines during elementary time period j, $j \in \mathbf{N}$, $P_j \in \mathbf{N}$, where $\mathbf{N}$ is the set of natural numbers. In the *discrete time* $j = 0,1,2,\ldots$, the rational machine replacement policy can be described as the *minimization* of the discounted total replacement cost

$$I(m_j, L_j, j = 1,...,T) = \sum_{j=1}^{T} \rho^j Đ_j m_j + \sum_{j=1}^{T} \rho^j \sum_{k=j-L_j}^{j} M_{jk} m_k \qquad (1)$$

under the condition

$$\sum_{j=t-L_i}^{i} m_j = P_i, \quad i = 1,...,T, \qquad (2)$$

with the unknown numbers m_j of purchased new machines and machine lifetimes L_j, $1 \le j \le T$, $T \le \infty$.

The replacement problem (1)-(2) is a *discrete-time IP* problem with the unknowns $m_j \in \mathbf{N}$ and $L_j \in \mathbf{N}$, $0 \le m_j \le m_{\max}$, $0 \le L_j \le L_{j+1}$, $1 \le j \le T$, subjected to constraint (2).

Despite its formal simplicity, model (1)-(2) is pretty general and covers many replacement models. It assumes that the industry operates under conditions of improving technology when newer vintages of machines require less maintenance. In economics, these conditions are known as

the *technological change* embodied in new capital equipment (new *vintages* of machines).

Analysis of problem (1)-(2), including extremum conditions, is difficult. Three assumptions that make (1)-(2) an IP problem are: the time is discrete and integer ($j \in \mathbf{N}$), machine numbers are integer ($m_j \in \mathbf{N}$), and machine lifetimes are integer ($L_j \in \mathbf{N}$). As usually for similar problems, it is beneficial to consider a real-valued analogue of the IP problem. In this talk, we analyze what happens if we relax *all* or *some* of these assumptions. In particular, our approach helps to construct efficient numeric algorithms.

2. Continuous–time replacement model. If we switch from the discrete time $j=1,2,\ldots,T$ to the continuous time $t \in [0,T)$, then the IP problem (1)-(2) leads to the following *optimal control problem*: find the unknown functions $m(t)$ and $L(t)$, $0 \le m(t) \le m_{\max}$, $L(t)' \le 1$, $t \in [0,T)$, that maximize

$$I = \int_0^T e^{-(1-r)t} [Đ(t)m(t) + \\ + \int_{t-L(t)}^{t} M(\tau,t)m(\tau)d\tau]dt, \qquad (3)$$

and satisfy constraint

$$P(t) = \int_{t-L(t)}^{t} m(\tau)d\tau, \quad t \in [0, T), \qquad (4)$$

and a certain initial condition on a prehistory $[L(0), 0]$.

Problem (3)-(4) describes the well-known vintage capital model of a firm, whose modifications have been investigated by Malcomson, van Hilten, Boucekkine, Germain & Licandro, Hritonenko & Yatsenko, and others. We prove that the problem (3)-(4) is convex and derive the *necessary and sufficient condition for an extremum*. It allows us to describe the complete dynamics of the optimal trajectories in the cases of infinite ($T=\infty$) and finite ($T<\infty$) horizons.

The structure of the (3)-(4) solutions appears to be determined by the solution $\tilde{a}(t)$, $t \in [0,\infty)$, of the integral equation

$$\int_t^{a^{-1}(t)} e^{-r(\tau-t)} [M(a(\tau),\tau) - \\ - M(t,\tau)]d\tau = \Pi(t), \quad t \in [0,\infty), \qquad (5)$$

where $a^{-1}(t)$ is the inverse of the function $a(t)=t-L(t)$.

Equation (5) is a key for the optimal replacement decision. There is no general theory for such equations, but our technique allows to analyze and numerically solve (5) in many meaningful special cases. The obtained properties of (5) solutions describe the qualitative dynamics of the optimal asset lifetime; in particular, show how the optimal lifetime depends on the intensity of technological change.

3. Numeric simulation. To demonstrate theoretic advantages and applied benefits of the proposed technique, a numeric example on real automotive industry data about the optimal replacement of passenger cars is considered. We provide a series of experiments with the variable asset lifetime, which confirm the theoretical findings of the paper. In particular, that more intensive technological change decreases the optimal lifetime of assets (and the inverse).

4. Possible generalizations. Modifications of the models (1)-(2) and (3)-(4) can take into account additional assumptions about endogenous technological change, resource restrictions, the environmental impact, economies and diseconomies of scale, fixed and adjustment costs, various financial, demographic, social, and other issues.

In conclusion, some open issues in mathematical modeling of the optimal asset replacement are highlighted.

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On variational aspects of the economic equilibrium problem with application to Pareto optimality

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The variational inequality approach to the economic equilibrium problem in reflexive Banach spaces based on the theory of pseudomonotone multivalued mappings (see [1] and [2]) turns out to be useful to establish some existence results for a class of Pareto optimal problems. The main advantage of this approach is that no interior points of the effective domains of the multiobjective functions under considerations are required.

Let X be a separable, reflexive Banach space, $X^\star$ its dual and $\langle \cdot\,, \cdot \rangle$ the pairing over $X^\star \times X$. Assume $\mathcal{K} \subset X$ to be a closed convex cone with its positive polar $\mathcal{K}^+ = \{\tau \in X^\star \colon \langle \tau, x\rangle \geq 0 \ \ \forall x \in \mathcal{K}\}$. It is not required that $\mathcal{K}$ contains interior points.

Assume that $V_j : X \to \mathbb{R} \cup \{+\infty\}, \quad j = 1, \ldots, m$, are convex, proper and lower semicontinuous functions and $\phi_j : \mathcal{K}^+ \to \mathbb{R}$ with $\phi_j(\tau) \geq 0, \quad \forall\, \tau \in \mathcal{K}^+, \quad j = 1, \ldots, m$, are continuous functions on $\mathcal{K}^+$ with nonnegative values. Set $\overline{V}_j \colon = V_j + \mathrm{ind}_{\mathcal{K}}$, $j = 1, \ldots, m$. Moreover, assume $\Phi = \sum_{j=1}^m \phi_j$.

Consider the following two problems:

Economic Equilibrium Problem: Find $\pi \in \mathcal{K}^+$ and $x_j \in \mathcal{K}$, $j = 1, \ldots, m$, such as to satisfy the conditions:

$$\left.\begin{array}{l} V_j(x_j) = \min\left\{V_j(x) \colon \langle \pi, x\rangle \leq \phi_j(\pi), \ \ x \in \mathcal{K}\right\}, \ j = 1, \ldots, m, \\ \left\langle -\sum\limits_{j=1}^m x_j, \tau - \pi \right\rangle + \Phi(\tau) - \Phi(\pi) \geq 0, \quad \forall\, \tau \in \mathcal{K}^+; \end{array}\right\} \tag{EEP}$$

and

Multiobjective Optimization Problem: Find $\pi \in \mathcal{K}^+$ such that

$$\left.\begin{array}{ll} \text{Minimize} & \left(\Phi(\pi), \overline{V}_1^\star(-\pi), \ldots, \overline{V}_m^\star(-\pi)\right) \\ \text{subject to} & \pi \in \mathcal{K}^+ \setminus \{0\}. \end{array}\right\} \tag{MOP}$$

Based on the existence results established for (EEP) some sufficient conditions for (MOP) will be shown without any requirements concerning the existence of interior points in $\mathcal{K}^+$ for a class of positive homogeneous multiobjective vector functions of an arbitrary positive degree.

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OPTIMAL CONTROL SYSTEMS OF SECOND ORDER WITH INFINITE TIME HORIZON *

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Keywords: infinite horizon systems, optimal control

Let us consider a control system described by the following system of the second order equations

$$\ddot{x}(t) = G_x(t, x(t), u(t)),\ t \in I := (0, \infty)\ a.e, \tag{1}$$

with the initial condition

$$x(0) = 0, \tag{2}$$

where $G : I \times \mathbb{R}^n \times M \to \mathbb{R}$, G_x is the gradient of G with respect to $x \in \mathbb{R}^n$, $M \subset \mathbb{R}^m$ is a fixed set. On the controls $u(\cdot)$ we assume that they belong to a set $\mathcal{U}^p$ of functions belonging to $L^p(I, \mathbb{R}^m)$ that take the values in the set M, $p \in [1, \infty]$. The space of solutions to the above system we define as the classical Sobolev space $H^1(I, \mathbb{R}^n)$ of functions $x : I \to \mathbb{R}^n$ being absolutely continuous on each bounded interval $[0, T] \subset I$ and satisfying the following conditions

$$\int_I |x(t)|^2\, dt < \infty \text{ and } \int_I \left|\dot{x}(t)\right|^2 dt < \infty.$$

Each of the functions $x(\cdot) \in H^1(I, \mathbb{R}^n)$ possesses limits at $t = 0$, $t = \infty$ and $\lim\limits_{t\to\infty} x(t) = 0$. By $H_0^1(I, \mathbb{R}^n)$ we denote the subspace of $H^1(I, \mathbb{R}^n)$ consisting of all functions satisfying initial condition $x(0) = 0$.

We say that a function $x(\cdot) \in H_0^1(I, \mathbb{R}^n)$ is a weak solution to (1)-(2), if

$$\int_I \left\langle \dot{x}(t), \dot{h}(t) \right\rangle + \langle G_x(t, x(t), u(t)), h(t)\rangle\, dt = 0$$

for any $h(\cdot) \in H_0^1(I, \mathbb{R}^n)$.

One can show that weak solution $x(\cdot)$ to (1)-(2) possesses a second order (classical) derivative $\ddot{x}(t)$ for $t \in I$ a.e. and satisfies the control system (1) a.e. on I (we say in such a case that $x(\cdot)$ is a Caratheodory solution to (1)-(2)).

To study optimal control problems connected with control systems defined on unbounded interval I one uses different concepts of optimality of an integral type.

Definition 1 *Let $f : I \times \mathbb{R}^n \times M \to \mathbb{R}$. We say that an admissible pair (i.e. satisfying control system (1)) $(x_*, u_*) \in H_0^1(I, \mathbb{R}^n) \times \mathcal{U}^p$ is*

a) *classically optimal, if*

$$\int_I f(t, x_*(t), u_*(t))dt \le \int_I f(t, x(t), u(t))dt$$

for any admissible pair $(x, u) \in H_0^1(I, \mathbb{R}^n) \times \mathcal{U}^p$;

b) *strongly optimal, if*

$$\lim_{T\to\infty} \Big(\int_0^T f(t, x_*(t), u_*(t))dt - \int_0^T f(t, x(t), u(t))dt\Big) \le 0$$

for any admissible pair $(x, u) \in H_0^1(I, \mathbb{R}^n) \times \mathcal{U}^p$;

c) *overtaking, if*

$$\limsup_{T\to\infty} \Big(\int_0^T f(t, x_*(t), u_*(t))dt - \int_0^T f(t, x(t), u(t))dt\Big) \le 0$$

for any admissible pair $(x, u) \in H_0^1(I, \mathbb{R}^n) \times \mathcal{U}^p$;

d) *weakly overtaking, if*

$$\liminf_{T\to\infty} \Big(\int_0^T f(t, x_*(t), u_*(t))dt - \int_0^T f(t, x(t), u(t))dt\Big) \le 0$$

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for any admissible pair $(x,u) \in H_0^1(I,\mathbb{R}^n) \times \mathcal{U}^p$.

Optimal control problems connected with systems defined on unbounded time interval are called infinite horizon optimal control problems. In the case of bounded interval I, one investigates, in general, one type of cost functional, namely, that given in definition a). When $I = (0,\infty)$ assumptions concerning the integrability of the function $I \ni t \longmapsto f(t,x(t),u(t)) \in \mathbb{R}$ are often too restrictive and they are not fulfilled in some (for example, economical) applications. So, in such a case it is necessary to consider some other concepts of optimality, for instance that given in definitions b), c), d). A review of the concepts of optimality for problems with infinite horizon and their interrelationships are given in (1) (cf. also (2)).

Assuming, among other things, that

a) G, G_x and f are measurable in $t \in I$, continuous in $(x,u) \in \mathbb{R}^n \times M$ and satisfy the following growth condition: there exist constants a_1, a_2, $c_3 > 0$ and functions $b_1(\cdot)$, $b_2(\cdot) \in L^2(I,\mathbb{R})$, $c_1(\cdot)$, $c_2(\cdot)$, $b_3(\cdot) \in L^1(I,\mathbb{R})$, such that

$$a_1 |x|^2 + b_1(t)|x| + c_1(t) \leq G(t,x,u) \leq a_2 |x|^2 + b_2(t)|x| + c_2(t),$$

$$|G_x(t,x,u)| \leq c_3 |x|^2 + b_3(t),$$

for $t \in I$ a.e., $x \in \mathbb{R}^n$, $u \in M$,

b) G is convex in x and lipschitzian in u

we prove that for any admissible control $u(\cdot) \in \mathcal{U}^p$ there exists a unique solution $x_u(\cdot) \in H_0^1(I,\mathbb{R}^n)$ to control system (1)-(2) and it depends continuously on controls. More precisely, if a sequence $(u_k)_{k\in\mathbb{N}} \subset \mathcal{U}^p$ of controls converges in $L^p(I,\mathbb{R}^m)$ with respect to the norm topology to a control $u_0 \in \mathcal{U}^p$, then the sequence $(x_k)_{k\in\mathbb{N}}$ of corresponding trajectories converges weakly in $H_0^1(I,\mathbb{R}^n)$ to x_0 being the trajectory of system (1)-(2), corresponding to control u_0. Consequently, the sequence $(x_k)_{k\in\mathbb{N}}$ converges to x_0 uniformly on each bounded interval $[0,T] \subset I$. If the function G is affine in u and $p = \infty$, the norm convergence of controls can be replaced by the weak-* convergence in $L^\infty(I,\mathbb{R}^m)$.

Using these stability results we prove two theorems (in general case and when G is affine in u) on the existence of classically optimal solution to system (1)-(2). Next, as in (2) for the first order systems, we derive an optimality principle and prove a maximum principle which gives necessary conditions for optimality in the sense of each optimality definition given in Definition 1.

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FLOW-INVARIANCE AND CONTROLLABILITY

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Keywords: flow-invariance; controllability

1. INTRODUCTION

Let X be a Banach space, $a \in \mathrm{R}$, $A : D(A) \subseteq X \to 2^X$ such that $A-aI$ is an m-dissipative operator, $g : X \to X$ a given function, $\xi \in \overline{D(A)}$, and $c(\cdot)$ a measurable control taking values in $D(0,1)$. Here, the problem we consider is how to find a control $c(\cdot)$ in order to reach the origin starting from the initial point ξ in some time T, by C^0-solutions of the state equation

$$\begin{cases} u'(t) \in Au(t) + g(u(t)) + c(t) \\ u(0) = \xi. \end{cases} \tag{1}$$

Let us consider $G : X \to 2^X$, defined by $G(x) = ax + g(x) + D(0,1)$. We can rewrite the above problem as follows. For a given $\xi \in \overline{D(A)}$, find $T > 0$ and a C^0-solution of multi-valued fully nonlinear Cauchy problem

$$\begin{cases} u'(t) \in (A - aI)u(t) + G(u(t)) \\ u(0) = \xi, \end{cases} \tag{2}$$

that satisfies $u(T) = 0$.

2. RESULTS

The main result is given by the following theorem.

Theorem 1. Let X be a Banach space whose dual is uniformly convex, let $A : D(A) \subseteq X \to 2^X$ be such that $A-aI$ is an m-dissipative operator which is the infinitesimal generator of a compact semigroup of contractions, $\{S(t) : \overline{D(A)} \to \overline{D(A)};\ \ t \geq 0\}$, let $g : X \to X$ be a continuous function such that for some $L > 0$ we have

$$\|g(x)\| \leq L\|x\|, \tag{3}$$

for every $x \in X$. Assume $0 \in D(A)$ and $0 \in A0$. Then, for every $\xi \in \overline{D(A)}$ with $\xi \neq 0$ there exists a C^0-solution $u : [0, \infty) \to X$ of (2) which satisfies the inequation

$$\|u(t)\| \leq \|\xi\| - t + (L + a) \int_0^t \|u(s)\| ds \tag{4}$$

for every $t \geq 0$ for which $u(t) \neq 0$.

From this theorem it follows

Corollary 1. Under the hypothesis of Theorem 1 the following properties hold.

(i) In case $L + a \leq 0$, for any $\xi \in \overline{D(A)}$, $\xi \neq 0$, there exist a control $c(\cdot)$ and a C^0-solution of (1) that reaches the origin of X in some time $T \leq \|\xi\|$ and satisfies

$$\|u(t)\| \leq \|x\| - t \tag{5}$$

for any $0 \leq t \leq T$.

(ii) In case $L+a > 0$, for every $\xi \in \overline{D(A)}$ satisfying $0 < \|\xi\| < 1/(L+a)$, there exist a control $c(\cdot)$ and a C^0-solution of (1) that reaches the origin of X in some time

$$T \leq \frac{1}{L+a} \log \frac{1}{1 - (L+a)\|\xi\|},$$

and satisfies

$$\|u(t)\| \leq e^{(L+a)t} \left(\|\xi\| - \frac{1}{L+a} \right) + \frac{1}{L+a} \tag{6}$$

for any $0 \leq t \leq T$.

The proof of Theorem 1 is based on recent flow-invariance results presented in (Cârjă et.al, 2007).

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WEAK SOLUTIONS TO STOCHASTIC INCLUSIONS AND THEIR PROPERTIES

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In the talk we present a martingale problem connected with stochastic inclusions driven by a general semi-martingale. This approach enables us to formulate equivalent results on existence of weak (or martingale) solutions to such inclusions and then analyze some properties of weak solutions set. Presented results extend some of those being known both for deterministic differential inclusions and stochastic differential inclusions driven by Brownian motion.

OPTIMAL CONTROL OF SEMILINEAR CONSTRAINED PARABOLIC INCLUSIONS

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This talk mainly concerns optimal control problems with general endpoint constraints for semilinear parabolic inclusions in reflexive and separable Banach spaces. First we consider the following optimal control problem for *unbounded semilinear evolution inclusions* with general endpoint constraints:

$$\text{minimize} \quad I[x] = \phi\big(x(1)\big)$$

over *mild* continuous trajectories $x\colon [0,1] \to X$ for the semilinear evolution inclusion

$$\dot{x}(t) \in Ax(t) + F(x(t),t), \quad x(0) = x_0 \in X$$

subject to the endpoint constraint

$$x(1) \in \Omega \subset X,$$

where $A\colon X \to X$ is an *unbounded* generator of the *compact* C_0-semigroup $\{e^{At}|\ t \geq 0\}$ and where $\Omega \subset X$ is a closed set of a reflexive and separable space X. A special case of $F(x,t) = f(x,U,t)$ with a control set U relates to semilinear control evolution *equations* considered in PDE control theory for *smooth* data.

Developing the method of *discrete approximations* [1, 2, 3], we establish *stability* of discrete approximations in the sense of the *uniform convergence* of their optimal solutions to the reference optimal solution for the original problem. Based on the advanced tools of variational analysis and generalized differentiation, we derive *necessary optimality conditions* for discrete-time problems and then, by passing to the limit from discrete approximations, obtain necessary conditions of the *Euler-Lagrange type* for the above problem governed by unbounded evolution inclusions.

The method of discrete approximations and the necessary optimality conditions derived for the above control problem governed by evolution inclusions are applied to the following

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optimal control problem governed by *multidimensional semilinear parabolic inclusions*:

$$\text{minimize} \quad J[y] = \int_0^T \int_\Omega \varphi\big(y(t,x)\big)\, dxdt$$

over continuous *mild* solutions $y\colon [0,T] \times I\!R^n \to I\!R^n$ to the semilinear parabolic partial differential inclusion

$$\begin{cases} y_t \in \Delta y + G(t,x,y), & (t,x) \in (0,T) \times \Omega, \\ y\,|_{\partial\Omega} = 0, & \\ y(0,x) = y_0(x), & x \in \Omega \subset I\!R^n, \end{cases}$$

where $G\colon [0,T] \times \Omega \times I\!R^n \rightrightarrows I\!R^n$ is a set-valued mapping between finite-dimensional spaces.

The results obtained on necessary optimality conditions seem to be among the first results in the literature dealing with optimization problems governed by *parabolic inclusions* vs. equations, although most of them are also new for *nonsmooth* equations. Their formulations involve the basic generalized differential constructions by the first author comprehensively developed in [1].

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EVOLUTION OF VISCOELASTIC CONTACT PROBLEMS FOR PIEZOELECTRIC MATERIALS WITH ADHESION *

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Keywords: Hemivariational inequality, piezoelectric, Clarke subdifferential, adhesion, pseudomonotone, viscous, evolution inclusion.

In this paper we consider a second order evolution inclusion with a coercive viscosity operator and a multivalued term of subdifferential form. The study is motivated by the dynamic problem of frictional contact between a viscoelastic piezoelectric deformable body and a foundation. The interaction between the body and the foundation is described, due to the skin effects, by a nonmonotone possibly multivalued law between the bonding forces and the corresponding displacements. This law is expressed by the Clarke subdifferential of a locally Lipschitz nonconvex nonsmooth superpotential and leads to a hemivariational inequality of hyperbolic type. Such inequality results from the d'Alembert principle for a dynamic mechanical system (1; 6).

On the other hand our model concerns piezoelectric materials. Such materials are dielectrics which exhibit significant deformations in response to an applied electric field (direct efect) as well as dielectric polarization in response to mechanical strains (converse efect). Both effects were discovered by Jacques and Pierre Curie in 1880-1881 but only recently such bodies have been used in smart material technology. The linear constitutive equations coupling the mechanical and electrical quantities in the piezoelectric materials were formulated by Voigt in 1910.

Some materials are naturally piezoelectric, e.g. crystals, living bones, human skin, etc., other that are manufactured with piezoelectric characteristics are very important in many applications, e.g. in biomechanics, biomedicine, structural mechanics and in particular as sensors, actuators, transducers, speakers and electronic clocks.

The present paper is a continuation of (2; 3; 4; 5), where the existence and uniqueness results for the hemivariational inequalities modeling the frictional contact for the piezoviscoelastic materials were delivered. Our model problem consists of a system coupled with the evolution hemivariational inequality for the displacement, a time dependent stationary equation for the electric potential and an ordinary differential equation for the bonding field. We prove the existence of a weak solution to an abstract formulation of the mechanical problem. Applications to contact problems of electro-viscoelasticity are discussed.

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ON INTEGRODIFFERENTIAL HEMIVARIATIONAL INEQUALITIES FOR VISCOELASTIC MATERIALS WITH LONG MEMORY TERM *

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Keywords: Hemivariational inequality, Clarke subdifferential, evolution inclusion, viscoelasticity, Volterra integral term, frictional contact problem, weak solution.

Phenomena of contact between deformable bodies abound in industry and everyday life. Contact of braking pads with wheels, tires with roads, pistons with skirts are just a few simple examples. Common industrial processes such as metal forming, metal extrusion, involve contact evolutions. Owing to their inherent complexity, contact phenomena are modelled by nonlinear evolutionary problems.

We consider a class of abstract evolution hemivariational inequalities in the study of frictional contact problems for viscoelastic materials with long memory term. In the model dynamic equation of motion is considered with the viscoelastic constitutive relationship of the Kelvin-Voigt type, the contact is bilateral and the friction is modeled with Tresca's law. The term responsible for memory of the body is given in the integral form of a linear continuous operator. The multivalued boundary condition comes from the nonconvex superpotential and can be written in the form of a general subdifferential. The latter leads to hemivariational inequalities as a variational formulation of our problem. The aim of this presentation is to establish the existence of weak solutions to the problem by using arguments of evolution hemivariational inequalities, in particular a surjectivity result for pseudomonotone mappings and a fixed point theorem.

We also study the dependence of the solution on the memory term and derive a convergence result. We show that a sequence of solutions corresponding to a long memory material converges to a solution of the problem with short memory as the relaxation coefficient tends to zero.

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Quasilinear parabolic variational inequalities: Existence and Comparison

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Keywords: Parabolic variational inequality; Sub-supersolution; Existence; Comparison

1. Abstract

Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with Lipschitz boundary $\partial\Omega$, $Q = \Omega \times (0,\tau)$ and $\Gamma = \partial\Omega \times (0,\tau)$, $\tau > 0$. In this note we are concerned with existence and comparison results of the following parabolic variational inequality:

$$u \in Y_0 \cap K,\ u(\cdot,0) = 0 :$$

$$\langle u_t + A(u) + F(u) - h, v - u\rangle \geq 0, \qquad (1)$$

for all $v \in K$, where K is a closed, convex subset of $X_0 := L^p(0,\tau; W_0^{1,p}(\Omega))$, $Y_0 = \{u \in X_0 : u_t \in X_0^*\}$, $\langle\cdot,\cdot\rangle$ denotes the duality pairing between X_0^* and X_0, and $p \in [2,\infty)$. The operator $A : X_0 \to X_0^*$ is related with a nonlinear elliptic operator of Leray-Lions type in divergence form given by

$$A(u)(x,t) = -\sum_{i=1}^{N} \frac{\partial}{\partial x_i} a_i(x,t,\nabla u(x,t)),$$

and F is the Nemytskij operator associated with the Carathéodory function $f :\ Q\times\mathbb{R}\times\mathbb{R}^N \to \mathbb{R}$ by

$$F(u)(x,t) = f(x,t,u(x,t),\nabla u(x,t)).$$

We assume that $h \in L^{p'}(Q) \subset X_0^*$, where p' is the Hölder conjugate of p.

Solutions of the variational inequality (1) are usually referred to as *strong* solutions. There is a large number of papers dealing with parabolic inequalities under different structure and regularity hypotheses of the data such as, e.g., (Charrier et.al, 1978; Chipot et.al, 1988; Nagase, 1989; Papageorgiou et.al, 1997; Puel, 1976; Troianiello, 1983; Vivaldi, 1987) and the recent survey paper (Rudd et.al, 2002).

Our main goal is to provide a systematic development of the method of sub-supersolutions for the parabolic variational inequality (1) for general convex sets K. While the sub-supersolution method is well established for parabolic equations that result from (1) in case that K is the entire space X_0, there are only a few papers dealing with sub-supersolutions for (1) for special K. Also, as will be seen in the sequel, the arguments for parabolic variational inequalities do not follow straightforwardly from neither those for elliptic inequalities, nor those for parabolic equations.

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Scalar Periodic Problems at Resonance with p-Laplacian-Like Operator

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Keywords: hemivariational inequality, Clarke subdifferential, resonance, p-Laplacian-like operator, critical point theory

1. STATEMENT OF PROBLEM

In this paper we prove the existence of multiple solutions for the following nonlinear periodic problem:

$$\begin{cases} \big(a(t,u'(t))\big)' + \partial j(t,u(t)) \ni 0 \\ \qquad\qquad \text{for a.a. } t \in (0,T), \\ u(0) = u(T), \quad u'(0) = u'(T). \end{cases} \tag{1}$$

Here $(t,y) \longmapsto a(t,y)$ is a set-valued map and $\partial j(t,\zeta)$ is the generalized subdifferential of a generally nonsmooth locally Lipschitz potential $\zeta \longmapsto j(t,\zeta)$. Let $p \in (1,+\infty)$ and consider the Sobolev space $W^{1,p}_{per}((0,T)) = \{u \in W^{1,p}((0,T)) : u(0) = u(T)\}$. Recall that $W^{1,p}((0,T))$ is embedded into $C([0,T])$ and so the pointwise evaluation at $t=0$ and $t=T$ make sense. For a given $u \in W^{1,p}_{per}((0,T))$, the multivalued term $\big(a(t,u'(t))\big)'$ is interpreted as follows: $\big(a(t,u'(t))\big)' = \{v' \in L^{p'}((0,T)),\ v(t) \in a(t,u'(t)) \quad \text{for a.a. } t \in (0,T)\}$, where $\frac{1}{p} + \frac{1}{p'} = 1$. Here derivative v' is understood in the sense of distributions. By a solution of problem (1) we mean a function $u \in C^1([0,T])$, such that $v'(t) = -u^*(t) \quad \text{for a.a. } t \in (0,T)$, with $v' \in \big(a(\cdot,u'(\cdot))\big)'$ and $u^* \in L^{p'}((0,T))$, $u^*(t) \in \partial j(t,u(t))$ for almost all $t \in (0,T)$.

Our hypotheses on the set-valued map $a(t,y)$, include as a special case the scalar p-Laplacian differential operator. Recently there has been increasing interest for second order scalar periodic differential equations involving the p-Laplacian differential operator. We mention the works of (Dang and Oppenheimer, 1996), (del Pino et.al, 1992), (Fabry and Fayyad, 1992), (Gasiński and Papageorgiou, 2002, 2003), (Guo, 1993), (Papageorgiou and Papageorgiou, 2004), (Gasiński, to appear , a,b).

2. EXISTENCE RESULT

The precise hypotheses on the data of (1) are the following:

$\underline{H(a)}$: $a(t,y) = \partial G(t,y)$, where $G\colon (0,T) \times \mathbb{R} \longrightarrow \mathbb{R}$ is a functional, such that:

(i) the function $(t,y) \longrightarrow G(t,y)$ is continuous;

(ii) for every $t \in (0,T)$, the function $y \longmapsto G(t,y)$ is strictly convex, $G(t,0) = 0$ for all $t \in (0,T)$ and

$$\partial G(0,\cdot) = \partial G(T,\cdot);$$

(iii) for all $t \in (0,T)$, all $y \in \mathbb{R}$ and all $v^* \in a(t,y) = \partial G(t,y)$, we have

$$|v^*| \leqslant a_1(t) + c_1|y|^{p-1},$$

with $a_1 \in L^{p'}((0,T))_+$ (where $\frac{1}{p} + \frac{1}{p'} = 1$), $c_1 > 0$;

(iv) for all $t \in (0,T)$, all $y \in \mathbb{R}$ and all $v^* \in a(t,y)$, we have

$$v^* y \leqslant pG(t,y);$$

(v) for all $t \in (0,T)$ and all $y \in \mathbb{R}$, we have

$$c_0|y|^p \leqslant G(t,y),$$

for some $c_0 > 0$.

Suppose that $\beta \in C_{per}([0,T])$, $\beta \geqslant \gamma > 0$ for all $t \in (0,T)$ and

$$G(t,y) = \frac{1}{p}\beta(t)|y|^p.$$

Then

$$a(t,y) = \partial G(t,y) = \beta(t)|y|^{p-2}y$$

satisfies hypotheses $H(a)$ and the resulting differential operator is a weighted p-Laplacian. If $\beta \equiv 1$, then we have the p-Laplacian. We remark that hypotheses $H(a)$ do not require that the differential operator is homogeneous.

Another possibility of G is the following

$$G(t,y) \;=\; \frac{\beta(t)}{p}\big[(1+y^2)^{\frac{p}{2}}-1\big],$$

with $p>1$ and $\beta\in C_{per}([0,T])$, $\beta(t)\geqslant\gamma>0$ for all $t\in(0,T)$.

One more possibility of G is the following

$$G(t,y) \;=\; \frac{\beta(t)}{p}\big[(1+|y|)^{p}-1\big],$$

where $p>1$ and β are as above. In this case, the map a is really multivalued and it still satisfies hypotheses $H(a)$.

As for the potential function j we will assume the following basic assumptions.

$\underline{H(j)_1}$ $j\colon(0,T)\times\mathbb{R}\longrightarrow\mathbb{R}$ is a function, such that

(i) for every $\zeta\in\mathbb{R}$, the function $t\longrightarrow j(t,\zeta)$ is measurable;

(ii) for almost all $t\in(0,T)$, the function $\zeta\longmapsto j(t,\zeta)$ is locally Lipschitz with $L^{p'}((0,T))_+$-Lipschitz constant;

(iii) for every $M>0$, there exists $\widehat{a}_M\in L^1((0,T))_+$, such that for almost all $t\in(0,T)$, all $|\zeta|\leqslant M$ and all $u^*\in\partial j(t,\zeta)$, we have

$$|u^*| \;\leqslant\; \widehat{a}_M(t);$$

Besides, we will assume also resonance conditions of various type: Landesman-Lazer-type, Tang-type or some other known in the literature. Under all these hypothesis we will show several existence results for problem (1).

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Five nontrivial solutions with precise sign data for a p-Laplacian equation

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Abstract: We consider nonlinear elliptic problems driven by the p-Laplacian with a nonsmooth potential depending on a parameter $\lambda > 0$. The main result guarantees the existence of two positive, two negative and a nodal (sign-changing) solution for the studied problem whenever λ belongs to a small interval $(0, \lambda^*)$ and $p \geq 2$. We do not impose any symmetry hypothesis on the nonlinear potential. The constant-sign solutions are obtained by using variational techniques based on nonsmooth critical point theory (minimization argument, Mountain Pass theorem, and a Brezis-Nirenberg type result for C^1-minimizers), while the nodal solution is constructed by an upper-lower solutions argument combined with the Zorn lemma and a nonsmooth second deformation theorem.

Nodal and multiple constant sign solutions for equations with the p-Laplacian

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Abstract: We consider nonlinear elliptic equations driven by the p-Laplacian with a nonsmooth potential (hemivariational inequalities). We obtain the existence of multiple nontrivial solutions and we determine their sign (one positive, one negative and the third nodal). Our approach uses nonsmooth critical point theory coupled with the method of upper-lower solutions.

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NONHOMOGENOUS BOUNDARY VALUE PROBLEM FOR SEMILINEAR HYPERBOLIC EQUATION. STABILITY

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Keywords: Nonhomogenous boundary value problem, semilinear equation of vibraiting string, dual variational method

Let Ω be an open bounded domain in R^n, with boundary Γ, assumed to be sufficiently smooth. The aim of the paper is to study the second order hyperbolic semilinear mixed problem with Dirichlet boundary condition:

$$\begin{aligned} &x_{tt}(t,y)-\Delta x(t,y)+f(t,y,x(t,y))=0\\ &x(0,y)=x^0(y),\ x_t(0,y)=x^1(y),\ y\in\Omega\\ &x(t,y)=u(t,y),\ (t,y)\in\Sigma=(0,T)\times\Gamma. \end{aligned} \tag{1}$$

We study existence of solutions to (1) over a finite interval $[0,T]$, depending on smoothness of the data. We exlude blowing up in finite time of solutions to (1) imposing hypothesis **Gw3,** which relates some interaction between growth of f and length of time T.The importance of the problem with control on the boundary appears in optimal control theory see e.g. [1].

We study (1) by variational method, i.e. we shall consider (1) as the Euler—Lagrange equation of the functional:

$$\begin{aligned} J^w(x)=\int_0^T\{&\frac{1}{2}\left\|\Lambda^{-1}\nabla x(t,\cdot)\right\|^2_{H^{-1}(\Omega)}\\ &-\frac{1}{2}\left\|\Lambda^{-1}x_t(t,\cdot)\right\|^2_{H^{-1}(\Omega)}\}dt\\ &+\int_0^T\int_\Omega F(t,y,x(t,y))\,dydt\\ &-\left\langle x(T,\cdot),\Lambda^{-1}x^1(\cdot)\right\rangle_{L^2(\Omega)} \end{aligned} \tag{2}$$

where $F_x=f$, defined on some subspace of functions of the space $C([0,T];H^{-1}(\Omega))$.

Our purpose is to investigate (1) by studying critical points of functional (2). To this effect we apply a new duality approach which is based on ideas developed in [2]. Our aim is to find a nonlinear subspace X^w of $C([0,T];H^{-1}(\Omega))$ and study (2) just only on X^w. The main difficulty in our approach is just the construction of the set X^w.

Let $\mathcal{L}^w=\left\{g:g\in L^1(0,T;H^{-1}(\Omega))\right\}$ and let $x^0\in L^2(\Omega)$, $x^1\in H^{-1}(\Omega)$ and $u\in L^2(\Sigma)$

$$\begin{aligned} U^w=\{&x:x\in C([0,T];L^2(\Omega)),\\ &\frac{\partial x}{\partial t}\in C([0,T];H^{-1}(\Omega)),x_{tt}-\Delta x\in\mathcal{L}^w,\\ &x(0,\cdot)=x^0(\cdot),\ x_t(0,\cdot)=x^1(\cdot),\\ &x(t,y)=u(t,y),\ (t,y)\in\Sigma=(0,T)\times\Gamma\},\\ U^{w1}&=C([0,T];L^2(\Omega)),\\ U^{w2}&=C([0,T];H^{-1}(\Omega)). \end{aligned}$$

We know: $\Delta:H^1_0(\Omega)\to H^{-1}(\Omega)$, $\Delta=\Lambda^2$ where $\Lambda:H^1_0(\Omega)\to L^2(\Omega)$.

We assume the following hypotheses:

Gw1 *there exists a function* $\overline{z}^w\in U^{w1}$ *such that* $F_x(\overline{z}^w)\in\mathcal{L}^w$; $(F_x(h)=F_x(\cdot,\cdot,h(\cdot,\cdot)))$.

Gw2 F *is differentiable with respect to the third variable in* R *and for almost all* $(t,y)\in(0,T)\times\Omega$ $F_x(t,y,\cdot)$ *is continuous in* R.

Let $I^w=\left[-TB^w\sup_{t\in(0,T)}\|\overline{z}^w(t,\cdot)\|_{L^2(\Omega)},\ TB^w\sup_{t\in(0,T)}\|\overline{z}^w(t,\cdot)\|_{L^2(\Omega)}\right]$.
We define the set $\overline{X}^w=\left\{x\in U^w:\ \|x(t,\cdot)\|_{L^2(\Omega)}\in I^w,\ t\in(0,T)\right\}$.

Gw3 $F_x(t,y,0)\neq 0$, *for a.e.* $(t,y)\in(0,T)\times\Omega$; $(t,y)\to F(t,y,x(t,y))$ *is integrable on* $(0,T)\times\Omega$ *for* $x\in\overline{X}^w$ *and*

$$\begin{aligned} &\sup_{x\in\overline{X}^w}\|F_x(t,\cdot,x(t,\cdot))\|_{H^{-1}(\Omega)}\\ \leq\ &\sup_{t\in(0,T)}\|\overline{z}^w(t,\cdot)\|_{L^2(\Omega)},\ t\in(0,T), \end{aligned} \tag{3}$$

Gw4 $F_x(\cdot,\cdot,x(\cdot,\cdot)) \in \mathcal{L}^w$, $F_x(\cdot,\cdot,x(\cdot,\cdot)) \in L^2(\Sigma)$, *for* $x \in \overline{X}^w$, $F(t,y,x) \geq a(t,y)x + b(t,y)$, *for some* $a, b \in L^1((0,T)\times\Omega)$, $x \in \mathbf{R}$.

The dual functional reads

$$J_D^w(p,q) = -\int_0^T \int_\Omega F^*(t,y,\Lambda^{-1}(p_t(T-t,y) + div\ q(t,y)))dydt \quad (4)$$
$$-\frac{1}{2}\int_0^T \left\|\Lambda^{-1}q(t,\cdot)\right\|^2_{H^{-1}(\Omega)} dt$$
$$+\frac{1}{2}\int_0^T \left\|\Lambda^{-1}p(T-t,\cdot)\right\|^2_{H^{-1}(\Omega)} dt$$
$$+\left\langle x^0(\cdot), \Lambda^{-1}p(T,\cdot)\right\rangle_{L^2(\Omega)}$$
$$-\int_\Sigma \left\langle u(t,y), \Lambda^{-1}q(t,y)\,\nu(y)\right\rangle dydt$$

where, for a.e. $t \in [0,T]$, $p_t(T-t,\cdot) + div\ q(t,\cdot)$ is an element of $H^{-1}(\Omega)$, ν is outer normal to Ω and F^* is Fenchel conjugate to F.

The main results of the paper are the following existence theorem.

Theorem 1. *There is* $\overline{x} \in X^w$, *that* $\inf_{x\in X^w} J^w(x) = J^w(\overline{x})$. *Assume that the functional* $x \to \int_0^T \int_\Omega F(t,y,x(t,y))dydt$ *is subdifferentiable (in the sense of convex analysis) at the point* $\bar{x} \in U^w$. *Then there is* $(\overline{p},\overline{q}) \in U_D$ *such that* $J_D^w(\overline{p},\overline{q}) = \inf_{x\in X^w} J^w(x) = J^w(\overline{x})$ *and the following system holds, for* $t \in [0,T]$, $\Lambda^{-1}\overline{x}_t(t,\cdot) = \Lambda^{-1}\overline{p}(T-t,\cdot)$, $\Lambda^{-1}\nabla\overline{x}(t,\cdot) = \Lambda^{-1}\overline{q}(t,\cdot)$, $\Lambda^{-1}(-\overline{p}_t(T-t,\cdot) - div\ \overline{q}(t,\cdot)) = -\Lambda^{-1}F_x(t,\cdot,\overline{x}(t,\cdot))$.

and stability

Theorem 2. *Let* $\{u_n\}$, $\{x_n^0\}$, $\{x_n^1\}$ *given sequences in* $L^2(\Sigma)$, $L^2(\Omega)$, $H^{-1}(\Omega)$ *respectively, converging to* $\bar{u}$, $\bar{x}^0$, $\bar{x}^1$ *in* $L^2(\Sigma)$, $L^2(\Omega)$, $H^{-1}(\Omega)$ *respectively. Then there is a subsequence of* $\{x_n\}$ *- solutions to (1) corresponding to* $\{u_n\}$, $\{x_n^0\}$, $\{x_n^1\}$, *which we denote again by* $\{x_n\}$ *weakly convergent in* $L^2(0,T,L^2(\Omega))$ *to an element* $\bar{x} \in U^w$ *being the solution to (1) corresponding to* $\bar{u}$, $\bar{x}^0$, $\bar{x}^1$.

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SHAPE OPTIMIZATION IN 3D CONTACT PROBLEMS WITH COULOMB FRICTION

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Keywords: equilibrium constraint, contact problem, quasi-variational inequality

1. INTRODUCTION

Since 1980, a considerable attention of applied mathematicians has been devoted to unilateral contact problems with Coulomb friction, cf. [2] and the references therein. Concerning the static case, our comprehension has reached a fairly satisfactory level. In [1], the authors have developed a numerical approach to a class of optimization problems, where one computes optimal shape of a 2D elastic body in contact with a rigid obstacle which obeys the Coulomb friction law. The problem has been formulated as a mathematical program with equilibrium constraints (MPEC) and solved via the so called implicit programming approach (ImP), cf. [5]. The technique from [1] cannot be, however, extended to the 3D case in a straightforward way. The reason is the nonpolyhedral nature of the subdifferential map of the Euclidean norm in $\mathbb{R}^n$, whenever $n \geq 2$. Whereas the stability and sensitivity analysis of variational inequalities/generalized equations over polyhedral constraint sets has been developed quite deeply so far, much less is known about the nonpolyhedral case. This holds in particular for the generalized equation (GE) modeling the investigated 3D contact problem. Further, also the numerical solution of this GE with a fixed shape of the body (which is the state problem in our MPEC) is substantially more demanding. The main aim of this contribution is to extend the ImP technique of [1] to the 3D case, which requires to discretize this MPEC by finite elements, to construct a fast and precise solver for the state problem and, by using tools of sensitivity analysis, to compute a "subgradient" information, needed in the used nonsmooth optimization method.

2. NUMERICAL APPROACH

Our workhorse in sensitivity analysis is the generalized differential calculus of B. Mordukhovich ([4]) which is applied to the solved (discretized) MPEC along the lines of [3]. The main difficulty arises thereby in the treatment of the generalized equation

$$\begin{array}{rcl} 0 & \in & A_{\tau\tau}(x)u_\tau + A_{\tau\nu}(x)u_\nu - l_\tau(x) \\ & & \qquad\qquad + \widetilde{Q}(u_\tau, \lambda), \\ 0 & = & A_{\nu\tau}(x)u_\tau + A_{\nu\nu}(x)u_\nu - l_\nu(x) \\ 0 & \in & u_\nu + x + N_{\mathbb{R}^p_+}(\lambda), \end{array} \tag{1}$$

defining the discretized state problem. In this model we have to do only with nodes laying on the contact boundary which shape is subject to optimization. The state variable $y = (u_\tau, u_\nu, \lambda) \in \mathbb{R}^{2p} \times \mathbb{R}^p \times \mathbb{R}^p_+$, where p is the number of nodes, u_τ is the vector of tangent displacements, u_ν is the vector of normal displacements and λ is the multiplier associated with the nonpenetrability constraint

$$u_\nu + x \geq 0. \tag{2}$$

In (1), (2) the control $x \in \mathbb{R}^p$ specifies the shape of the contact boundary. $A_{\tau\tau}, A_{\tau\nu}, A_{\nu\tau}$ and $A_{\nu\nu}$ are blocks of the appropriate restriction of the stiffness matrix which depend on x in a continuously differentiable way. This holds true also for the vectors l_τ, l_ν reflecting the action of external forces. The multifunction $\widetilde{Q}$ in the first line of (1) is given by

$$\widetilde{Q}(u_\tau, \lambda) = \lambda \bullet \partial j(u_\tau), \quad j(u_\tau) = \mathcal{F} \sum_{i=1}^{p} \|u_\tau^i\|,$$

where u_τ^i is the tangential displacement of the ith node, $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^2, \mathcal{F} > 0$

is the friction coefficient and " $\bullet$ " denotes the Hadamard product.

The shape optimization problem is defined as follows:

$$\begin{array}{ll} \text{minimize} & f(x,y) \\ \text{subject to} & \\ & y \text{ solves the GE (1)} \\ & x \in \omega, \end{array} \tag{3}$$

where f is the objective and ω is the set of admissible controls. Since (1) defines a single-valued and locally Lipschitz map S assigning x the corresponding state variable y, problem (3) amounts to the nonsmooth program

$$\begin{array}{ll} \text{minimize} & \Theta(x) := f(x, S(x)) \\ \text{subject to} & \\ & x \in \omega. \end{array} \tag{4}$$

The step from (3) to (4) is the core of ImP. To solve (4) numerically, one needs to be able to compute at each $x \in \omega$ the corresponding state variable $y = S(x)$ and one arbitrary vector ξ from the Clarke subdifferential of Θ. In our approach this is done by solving the (regular) *adjoint generalized equation*.

$$0 \in \nabla_y f(x,y) \quad + \quad (\nabla_y F(x,y))^T v + \widehat{D}^* Q(y, -F(x,y))(v) \tag{5}$$

in variable v, where $y = S(x)$ and F, Q denote the single-valued and the multi-valued part in (1), respectively. $\widehat{D}^*Q$ is the regular coderivative which is replaced sometimes by the limiting coderivative D^*Q, cf.[3]. Having computed a solution v of (5), we use the formula

$$\xi = \nabla_x f(x,y) + (\nabla_x F(x,y))^T v$$

to arrive at the desired subgradient. As nonsmooth optimization solver, we use the classical bundle-trust algorithm from (6). We provide numerical results of several test examples to illustrate the properties of the proposed approach.

3. CONCLUSION

The investigated optimization problem belongs to the hardest MPECs ever solved. This concerns both the applied tools from variational analysis as well as numerical complexity and dimensionality. In the numerical treatment some other alternatives are available and deserve a proper testing.

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ELLIPTIC CONTROL SYSTEMS IN UNBOUNDED SETS

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Keywords: elliptic systems, continuous dependence on parameters, Sobolev spaces

1. Introduction

Let $0 \leq N_+ \leq N$. Consider the boundary value problem

$$\begin{cases} \operatorname{div}\left[A_i(x)\nabla z_i(x)\right] - c_i(x)\, z_i(x) = \\ = \dfrac{\partial F}{\partial z_i}(x, z(x), u(x)), \ 1 \leq i \leq N_+, \\ \operatorname{div}\left[A_i(x)\nabla z_i(x)\right] - c_i(x)\, z_i(x) = \\ = -\dfrac{\partial F}{\partial z_i}(x, z(x), u(x)), \ N_+ < i \leq N, \\ z_1(x) = \ldots = z_N(x) = 0 \text{ for } x \in \partial\Omega, \end{cases}$$

in the variational setting.

The system is defined in an open set $\Omega \subseteq \mathbb{R}^n$, $n \geq 1$, that ensures the compact embedding of the Sobolev space $H_0^1(\Omega)$ into $L^2(\Omega)$. A sufficient condition of the compactness is the equality

$$\lim_{|x|\to+\infty} \lambda_n(\Omega \cap B(x,1)) = 0,$$

where λ_n denotes the Lebesgue measure and $B(x,1)$ is the unit ball centered at x; see [2].

The functions $F = F(x,z,u) : \Omega \times \mathbb{R}^N \times \mathbb{K} \longmapsto \mathbb{R}$, $c_1, \ldots, c_N : \Omega \longmapsto \mathbb{R}$ and the matrix mappings $A_1, \ldots, A_N$ are assumed to be known.

The parameter u is an element of the set

$$\mathfrak{U}^p_{r,\mathbb{K}} := \{u \in L^p(\Omega)^m : \|u\|_{L^p} \leq r, \ u(x) \in \mathbb{K} \text{ for a.e. } x \in \Omega\}$$

with the chosen measurable set $\mathbb{K} \subseteq \mathbb{R}^m$ and numbers $r > 0$ and $p \in [1, +\infty)$. The set $\mathfrak{U}^p_{r,\mathbb{K}}$ can be interpreted as the set of admissible controls.

If $N_+ = N$, the system takes on the form

$$\begin{cases} \operatorname{div}\left[A_i(x)\nabla z_i(x)\right] - c_i(x)\, z_i(x) = \\ = \dfrac{\partial F}{\partial z_i}(x, z(x), u(x)), \ 1 \leq i \leq N, \\ z_1(x) = \ldots = z_N(x) = 0 \text{ for } x \in \partial\Omega. \end{cases}$$

A similar reduction happens when $N_+ = 0$.

The paper concerns weak solutions to the system: the existence, the continuous dependence on a parameter, and the optimality with respect to a cost functional. The solutions of the system are examined through the associated functional of action

$$\mathcal{F}^u(z) := \frac{1}{2}\left(\sum_{i=1}^{N_+} \|z_i\|_i^2 - \sum_{i=N_++1}^{N} \|z_i\|_i^2\right) + \int_\Omega F(x, z(x), u(x))\, dx, \tag{1}$$

where $\|\cdot\|_i$, $1 \leq i \leq N$, are the $H_0^1(\Omega)$-norms related to the system:

$$\|v\|_i^2 := \int_\Omega A_i(x)\nabla v(x) \cdot \nabla v(x)\, dx + \int_\Omega c_i(x)\, |v(x)|^2\, dx$$

for each $v \in H_0^1(\Omega)$. The critical points of the functional and the weak solutions of the system are the same, which follows from the assumptions made about the system. Among other things, the function F is supposed to be of Carathéodory type and satisfy certain growth conditions, so that functional (1) is

well defined and Gâteaux-differentiable:

$$\langle D\mathcal{F}^u(z), h\rangle := \sum_{i=1}^{N_+}(z_i,h_i)_i - \sum_{i=N_++1}^{N}(z_i,h_i)_i + \int_\Omega \frac{\partial F}{\partial z}(x,z(x),u(x))\cdot h(x)\,dx$$

for each $z, h \in H_0^1(\Omega)^N$.

2. Main results

First comes a theorem on the existence of weak solutions to the system; the proof uses Ky Fan's minimax theorem [4] or, for the reduced system, the coercivity argument. The set of weak solutions turns out to be compact in the Sobolev space.

Second, the author addresses the continuous dependence of weak solutions on the parameter u. The results involve the strong Painlevé-Kuratowski convergence of sets on the side of solutions and the three topologies—strong, of convergence in measure, and weak—on the side of parameters. It is crucial here to use the compactness of the embedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$.

The paper uses the following definition of the Painlevé-Kuratowski convergence. If X is a metric space and $\{A^k\}_{k=1}^{+\infty} \subseteq 2^X$, then the set of all cluster points of all sequences $\{a^k\}_{k=1}^{+\infty}$ with $a^k \in A^k$, $k = 1, 2, ...$, is said to be the upper limit of the sequence $\{A^k\}$.

Next, the author deals with the optimality of solutions to the system when it is affine in the parameter. The optimality is understood as the minimization of the cost functional

$$\mathcal{J}(u,z) := \int_\Omega \Phi(x, z(x), \nabla z(x), u(x))\,dx.$$

Under suitable assumptions it is sequentially lower semicontinuous in the weak-strong topology of $L^p(\Omega)^m \times H_0^1(\Omega)^N$. This fact makes it possible to prove the existence of an optimizer.

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EXISTENCE OF OPTIMAL CONTROLS FOR SOME STOCHASTIC SYSTEMS WITH A FRACTIONAL BROWNIAN MOTION

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Keywords: stochastic control, fractional Brownian motion, stochastic systems

1. INTRODUCTION

A sizable amount of work has been done on the control of stochastic systems that are described by stochastic differential equations with a Brownian motion and a drift term that contains the state and the control. Relatively little work has been done for the control of stochastic systems where the Brownian motion is replaced by a fractional Brownian motion with the Hurst parameter that is allowed to assume some value from an open interval of possible values.

2. MAIN TOPIC

A stochastic control problem is formulated where the stochastic system is a stochastic differential equation containing a fractional Brownian motion and a nonlinear drift term that contains the state and the control. Since it is undesirable to require the smoothness of the control on the state, it is typically necessary to verify only a weak solution of the stochastic system.

For the Hurst parameter of the fractional Brownian motion in the interval (0, ½), weak solutions of the stochastic systems are given with only some growth conditions on the drift. The weak solutions are obtained by a transformation of the measure for a fractional Brownian motion by absolute continuity and the corresponding Radon-Nikodym derivatives are given explicitly. With a convexity condition on the drifts of the stochastic equations, there is a convexity of the corresponding Radon-Nikodym derivatives. For a bounded, continuous cost function the existence of an optimal control is verified.

PENSION FUND WITH A MINIMUM GUARANTEE: A STOCHASTIC CONTROL APPROACH

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Keywords: Defined contribution pension fund, minimum guarantee, stochastic optimal control, dynamic programming, Hamilton-Jacobi-Bellman equation, viscosity solutions.

In this paper we propose and study a continuous time stochastic model of optimal allocation for a defined contribution pension fund with a minimum guarantee. Usually, portfolio selection models for pension funds maximize the expected utility from final wealth over a finite horizon (the retirement time), whereas our target is to maximize the expected utility from current wealth over an infinite horizon since we adopt the point of view of the fund manager. In our model the dynamics of wealth takes directly into account the flows of contributions and benefits and the level of wealth is constrained to stay above a "solvency level". The fund manager can invest in a riskless asset and in a risky asset but borrowing and short selling are prohibited. We concentrate the analysis on the effect of the solvency constraint, analyzing in particular what happens when the fund wealth reaches the allowed minimum value represented by the solvency level.

The model is naturally formulated as an optimal stochastic control problem and is treated by the dynamic programming approach. We show that the value function of the problem is a regular solution of the associated Hamilton-Jacobi-Bellman equation. Then we apply verification techniques to get the optimal allocation strategy in feedback form and to study its properties. We finally give a special example with explicit solution.

Hamilton-Jacobi-Bellman equations and large deviations for stochastic PDE

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Keywords: Hamilton-Jacobi-Bellman equations, viscosity solutions, large deviations

1. Introduction

We will discuss how recent results on Hamilton-Jacobi-Bellman (HJB) equations in Hilbert spaces can be used to provide an easy way to establish large deviation principle for a class of stochastic PDE with small noise intensities. The key ingredients in this procedure are viscosity solutions and an infinite dimensional version of the method of half-relaxed limits for HJB equations to obtain the existence of the so called Laplace limit for the large deviation problem at single times. The approach uses a lot of ideas recently developed by Feng and Kurtz in their work on large deviations [1].

2. Large deviations for stochastic PDE

We will study large deviation principle for solutions of stochastic PDE of the form

$$\begin{cases} dX_n(s) = (-AX_n(s) + b(s, X_n(s))ds \\ \qquad\qquad + \frac{1}{\sqrt{n}} Q^{\frac{1}{2}} dW(s) \quad s > t, \\ X_n(t) = x \in H, \end{cases}$$

where A is a linear, densely defined maximal monotone operator in a real, separable Hilbert space H, Q is a bounded, nonnegative, self-adjoint operator of trace class in H, and W is a cylindrical Wiener process in H. The operator A and the function b must satisfy some additional conditions. The goal is to show how results on HJB equations can be used to obtain that the sequence $\{X_n\}$ satisfies the large deviation principle in $C([t, +\infty); H_{-1})$, where H_{-1} is the completion of H with respect to some weaker topology. The procedure we propose is the following. We first establish that the sequence of processes $\{X_n(T)\}$ satisfies large deviation principle in H for every $T > t$ and then adapt the methods of [1] to show that the large deviation principle holds in the path space. To get the large deviation principle at a single time T one has to prove that the sequence $\{X_n(T)\}$ is exponentially tight and that for every $f \in C_b(H_{-1})$ the Laplace limit $\lim_{n\to\infty} u_n(t, x)$ exists, where

$$u_n(t, x) = -\frac{1}{n} \log \mathbb{E}[e^{-nf(X_n(T))}].$$

Exponential tightness is obtained by showing exponential moment estinmates for X_n.

3. HJB equations and the existence of the Laplace limit

We use here recent results on relaxed limits for HJB equations [2]. These results allow to pass to very weak limits with solutions of HJB equations without any apriori estimates. Adapting them to the current situation we can show that the functions u_n are the unique bounded viscosity solutions of equations

$$\begin{cases} (u_n)_t + \frac{1}{2n}\mathrm{tr}(QD^2u_n) - \frac{1}{2}\|Q^{\frac{1}{2}}Du_n\|^2 \\ \qquad\qquad + \langle -Ax + b(t, x), Du_n\rangle = 0, \\ u_n(T, x) = f(x) \quad \text{in } (0, T) \times H, \end{cases} \tag{1}$$

and that comparison holds for bounded viscosity solutions the above equations for $n \geq 1$ and $n = +\infty$. Finally the functions u_n converge to the unique viscosity solution u of (1) with $n = +\infty$, which is the limiting first order HJB equation. This yields the existence of the Laplace limit $u(t, x)$. Moreover the limiting HJB equation can also be used to express the limit as the value function of an optimal control problem and thus give a representation for the rate

function. Further, mostly stochastic arguments, establish the large deviation principle for the sequence $\{X_n\}$ in the path space.

Similar results can be obtained for problems with multiplicative noise using slightly more complicated techniques.

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ASYMPTOTIC BEHAVIOR OF A STOCHASTIC GENE EXPRESSION MODEL

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Keywords: stochastic process,gen expression,semigroups of operators,asymptotic stability

In my talk I am going to present a stochastic process modelling gene expression in eukaryotes. This phenomenon is modeled by means of piecewise-deterministic processes. We show that distributions of the process satisfy a (Fokker-Planck–type) system of partial differential equations:

$$\frac{\partial f_0}{\partial t} + \frac{\partial}{\partial x_1}(-x_1 f_0) + r\frac{\partial}{\partial x_2}((x_1 - x_2)f_0) = q_1 f_1 - q_0 f_0,$$

$$\frac{\partial f_1}{\partial t} + \frac{\partial}{\partial x_1}((1 - x_1)f_1) + r\frac{\partial}{\partial x_2}((x_1 - x_2)f_1) = q_0 f_0 - q_1 f_1.$$

Then, we construct a c_0 Markov semigroup in L^1 space corresponding to this system. The main result is asymptotic stability of the involved semigroup in the set of densities. The strategy of the proof of this result is as follows. First we show that the transition function of the related stochastic process has a kernel (integral) part. Then we find a set E on which the density of the kernel part of the transition function is positive. Next we show that the set E is an "attractor". Then we apply results concerning asymptotic behavior of partially integral Markov semigroups discussed in (2). We show that the semigroup satisfies the "Foguel alternative", i.e. it is either asymptotically stable or "sweeping". Since the attractor E is a compact set, we obtain that the semigroup is asymptotically stable.

My talk is based on the paper (1). A similar technique was applied to study asymptotic behavior of a large class of transport equations. The paper (3) can be consulted for a survey of many results on this subject.

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A Linear Control System Model for Risk Reserves

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Keywords: Linear system, stochastic control, risk reserves

1. Introduction

Linear control theory was apparently initially applied to the modelling of the reserve funds for a property/casualty insurance company by Martin-Löf ((4)). Even at that time an intensive development of computer simulation models of the insurance industry had been initiated. Most of the current large scale models concentrate on financial modelling and on testing deterministic scenarios. Nonetheless, as it is documented in (2) on workmen's compensation insurance, stochastic simulation models are required for the evaluation of the uncertainty in the claims' reserves. Therefore it is important to consider this facet of insurance models and to devote research to their mathematical aspects. It has been noted that the scope of the computational risk theory methods is wider than was expected when some approximations to probability distributions, that were a substantial part of risk theory until the 1980's, are employed.

2. Main Topics

A discrete time, linear, stochastic control system is constructed to model the risk reserves for an insurance company. The model has the autoregressive form. A control is used to regulate the risk reserve. The sequence of controls is determined by two approximations, the normal power approximation of order two and a log normal approximation. These approximations use the first three moments which incorporate the skewness of the distributions that is important for these problems. An example of automobile insurance is considered to compare the two approximations for the stationary control law. It is shown that the two approximations are given stationary controls that closely agree.

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LIMITING DISTRIBUTIONS FOR MINIMUM RELATIVE ENTROPY CALIBRATION

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Keywords: Model calibration, entropy, weak convergence, Monte Carlo.

1. MRE CALIBRATION

Model calibration is an important part of Applied Mathematical Finance. An asset pricing model is calibrated if it reproduces the current market prices of certain specified benchmark instruments.

In this talk we examine some features of the minimum relative entropy (MRE) calibration algorithm. Its idea is to find the probability measure which prices correctly a given set of benchmark instruments and minimizes the Kullback-Leibler entropy distance to a given prior distribution, corresponding to the modeller's a priori information or beliefs. The MRE method was applied to one-period models in (Buchen and Kelly, 1996; Gulko, 1998) and to multiperiod models in (Platen and Rebolledo, 1996; Avellaneda et. al, 1997; Avellaneda, 1998). In the latter case, lattice methods for nonlinear parabolic equations were applied for computational purposes.

2. WEIGHTED MONTE CARLO

In (Avellaneda et. al, 2000), a MRE method for calibrating Monte Carlo simulations of stochastic processes was introduced. Starting from a given model of market dynamics, the algorithm corrects price misspecifications by assigning probability weights to the simulated paths. These weights are chosen by minimizing the Kullback-Leibler entropy distance of the posterior measure to the empirical measure. Let us mention that this algorithm has already been implemented by some investment banks.

3. LIMITING DISTRIBUTIONS

A natural question which arises is stability of the MRE method under perturbations of the prior measure. This seems to be particularly important for the Monte Carlo calibration (and, in fact, other numerical methods), where we work with a simulated approximation to the prior distribution rather than the prior itself. In this context, a stability result characterizes the limiting distribution which is approximated by the calibrated measures as the number of simulated paths increases and the time step decreases to zero.

Following (Kruk, 2004), we show that the MRE calibration of probability distributions on a separable metric space to a (fixed) finite set of moment constraints is stable, i.e., continuous in the weak topology. This means that if a sequence of priors P_n converges weakly to P, then Q_n, the calibrated measures under P_n, converge weakly to Q which calibrates P to the same constraints. We also characterize the limiting distributions approached (in the variation distance) by the measures calibrating the same prior to an increasing number of option price constraints. Finally, we explain the limiting properties of the MRE Monte Carlo calibration algorithm.

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Numerical approximation for super-replication problems under gamma constraints

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Keywords: super-replication problem, Hamilton-Jacobi-Bellman equation, numerical approximation, generalized finite differences scheme

In a financial market, consisting in a non-risky asset and some risky assets, people are interested to study the minimal initial capital needed in order to super-replicate a given contingent claim, under gamma constraints.

Many authors have studied this problem in different cases and with different constraints: for example, see [7, 8], for problems in dimension 1, [4] for problems in dimension 2, and [6] for problems in a general dimension d.

In the literature, the super-replication price is carachterized as the viscosity solution of an HJB-equation with terminal and boundary conditions. In a particular case, the dual formulation of the super-replication problem leads to a standard form of optimal stochastic control problem [4].

In this paper we study numerically an HJB-equation coming from the super-replication problem in dimension 2. We discretize the HJB equation using the Generalized Finite Differences scheme [2, 3], then we study existence and uniqueness of the discrete solution. Finally we prove the convergence of the numerical solution to the viscosity solution. In particular, we are interested on the HJB equation which comes from the two dimensional dual problem introduced in [4]:

$$\vartheta(t,x,y) = \sup_{(\rho,\xi)\in\mathcal{U}} \mathbb{E}\left[g\left(X^{\rho,\xi}_{t,x,y}(T)\right)\right], \quad (1)$$

where (ρ,ξ) are valued in $[-1,1]\times(0,\infty)$, the process $(X^{\rho,\xi}_{t,x,y}, Y^{\rho,\xi}_{t,y})$ is a 2-dimensional positive process, and g is a payoff function. The main difficulty of the above problem is due to the non-boundness of the control set, this fact implies that the Hamiltonian associated to (1) is not bounded, and numerical approximation for such a problem becomes more complicate.

In the literature, problems with unbounded control have been studied by many authors (for example, [1, 5]). In all these cases, the authors decide to truncate the set of controls to make it bounded. This truncation simplifies the numerical analysis of the problem. However, there is no theoretical result justifying this truncation.

In this paper we do not truncate the set of controls, because we have a particular form of our HJB equation which leads us to avoid the difficulty of unbounded control. In fact, our HJB equation can be reformulated in the following way

$$\Lambda^-(J(t,x,y,D\vartheta(t,x,y),D^2\vartheta(t,x,y))) = 0,$$

where J is a symetric matrix differential operator associated to the Hamiltonian, and where $\Lambda^-(J)$ means the smallest eigenvalue of the matrix operator J. J does not depend on the control, but when we look for the first time at this equation, it seems that it is very difficult to treat. From standard computations on algebra, we rewrite the smallest eigenvalue as follows:

$$\Lambda^-(J) = \min_{\|\alpha\|=1} \alpha^T J\alpha,$$

where $\alpha\in\mathbb{R}^2$, and the HJB equation becomes:

$$\min_{\alpha_1^2+\alpha_2^2=1} \alpha^T J\alpha = 0,$$

where this time α is the control and it is bounded. Then we have transformed our problem into a bounded control problem, and now the numerical analysis is possible.

We consider the discretization of the HJB equation, and recall the main properties of the Generalized Finite Differences Scheme and we prove the consistency of this scheme. Moreover,

we prove existence and uniqueness of a bounded discrete solution, and finally we prove the convergence of the numerical approximation.

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Adaptive Shooting Methods for Dynamic Optimization - Concepts, Algorithms and Applications

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Keywords: optimal control, single shooting, adaption, structure detection

1. INTRODUCTION

This contribution will review some of the work on the development of adaptive shooting methods for the solution of optimal control problems carried out in our research group in recent years. The basic feature of the shooting method is an adaptive choice of the control vector parameterization in a shooting type of solution strategy. The following class of multi-stage dynamic optimization problems is considered:

$$\begin{aligned}
\min_{(u_k(t),p_k,t_k)_{k=1,\ldots,S}} & \sum_{k=1}^{S} \Phi(t_k, x(t_k), p_k) \\
\text{s. t. } & M_k\, \dot{x}_k(t) = f_k(t, x_k(t), u_k(t), p_k)\,, \\
& x_1(t_0) = x_0(p_1) \in \mathbb{R}^{n_{x_k}}\,, \\
& x_k(t_k) = B_k\, x_{k-1}(t_k)\,, \\
& g_k(t, x_k(t), u_k(t), p_k) \le 0\,, \\
& h_k(t_k, x_k(t_k), p_k) \le 0\,, \\
& u_k(t) \in U_k, \quad p_k \in P_k, \\
& \text{for } t_{k-1} < t \le t_k,\ k = 1, \ldots, S.
\end{aligned}$$

The dynamic optimization problem comprises S stages, each with possibly different differential-algebraic equations of index less than or equal to one.

2. ADAPTION

The control variables are adaptively discretized by multi-scale basis functions to resolve local detail with an appropriate number of parameters. In detail, the basis functions are wavelets generated from the *Haar basis* or the *hat basis*, respectively. At the beginning of the adaption procedure, an optimization problem with a small number of basis functions is solved. Depending on the wavelet coefficients of the optimal solution, some basis functions are deleted and a number of additional basis functions of the next resolution level are added. Details of the adaption algorithm and numerical case studies are given by Schlegel et al. [8].

3. STRUCTURE DETECTION

Furthermore, for single-stage problems ($S = 1$) the control switching structure of the solution is automatically detected during the refinement process of the adaptation of the control vector parameterization which gives insight into the solution features facilitating the interpretation of the result. The such detected structure is exploited to reparameterize the single-stage into a multi-stage problem with a close to minimal number of control vector parameters (Schlegel and Marquardt [6, 5]).

4. SENSITIVITIES

First and second order derivatives are computed by novel and highly efficient numerical algorithms exploiting forward as well as backward mode differentiation. Schlegel et al. [7] provide an efficient numerical algorithm based on the extrapolated linear-implicit Euler's method for the computation of first order sensitivities. Hannemann and Marquardt [1] modify the second-order adjoint sensitivity analysis (Haug and Ehle [3]) to efficiently compute the Hessian of the Lagrangian for path-constrained optimal control problems in shooting algorithms.

5. ONLINE APPLICATIONS

Kadam and Marquardt [4] introduce a two-level strategy for the dynamic real-time optimization of industrial processes. A parametric sensitivity-based technique is used to calculate optimal first-order updates to a nominal reference solution. The technique does not assume that the active constraint set remains the same after changes in uncertain parameters.

The structure detection algorithm (cf. section 3) is adapted for nonlinear model predictive control (Hartwich et al. [2]). The achieved reduction in terms of degrees of freedom in the concerned nonlinear program decreases the computational time.

6. CONCLUSIONS

Our numerical method conceptually links single-shooting and multiple type shooting on the one hand as well as direct and indirect methods on the other. The robustness and performance of the algorithms will be illustrated by different kinds of examples from chemical engineering of different complexity. The implementation has been proven to be very robust and highly efficient for large-scale optimal control problems with up to 15 000 differential-algebraic equations with a number of control variables and many inequality path and endpoint constraints. Some extensions of the algorithm to cover real-time applications in nonlinear model-predictive and neighboring extremal control will be briefly discussed together with illustrating examples.

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The Lifted Newton Method and its Use for Large Scale Dynamic Optimization and NMPC in Chemical Engineering

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Keywords: Nonlinear Optimization, Optimal Control, Optimization with DAE Systems, Nonlinear Model Predictive Control

We present a new full space exact Hessian SQP algorithm for large scale dynamic optimization that makes mainly use of two ingredients:

- We start by a process simulator (the adaptive DAE solver DAESOL-II [1]) that is able to generate adjoint sensitivities by the principle of internal numerical differentiation. Thus, a gradient computation is available at the cost of about five process simulations.
- Second, we work in the framework of Bock and Plitt's direct multiple shooting method [2] by introducing intermediate but constrained "node" variables into the optimization problem. It is a well known technique for reducing nonlinearity and increasing robustness of the optimization procedure, in particular for boundary value problems e.g. with end point quality constraints.

By a combination of both ingredients, we are able to derive a full space exact hessian SQP method that iterates in the very large space of all node variables, yet needs to evaluate only the same amount of derivatives as would be needed in a single shooting approach. This is similar to Schloeder's trick [4] which was however only applicable to least squares cost functions and not yet combined with adjoint techniques.

By a smart programming trick, the algorithm can easily be derived by "lifting" a standard single shooting SQP method, thus avoiding the tedious programming work usually avoided with new variants of direct multiple shooting.

We consider here the following type of nonlinear optimization problem

$$\begin{aligned} \min_{u} \quad & F(u) & = 0 \\ \text{s.t.} \quad & H(u) & \geq 0. \end{aligned}$$

This problem is then lifted by introducing intermediate node values x and corresponding constraints G to a problem of type

$$\begin{aligned} \min_{u,x} \quad & F(u,x) & = 0 \\ \text{s.t.} \quad & G(u,x) & = 0 \\ & H(u,x) & \geq 0. \end{aligned}$$

We can then efficiently calculate the quantities needed for the SQP method by evaluating directional derivatives only with respect to the original degrees of freedom u, and after solving a quadratic problem in Δu we need just another directional derivative to expand this QP solution to a step in the full variable space.

The algorithm is advantageous in case of large process models with few degrees of freedom. We present also an extension to online optimization in nonlinear model predictive control. Here we use the ideas of real-time iterations and initial value embedding as presented in [3]. We extend the latter idea to a more general parameter embedding. We consider the lifted online optimal control problem as dependent on some process parameters p

$$\begin{aligned} \min_{u,x} \quad & F(u,p,x) & = 0 \\ \text{s.t.} \quad & G(u,p,x) & = 0 \\ & H(u,p,x) & \geq 0, \end{aligned}$$

which could include the current process state. Then we embed these parameters in our problem by adding new nodes $\bar{p}$ and the trivial constraint $\bar{G} = \bar{p} - p$ to the optimization problem. We end up with

$$\begin{aligned} \min_{u,\tilde{x}} \quad & F(u,p,\tilde{x}) \quad = 0 \\ \text{s.t.} \quad & \tilde{G}(u,p,\tilde{x}) \quad = 0 \\ & H(u,p,\tilde{x}) \quad \geq 0, \end{aligned}$$

where $\tilde{x} = (x, \bar{p})$ and $\tilde{G} = (G, \bar{G})$. This allows us a smoother transition between two successive optimization problems, while the linearity of the constraints ensure that they are fulfilled after one SQP iteration.

Finally we demonstrate the performance of our approach at examples from chemical engineering.

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OPTIMISATION PROBLEMS IN ADVANCED OPERATING MODES OF CONTINUOUS CHROMATOGRAPHY

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Keywords: Simulated moving bed chromatography, Periodic operation, Process combinations, Reactive separations

1. BACKGROUND

Chemical processes most generally consist of a reaction step (synthesis) and a subsequent resolution of reactants and products (separation). The separation step can be very difficult (and expensive), in particular in the production of valuable pharmaceuticals and fine chemicals. In this context, chromatographic processes are an important option.

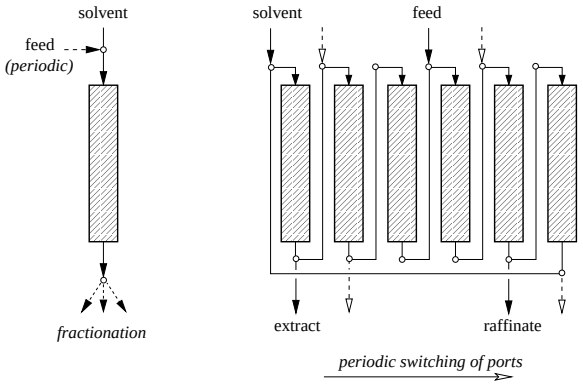

Fig. 1. Process schemes for discontinuous batch chromatography (left) and the continuous simulated moving bed (SMB) process (right).

Chromatography is performed using columns containing a stationary phase. The figure shows two general process options – discontinuous batch chromatography (single column, periodic injection of small feed amounts; left), and Simulated Moving Bed (SMB) chromatography (periodic switching of multiple columns, continuous feed; right). Due to its superior economic performance, the SMB process is receiving more and more attention.

2. DESIGN PROBLEM

The design task in chromatographic processes is characterised by the need to minimise an economically motivated objective. However, typically a multi-objective optimisation problem arises, since different aspects like the productivity (i.e., the throughput or space-time-yield of the process), consumption of solvents, product concentration, and yield have to be considered. Operating parameters that can be manipulated are usually the flow rate(s) within the process, the feed concentration or composition, and the duration of the different time intervals involved (e.g., for feed injection or product collection). Generally, the desired purity of the products is formulated as non-linear constraints.

Mathematical models of chromatographic processes are computationally expensive, since they typically involve a set of non-linear partial differential equations that require numerical solution schemes, because the PDEs are coupled by the involved thermodynamic equilibria. Occurring phenomena like shock fronts often necessitate a fine spatial discretisation (up to several thousand grid points per column). Furthermore, the process includes discrete events; in particular when considering new operating modes for such processes.

Due to the computational efforts related this, optimisations of ”standard” SMB processes could be performed only recently. Different strategies have been proposed; for example, genetic algorithms (Zhang et al., 2002), sequential quadratic programming (SQP) (Kaspereit et al., 2005), a two-level approach (Minceva and Rodrigues, 2005), and the use of feedback control (Schramm et al., 2003).

3. ADVANCED PROCESS CONFIGURATIONS AND NEW OPTIMISATION PROBLEMS

Besides standard SMB configurations, currently different advanced operating modes are subject to investigations. These allow to further increase the economic performance of SMB processes and to broaden the range of applications. Examples for such operating concepts include:

- combinations of SMB and complementary separation processes (including recycle streams),
- additional periodic variation of parameters (e.g., column configuration, flow rates, feed concentration),
- introduction of gradients with respect to solvent strength or temperature,
- implementation of chemical reactions within SMB processes.

However, optimisation of such processes remains a challenge and only few results have been published. Mainly, processes with periodic variations (see above) have been considered using genetic algorithms (Zhang et al., 2004). More recently, non-linear optimisation with full discretisation was applied successfully to SMB processes with periodic variation of the column configuration and flow rates (Kawajiri and Biegler, 2006).

In the presentation, on overview will be given on optimisation problems related to (continuous) chromatographic processes. After an introductory review of fundamental principles and modelling approaches, recent developments with respect to advanced operating modes for SMB processes and optimisation problems will be explained. A main example to be discussed is the flow-sheet integration of SMB chromatography with selective crystallisation to separate pharmaceutically relevant isomers (Kaspereit, 2006). Related to that, the optimal design of SMB processes with arbitrary purity requirements will be explained (Kaspereit et al., 2007). Further examples include SMB processes with cyclic modulation of operating parameters, and integrated processes where chromatography and chemical reactions are performed within the same apparatus.

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On the Optimality of Superstructures for Simulated Moving Beds

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Keywords: dynamic optimization, simulated moving beds, bang-bang solutions

1. Abstract

The past decade has seen a variety of operating modifications for Simulated Moving Bed (SMB) processes, including Three-Zone, VARICOL, and PowerFeed. In recent studies, we have shown that these can all be embedded within a superstructure optimization problem with time-variant flow rates. Moreover, the resulting dynamic optimization problem has yielded a number of interesting and useful insights on novel SMB operations. In many cases, optimal solutions have a "bang-bang" character, i.e., at any instant of time, the feed, desorbent, extract and raffinate streams appear at only one location. Remarkably, this occurs even though the optimization is performed without the introduction of binary decision variables. In this study we analyze and present the conditions where "bang-bang" solutions are optimal. We also demonstrate cases where these conditions do not hold and where "bang-bang" solutions are suboptimal. To demonstrate that these properties are independent of the column model and solution strategy, we present both "bang-bang" and "non-bang-bang" cases for two different column models.

2. Summary

SMB chromatography is a realization of continuous chromatographic separation that is applied in many industrial applications including the sugar, food, petrochemical, and pharmaceutical industries. As shown in Figure 1, an SMB unit consists of multiple columns connected to each other in a cycle and divided into four zones by two inlet streams, feed (F) and desorbent (D), and two outlet streams, extract (E) and raffinate (R). The continuous, counter-current operation is simulated by switching the four streams in the direction of the liquid flow in the columns.

In standard SMB operation, the four stream flows are kept constant over a switching interval and treated as operating parameters; the switching interval, or step time, is also an optimization parameter. On the other hand, PowerFeed operation allows the stream flows to be time variant. Moreover, VARICOL systems perform asynchronous valve switching, where the four inlet/outlet ports are switched independently, not simultaneously (1). Finally, the Three-Zone SMB has a circulation loop that is cut open, and the recycle stream from Zone III to Zone I is withdrawn as the raffinate stream. Three-Zone SMB, and Three-Zone SMB with purging have also been investigated in recent experimental studies (2; 3).

The dynamics of this process are characterized by Cyclic Steady State (CSS) operation, where the same concentration profiles are generated repeatedly in every cycle. As a result, the Simulated Moving Bed (SMB) chromatographic separation process contains time–dependent discrete decisions (4; 5; 6), and related optimization problems are challenging as they combine periodic nonlinear optimal control problems and partial differential equations (PDE) with time–dependent discrete decisions. In previous studies (8; 7) we proposed optimization strategies to find optimal operating schemes with a general superstructure approach. In this study the PDAE model is discretized in both time and space domains, and the resulting large scale nonlinear optimization problem is solved using two approaches, an interior-point solver for a fully discretized, direct transcription approach and a multiple shooting approach that uses a large-scale SQP strategy. Moreover, in recent studies (8; 6)

we observed that solutions from the superstructure optimization naturally led to a "bang-bang" policy. In general, the term bang-bang solution refers to control trajectories that are at their respective bounds over the considered time horizon. Here, we also require the satisfaction of a *special ordered set* constraint, i.e., at each instant of time each stream appears only at one location within a cycle. Remarkably, the decision as to whether a specific flow is located at a given port or not need not be characterized with a binary variable. Instead, a continuous relaxation in space still satisfies the "bang-bang" conditions. On the other hand, more complex non-bang-bang solutions were also observed in (7) and these reveal further insight into advanced SMB designs.

This talk reconciles these two policies and provides a justification for the occurence of "bang-bang" features in optimal SMB designs. Such solutions are normally expected to require binary decision variables and mixed integer optimal control formulations. However, we show that under certain conditions such solutions derive from continuous variable optimization formulations as well, and (computationally more expensive) mixed integer formulations are not required.

In this talk, we describe the general superstructure model for SMB optimization. Following this, the superstructure formulation is abstracted to a mixed integer optimal control problem (MIOCP) and properties of the MIOCP are presented. In particular, we present properties under which "bang-bang" solutions are optimal as well as conditions where these properties are violated. We then consider two different SMB different column models and demonstrate that these results are independent of particular details of these models. This is supplemented with a variety of computational results that demonstrate these properties and exhibit exceptions to "bang-bang" policies when these properties are not satisfied.

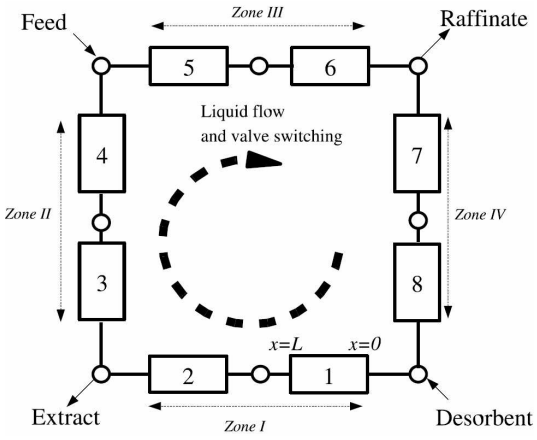

Fig. 1. Schematic diagram of standard SMB: 8 column type with two columns in each zone

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Robust Optimum Experimental Design Methods with Application to Parameter Estimation in Chemistry and Chemical Engineering

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Keywords: Parameter Estimation, Robust Optimum Experimental Design, Applications in Chemical Engineering

Estimating model parameters from experimental data is crucial to reliably simulate dynamic processes. In practical applications, however, it often appears that the experiments performed to obtain necessary measurements are expensive, but nevertheless do not guarantee sufficient identifiability. The optimization of one or more dynamic experiments in order to maximize the accuracy of the results of a parameter estimation subject to cost and other technical inequality constraints leads to very complex non-standard optimal control problems: find control variables ξ that minimize a function φ of a covariance matrix

$$\min_{\xi} \quad \varphi(C(x,p,\xi))$$

such that state variables x, parameters p and control variables ξ satisfy DAE model, control constraints

$$c_1(\xi) \geq 0 \quad \text{or} \quad = 0$$

and state constraints

$$c_2(x,p,\xi) \geq 0.$$

One of the difficulties is that the objective function is a function of a covariance matrix and therefore already depends on a generalized inverse of the Jacobian of the underlying parameter estimation problem. Another difficulty is that the optimization results depend strongly on the assumed values of parameters which are only known to lie in a - possibly large - confidence region. Hence, robust optimal experiments are required that solve worst-case (min-max) optimization problems

$$\min_{\xi\in\Omega} \max_{\|\Sigma(p-p_0)\|\leq\gamma} \varphi(C(x,p,\xi)).$$

We suggest new efficient solution methods for such problems. The methods have been applied successfully to real-world problems. The methods allow to estimate reliably unknown parameters and to reduce significantly experimental costs.

This is joint work with Hans Georg Bock, Stefan Körkel and Johannes P. Schlöder.

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Optimizing Control of a Reactive SMB Process

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Keywords: Simulated Moving Bed chromatography, Hashimoto process, optimizing control, experimental application

1. Introduction

In recent years, continuous chromatographic processes have been established as an efficient separation technology in industry, especially when temperature sensitive components or species with similar thermodynamic properties are involved. In SMB processes, a countercurrent movement of the liquid and of the solid phase is achieved by periodically switching the inlet and the outlet ports in a closed-loop of chromatographic columns. The integration of reaction and separation in one single plant is a promising approach to overcome chemical or thermodynamic equilibria and to increase process efficiency. Reactive chromatographic SMB processes in which the columns are packed with both catalyst and adsorbent have been proposed and demonstrated successfully. However, a full integration often is not efficient because the catalyst is not used in the separating zones that clean the eluent and the adsorbent or even counterproductive in the product purification zones. By placing reactors between the separation columns at specific positions around the feed port, a more efficient process, the Hashimoto SMB Hashimoto *et al.* (1983) process, can be established.

In this paper, the simulated and the experimental performances of optimizing control of the Hashimoto SMB process are presented. A nonlinear predictive controller for the Hashimoto SMB process is established that computes optimal control variables (flow rates and the switching time) while the purity requirements of the product streams and the conversion of the feed to the valuable product are considered as constraints. The concept is extended to the case of high product purities and applied to a pilot plant of the biochemical and chemical engineering department at the Universität Dortmund. As an oscillatory behavior of the controller was observed in some situations, an additional term was added to the cost function that prevents the breakthrough of impurities via the recycle loop.

2. Process Model

The Hashimoto SMB process is an integrated reaction and separation process. Both, reaction and chromatographic separation are performed in separate units such that optimal conditions for reaction and for separation can be chosen independently and the reactors can be constantly placed at positions where the forward reaction of the equilibrium limited reaction system is promoted. A relative movement of the adsorbent is implemented by switching the ports in the direction of the liquid flow. The reactors, however, remain at their positions relative to the ports. The columns are described accurately by the *general rate model*. The resulting partial differential

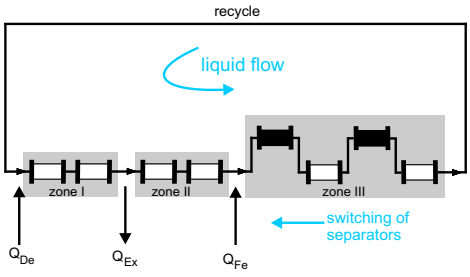

Fig. 1. Hashimoto three-zone configuration (reactors: black, separators: white)

equations are transformed into ordinary differential equations by a finite element discretization of the bulk phase and orthogonal collocation of the solid phase.

3. Predictive control strategy

3.1. Formulation of the optimization problem

The goal of the optimization is to minimize an economic objective (rather than e. g. a cost function involving a tracking error) while important plant specifications (purity and recovery requirements, pump limitations, process dynamics) are formulated as constraints. The objective function of the optimization consists of the eluent consumption over the horizon as the main objective of the optimizer and a regularization term that penalizes changes of the degrees of freedom and leads to a smooth behavior of the controlled system such that aggressive changes of the control variables only take place when needed to obtain a feasible operation (e.g. in the presence of a set point change). An additional penalty term is added to the objective in order to prevent a breakthrough of impurities via the recycle line.

4. Results

4.1. Simulation

For the simulation, a considerable plant/model mismatch is considered. The controller is switched on at period 80. The purity constraint is initially set to 85%, increased to 90% at period 184, further increased to 95% at period 368 and finally set to 99% at period 648. The controller manages to keep the product purity and the recovery at the specified minimal values for the full simulation run and to reduce the solvent consumption, see Figure 2.

4.2. Experiment

The desired purity was set to 80% and increased to 82% for the last two intervals of operation while the recovery set point was set to 70%. Due to the computation time of around 30 min, the flow rates and the switching period calculated by the optimizer are based on an error feedback that is delayed by one switching cycle.

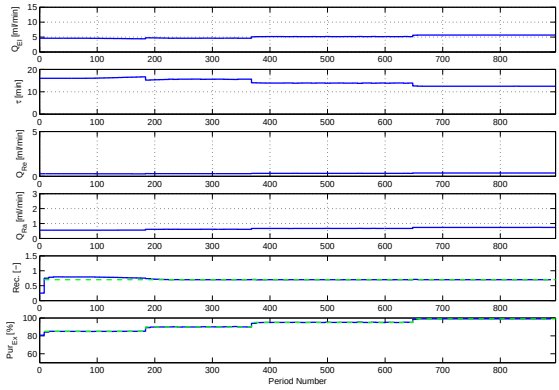

Fig. 2. Simulation: Manipulated and controlled variables

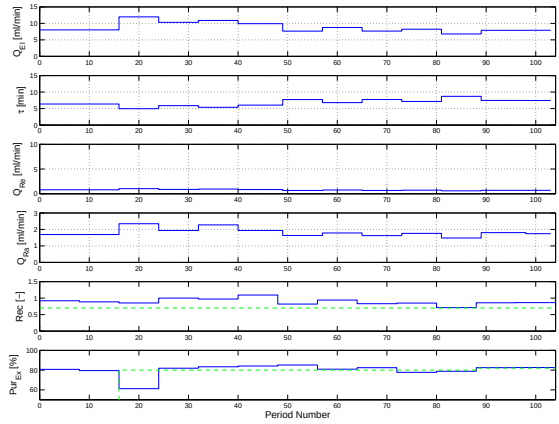

Fig. 3. Experiment: Manipulated and controlled variables

The recovery constraint was already met at the first interval since the plant had been in operation before. The controller was switched on in the second interval. A recycle pump failure occurred in the 3rd interval that reduced the liquid flow in all separation zones considerably and led to a drop of the purity. The controller managed to keep the purity above the desired 80% with the exception of interval 10 where a slight violation occurred, see Figure 3. The solvent consumption is reduced in a smooth fashion. Overall, the performance was satisfactory.

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INTERIOR-POINT QUASI-SEQUENTIAL APPROACH AND APPLICATION TO THE OPTIMIZATION OF THE TENNESSEE-EASTMAN-PROCESS

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Keywords: dynamic optimization, quasi-sequential, interior point, Tennessee Eastman process.

1. INTRODUCTION

In this contribution, we consider an extension of the quasi-sequential approach [Hong06] using an interior-point strategy for efficient solution of large-scale dynamic optimization problems with path constraints on state variables. The quasi-sequential approach is suitable for accomplishing this task. It utilizes advantages of both simultaneous approaches (where a complete discretization for both states and controls is adopted) and sequential approaches (where a model integration step is used for eliminating the states and equalities). Furthermore, the elimination of equality constraints simplifies the line-search problem considerably and therefore larger steps can be taken towards the optimum.

2. ACTIV-SET VERSUS INTERIOR-POINT

Within the quasi-sequential approach an active-set strategy has been used until now. It is well-known that this strategy will be inefficient for problems with a large number of inequality constraints. In the current work the active-set strategy is replaced by an interior-point method. Due to the handling of inequality constraints with barrier terms the eventual problem to be solved consists of merely an objective function. We chose a primal-dual interior-point approach [Waechter06] which presents excellent convergence properties and computational performances. This modification leads to a considerable reduction of computational costs in situations where the number of active constraints is high.

3. APPLICATION

The interior-point quasi-sequential approach is applied to the dynamic optimization of the Tennessee Eastman Process. The Tennessee Eastman process [Downs93] has been used in many studies with different aspects of process systems engineering. Due to its characteristics of being open-loop instable as well as highly nonlinear, it is even impossible to initialize the dynamic optimization problem [Jockenhövel04]. A two-step procedure is proposed to overcome this difficulty. The results from the interior-point quasi-sequential approach will be compared with those from the active-set quasi-sequential approach.

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Tools and Languages for Modeling and Optimization of Large-Scale Dynamical Systems

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Keywords: Large Scale Dynamic Optimization, Modelica, Modeling of Complex Systems

1. Introduction

High-level modeling languages are receiving increased industrial and academic interest within several domains, such as chemical engineering, thermo-fluid systems and automotive systems. One such modeling language is Modelica, [1]. Modelica is an open language, specifically targeted at multi-domain modeling and model reuse. Key features of Modelica include object oriented modeling, declarative equation modeling, a component model enabling acausal connections of submodels, as well as support for hybrid/discrete behaviour. These features have proven very applicable to large-scale modeling problems in various fields.

While there exist very efficient software tools for simulation of Modelica models, tool support for static and dynamic optimization is generally weak. Furthermore, specification of optimization problems is not supported by Modelica. Since Modelica models represent an increasingly important asset for many companies, it is of interest to investigate how Modelica models can be used also for optimization.

This contribution gives an overview of a project targeted at *i)* defining an extension of Modelica, Optimica, which enables high-level formulation of optimization problems, *ii)* developing prototype tools for translating a Modelica model and a complementary Optimica description into a representation suited for numerical algorithms, and *iii)* performing case studies demonstrating the potential of the concept.

The project integrates dynamical modeling and optimization with computer science and numerical algorithms. One of the main benefits of the suggested approach is that the high-level descriptions are automatically translated into an intermediate representation by the compiler front-end. This intermediate representation can then be further translated to interface with different numerical algorithms. The user is therefore relieved from the burden of managing the often cumbersome API:s of numerical algorithms. The flexibility of the architecture also enable the user to select the algorithm most suitable for the problem at hand.

2. Optimica

A key issue is the definition of syntax and semantics of the Modelica extension, Optimica. Optimica should provide the user with language constructs that enables formulation of a wide range of optimization problems, such as parameter estimation, optimal control and state estimation based on Modelica models.

At the core of Optimica are the basic optimization elements such as cost functions and constraints. It is also possible to specify bounds on variables in the Modelica model as well as to mark variables and parameters as optimization quantities, i.e., to express what to optimize over. While this type of information represents a canonical optimization formulation, the user is often required to supply additional information, related to the numerical method which is used to solve the problem. In this category we have e.g., specification of transcription method, discretization of control variables and initial guesses. Optimica should also enable convenient specification of these quantities.

3. Software Tools

In order to demonstrate the proposed concept, prototype software tools are being developed.

In essence, the task of the software is to read the Modelica and Optimica source code and then translate, automatically, the model and optimization descriptions into a format which can be used by a numerical algorithm. The Modelica/Optimica compiler is developed using the Java-based compiler construction tool JastAdd, [5]. For an overview of the computer science aspects of the compiler implementations, see [7].

Currently, the front-end of the Modelica/Optimica compiler supports a subset of Modelica and a basic version of Optimica. In addition, a code-generation back-end for AMPL, [3], has been developed. AMPL is a language intended for formulation of algebraic optimization problems. Accordingly, the compiler performs automatic transcription of the original continuous-time problem into an algebraic formulation which can be encoded in AMPL. In the transcription procedure, the problem is discretized by means of a simultaneous optimization approach based on collocation over finite elements, see e.g., [2] for an overview. Finally, the automatically generated AMPL description may be executed and solved by a numerical NLP algorithm. For this purpose we have used IPOPT, [6].

4. A Case Study

The prototype tools have been used to formulate and solve a start-up problem for a plate reactor system. The plate reactor is conceptually a tubular reactor located inside a heat exchanger, and offers excellent flexibility, since it is reconfigurable and allows multiple injection points for chemicals, separate cooling/heating zones and easy mounting of temperature sensors. In this case study, an exothermic reaction, $A + B \rightarrow C$, was assumed. The reactor was fed with a fluid with a specified concentration of the reactant A. The reactant B was injected at two points along the reactor.

The primary objective of the start-up sequence was to transfer the state of the reactor from an operating point where no reaction takes place, to the desired point of operation. This problem is challenging, since the dynamics of the system is fast and unstable in in some operating conditions. In addition, the temperature in the reactor must be kept below a safety limit, in order not to damage the hardware.

Optimal control and state profiles were calculated off-line and then used as feedforward and feedback signals in a PID-based mid-ranging control system.

The experiences from using the Modelica/Optimica compiler in this project are promising, in that the tools enable the user to focus on *formulation* of the problem instead of, which is common, *encoding* of the problem. For more details on this case study, see [4].

5. Summary

This contribution gives an overview of a project targeted at extending the Modelica language to also support optimization. The goals of the project include specification of Optimica, development of prototype software tools and case studies. The results are promising, and encourage further development.

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REOXYGENATION AND SPLIT-DOSE RESPONSE TO RADIATION IN A TUMOUR CORD MODEL

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Keywords: PDE models, Tumour cords, Radiotherapy, Reoxygenation

1. INTRODUCTION

After a single dose of radiation, important changes mainly due to cell death are expected to occur in the oxygenation and nutritional state of surviving cells. In particular, a transient increase of oxygenation (reoxygenation) may occur. Since cell radiosensitivity increases with oxygen concentration, reoxygenation is expected to induce a greater sensitivity of the tumour to a subsequent irradiation. Such a resensitization could counterbalance the sparing effect of dose splitting on cell survival caused by damage repair and cell repopulation. In previous papers (Bertuzzi et.al, 2003), (Bertuzzi et.al, 2004), we proposed a model for the response of tumour cords (cylindrical arrangements of tumour cells around tumour blood vessels) to single-dose treatments. That model has been extended to describe the response to impulsive irradiation (Bertuzzi et.al, 2007), incorporating the repair/misrepair process of the DNA double strand breaks (DSB) produced by radiation (Hlatky et.al, 2003). The model has been used to study the time course of reoxygenation and its role in the response to split doses.

2. MODEL EQUATIONS

We model the tumour vasculature as a regular array of parallel and identical vessels, as in the Krogh model of microcirculation. Thus, the tumour tissue can be partitioned into identical cylinders of tissue around central vessels (tumour cords). Let r be the radial distance, r_0 the vessel radius, and B the cord radius. Necrotic regions are supposed to be absent. Changes along the axial coordinate are disregarded. We denote by ν_P, ν_Q, $\nu^\dagger$, ν_N the volume fractions of proliferating (P) cells, quiescent (Q) cells, lethally damaged cells, and dead cells respectively. $u(r,t)$ denotes the (radially directed) velocity of the cellular component, and $\sigma(r,t)$ the oxygen concentration. We will assume $\nu_P+\nu_Q+\nu^\dagger+\nu_N=\nu^\star$, $\nu^\star$ constant. From the mass conservation, we can write

$$\frac{\partial \nu_P}{\partial t}+\nabla\cdot(\nu_P\,u)=\chi\nu_P+\gamma\nu_Q-\lambda\nu_P-m_P\nu_P\,, \tag{1}$$

$$\frac{\partial \nu_Q}{\partial t}+\nabla\cdot(\nu_Q\,u)=-\gamma\nu_Q+\lambda\nu_P-m_Q\nu_Q\,, \tag{2}$$

$$\frac{\partial \nu^\dagger}{\partial t}+\nabla\cdot(\nu^\dagger\,u)=m_P\nu_P+m_Q\nu_Q-\mu\nu^\dagger\,, \tag{3}$$

$$\frac{\partial \nu_N}{\partial t}+\nabla\cdot(\nu_N\,u)=\mu\nu^\dagger-\mu_N\nu_N\,. \tag{4}$$

In Eqs. (1)-(4) χ is the proliferation rate, and $\gamma(\sigma)$ and $\lambda(\sigma)$ are, respectively, the rates for the transitions $Q\to P$ and $P\to Q$. We suppose that γ and λ are nondecreasing and, respectively, nonincreasing functions of σ. $m_P(r,t)$ and $m_Q(r,t)$ are rates representing the production of lethal damage due to the misrepair process, μ is the death rate of lethally damaged cells. μ_N is the degradation rate of dead cells into liquid. Since $\nu^\star$ is constant, we obtain

$$\nu^\star\frac{1}{r}\frac{\partial}{\partial r}(ru)=\chi\nu_P-\mu_N(\nu^\star-\nu_P-\nu_Q-\nu^\dagger)\,, \tag{5}$$

that yields the cell velocity when completed with the boundary condition $u(r_0,t)=0$.

Concerning the equation for σ, we assume

$$\Delta\sigma=f(\sigma)(\nu_P+\nu_Q+\nu^\dagger)\,, \tag{6}$$

$$\sigma(r_0,t)=\sigma_b\,,\qquad \left.\frac{\partial\sigma}{\partial r}\right|_{r=B(t)}=0\,,$$

where $f(\sigma)$ denotes the ratio between the consumption rate per unit volume of live cells and

the diffusion coefficient, and σ_b is the oxygen blood concentration. The cord boundary $B(t)$ is given by

$$\dot{B} = u(B(t), t)\,, \quad B(0) = B_0\,, \qquad (7)$$

until $\sigma(B(t), t) > \sigma_N$, σ_N being the threshold under which necrosis occurs. According to the model in (Hlatky et.al, 2003), we have

$$m_P = \frac{1}{2}kX_P^2\,, \quad m_Q = \frac{1}{2}kX_Q^2\,,$$

where $X_P(r,t)$ and $X_Q(r,t)$ denote the mean number of DSBs in a P and, respectively, Q cell at the position r at time t. These quantities satisfy the following equations

$$\frac{\partial X_P}{\partial t} + u\frac{\partial X_P}{\partial r} = -\omega X_P - 2kX_P^2\,, \qquad (8)$$

$$\frac{\partial X_Q}{\partial t} + u\frac{\partial X_Q}{\partial r} = -\omega X_Q - 2kX_Q^2\,, \qquad (9)$$

where ω and k are the rate constants for the repair and the binary misrepair process.

Because we are considering only impulsive irradiation, the direct induction of lethal damages, as well as the production of repairable DSBs, will be represented in the initial conditions. If a sequence of impulsive irradiations is given with dose D_i at time t_i, $i=1,2,...,$ $t_1=0$, we have the following initial conditions for Eqs. (1)-(3),(8)-(9):

$$\nu_P(r,t_i^+) = \exp[-\alpha_P(\sigma(r,t_i^-))D_i]\nu_P(r,t_i^-)\,,$$

$$\nu_Q(r,t_i^+) = \exp[-\alpha_Q(\sigma(r,t_i^-))D_i]\nu_Q(r,t_i^-)\,,$$

$$\nu^\dagger(r,t_i^+) = (1-\exp[-\alpha_P(\sigma(r,t_i^-))D_i])\nu_P(r,t_i^-)$$

$$+(1-\exp[-\alpha_Q(\sigma(r,t_i^-))D_i])\nu_Q(r,t_i^-)+\nu^\dagger(r,t_i^-)\,,$$

$$X_P(r,t_i^+) = \delta_P(\sigma(r,t_i^-))D_i + X_P(r,t_i^-)\,,$$

$$X_Q(r,t_i^+) = \delta_Q(\sigma(r,t_i^-))D_i + X_Q(r,t_i^-)\,.$$

The dependence on the oxygen concentration of the radiosensitivity is expressed in terms of the parameters, α and β, of the standard linear-quadratic model (Wouters and Brown, 1997)

$$\alpha_P(\sigma) = \alpha_M^P\psi_\alpha(\sigma)\,, \quad \alpha_Q(\sigma) = \alpha_M^Q\psi_\alpha(\sigma)\,,$$

$$\beta_P(\sigma) = \beta_M^P\psi_\beta^2(\sigma)\,, \quad \beta_Q(\sigma) = \beta_M^Q\psi_\beta^2(\sigma)\,,$$

where $\psi_\alpha(\sigma)$, $\psi_\beta(\sigma)$ are Michaelis-Menten functions of σ. Since $\beta = \delta^2 k/(4\omega)$, $\delta_P(\sigma)$ and $\delta_Q(\sigma)$ are thus expressed by

$$\delta_{P,Q}(\sigma) = \sqrt{\frac{4\omega}{k}\beta_M^{P,Q}}\psi_\beta(\sigma)\,.$$

At $t = 0^-$, we have $\nu_P(r,0^-) = \nu_{P_0}(r)$, $\nu_Q(r,0^-) = \nu_{Q_0}(r)$, and all the other state variables are zero.

3. CONCLUSIONS

Numerical simulations of the model were able to predict the cellular response to a single dose of radiation and the time-course of reoxygenation. We compared the single-dose response to the response occurring when the dose is divided into two equal fractions (split-dose response). It was found that the reoxygenation reduces the sparing effect of fractionation, the maximal reduction being achieved when the second dose is delivered at the time of maximal reoxygenation. The prediction of the reoxygenation time course might thus be useful in determining the optimal time of dose delivery. Moreover, the sparing effect appears strongly influenced by the intervessel distance. The comparison of the effects of split-dose delivery in the tumour and in the normal tissue was also performed.

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Mathematical Modeling of Cellular Signaling in Macrophages: Lipid Signaling Kinetics

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1. Introduction

In recent years, mathematics has begun significantly impacting research in the biological sciences through the use of mathematical tools that are much more varied than traditional statistical techniques, which have long been used to analyze experimental data. One area that has benefited from such mathematical applications is the study of cellular signaling pathways, where mathematical models are providing insight into the structure and function of these complex cellular interactions. Our current work focuses on one such signaling pathway in a macrophage-like cell line. A macrophage is a type of white blood cell that surrounds and kills microorganisms, removes dead cells, and stimulates the action of other immune system cells.

To begin, a brief description of the underlying biology is given. Activation of cell surface G-protein coupled receptors (GPCRs) initiates diverse cellular signaling responses including mobilization of internal calcium (Ca^{2+}), cyclic adenosine monophosphate (cAMP) modulation and the activation of lipid hydrolases and kinases. These signaling pathways interact with one another, often in a non-linear manner, and the final biological response is shaped by the nature of these interactions. Recently there has been significant progress in modeling individual components of such pathways. For instance, Lemon (2) published a model in 2003 which included an extensive study of the activation and desensitization of the P2Y2 receptor post agonist stimulation with the nucleotide uridine triphosphate (UTP). The study and mathematical modeling of Ca^{2+} dynamics involved in similar signaling pathways has also been widely studied (3; 4). Utilizing the insights from such previously studied areas and modeling concepts, our focus is directed to a different yet equally important aspect of the P2Y6 signaling pathway. Although the model includes ordinary differential equations for the major pathway components, an emphasis is placed on the production and degradation of diacylglycerol (DAG), a cellular second messenger molecule which plays an important role in initiating various changes in cell behavior, including cell activation, differentiation, proliferation and tumor promotion.

2. Model Development

Our goal is the construction of a comprehensive mathematical model for the uridine 5-diphosphate (UDP) signaling pathway in the RAW 264.7 macrophage. This mathematical model incorporates modules for: (i) the ligand interaction with the P2Y6 receptor, the putative mode of action for UDP; (ii) the subsequent G-protein cascade; (iii) the activation of effector enzymes including phospholipase C (PLC), diacylglycerol kinase (DGK), and several forms of phosphatidylinositol kinase (PI4K, PI5K). In addition, small molecule dynamics for Ca^{2+}, IP3, and PIPn are either modeled or used as functional inputs to provide a comprehensive description of the signaling dynamics. Our model focuses on diacylglycerol (DAG) and phosphatidic acid

(PA), and lipidomic technology is utilized to measure the formation and fate of these important lipid second messengers.

Our current mathematical model is able to reproduce many of the response characteristics observed in the experimental data, including the correct order of magnitudes, appropriate timescales, and realistic kinetics. However, upon construction of the model based on the canonical pathway, which only includes a single pool of DAG produced from hydrolysis of phosphatidyl inositol 4,5 bisphosphate (PIP2), it became clear that there had to be other interactions taking place, as the model was unable to capture the initial dip in DAG seen experimentally. This discovery has led to the development of a newly proposed pathway in which two pools of DAG are present within the cell, and both are stimulated upon activation of the P2Y6 receptor. Inclusion of this second pool of DAG allows for more accurate modeling of the experimental results.

This talk will focus on the interactions involved in forming a collaborative relationship among researchers in diverse fields and the impact that mathematics has had on the experimental designs used to understand the pathway.

Joint work with H. Alex Brown and the Brown Laboratory, Department of Pharmacology, Vanderbilt University.

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Population-based models of anti-tumor anti-angiogenesis therapy: theory and biomedical inferences.

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Keywords: Tumor, Angiogenesis, Therapy, Qualitative Theory of Differential Equations.

1. ANGIOGENESIS, TUMORS AND ANTI-ANGIOGENIC THERAPIES

Primary tumors and metastases require the formation of new blood vessels in order to grow beyond about 1 to 2 mm^3. This process is sustained by different mechanisms: tumors may coopt existing vessels, may induce the formation of new vessels from pre-existing ones or may exploit endothelial precursors originating from the bone marrow. Vessel formation is regulated by a number of pro- and anti-angiogenic molecules, released by tumor cells. There is compelling evidence from experimental work, that inhibiting angiogenesis may induce tumor regression or sometimes cure. Targeting tumor vasculature, composed of genetically stable endothelial cells, has been regarded as a means to overcome acquired drug resistance. Angiogenesis inhibitors are commonly classified as direct inhibitors, acting on the endothelial cells and inhibiting their proliferation and migration or inducing their apoptosis, indirect inhibitors, blocking the production of angiogenic factors by malignant cells. Most angiogenesis inhibitors are cytostatic, inhibiting the formation of new blood vessels, but some direct inhibitors may result cytotoxic, inducing rapid destruction of existing blood vessels. Various anti-angiogenic drugs are undergoing clinical evaluation, with conflicting outcomes despite some encouraging results.

2. MATHEMATICAL MODELING ANTI-ANGIOGENESIS THERAPIES

Modelling the interaction between tumor growth and the development of its vascular network, as well as the action of angiogenesis inhibitors, could help to plan effective anti-angiogenic therapies. Some mathematical models have been recently proposed (Hahnfeldt et al 1999, Agur et al 2004, d'Onofrio and Gandolfi 2004). Among the factors influencing the clinical effectiveness of angiogenesis inhibitors, the administration schedule appears to be particularly relevant. Anti-angiogenic therapy has always been proposed as uninterrupted, long term treatment, to obtain effective tumor growth control. Despite this concept has pervaded the clinical development of anti-angiogenic drugs, a deeper insight into the relationships between drug pharmacokinetics and anti-vascular activity could be useful to improve clinical results.

Hahnfeldt et al. (1999) proposed a simple mathematical model which describes the vascular phase of tumor growth assuming that it is strictly controlled by the dynamics of the vascular network, and that the vascular dynamics is the result of the opposite influence of pro-angiogenic and anti-angiogenic factors produced by the tumor itself. This model

provides a framework to portray the effects of anti-angiogenic therapies, and it was successful in fitting experimental data on the growth and response to different anti-angiogenic drugs of Lewis lung carcinomas implanted in mice. A mathematical analysis of that model was presented in (d'Onofrio and Gandolfi 2004), focusing on the tumor eradication, under regimens of continuous or periodic anti-angiogenic therapy.

3. THE INTERPLAY BETWEEN MATHEMATICAL MODELS AND MEDICAL INFERENCES

In this work we illustrate some biological and clinical inferences derived from the analysis of the model by Hahnfeldt et al. (1999) and of variants and generalizations of it. In particular, we shall focus on the following topics:

- Analytically, we shall derive conditions for the globally asymptotically stable eradication of the disease;
- Concerning the class of anti-angiogenic drugs that act by altering the proliferation related parameters of the vascular cells, we shall show that these drugs, even though can exert tumor control, are ineffective in leading to tumor eradication unless there is a sufficiently high rate of spontaneous loss of the tumor vasculature (d'Onofrio and gandolfi, 2006);
- Through numerical simulations, we shall compare the effect of a constant continuous infusion of a drug that induces vascular loss to the effect of a periodic, bolus-based, therapy. We shall investigate the role of drug elimination rate and dose fractionation, and show that different schedulings guaranteeing the same mean value of drug concentration may exhibit very different long-term responses according to their concentration versus time profile, with the profiles that approach the constant one being more effective (d'Onofrio et Al, 2006);
- We shall briefly study the problem of optimization of therapies (Swierniak et al., 2006)(Ledzewicz and H. Schättler, 2007);
- Finally, we shall show as some biological problems related to the anti-angiogenic therapy may lead to more complex phenomena that may be modeled by differential equations with distributed delays. In turn, we shall see as this way of modeling might give some contribution to the improvement of the therapy (d'Onofrio, 2006).

4. CONCLUSIONS

Summarizing, in this work we shall show how classical biological and medical features may naturally be translated in classical topics of the qualitative theory of differential equations such as global stability, delay differential equations, singular perturbation methods, cooperative systems, periodic solutions, persistence theory and optimal control..

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Heuristic optimization of a mathematical model of the innate immune response to cancer vaccines.

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Keywords: mathematical model, cancer vaccine, immunotherapy, optimization

1. Introduction

Traditionally most immunisation regimes have been optimised in order to stimulate high levels of antibody. This is because for many diseases protection can be predominantly antibody mediated. However this is not the case for all diseases, for example cytotoxic immune responses are important for protection against intracellular bacteria and viruses, as well as in the treatment of cancer. It is more difficult to optimise vaccination regimes aimed at stimulating cytotoxic immune responses since cytotoxic immune responses are much more difficult to measure than antibody titres. In particular, ex vivo measurements are difficult, since these cells are present only at very low levels and are often difficult to detect following immunisation. Therefore, subjective markers for vaccine efficacy are often utilised. In the case of therapeutic cancer vaccines, these markers may be such things as disease free survival or time to disease progression. However as these parameters do not provide an immediate read out of the efficacy of the immunisation regime they provide little help for optimising the therapy. Therefore often the only option available for researchers and clinicians is the "Goldlilocks" approach to cancer vaccination: give not too much of the vaccine, or to little and give it not too often or too few times.

We present a new mathematical model of the immune kinetics in response to tumor antigen. The aim of this work is to model the T cell immune response to a vaccine with the goal that this can be used to aid in the optimisation of vaccine induced prophylactic and therapeutic cellular immune responses. The model is calibrated using data from mouse experiments where it is possible to directly measure cellular immune responses. Additionally in the mouse many parameters such as time to cell division, the rate of cell division and of cell death after exposure to antigen are known. Heuristic methods are then applied to the model to suggest immunization protocols that would produce the best cellular immune response. We will discuss the ultimate goals of the model, which are to understand the impact of clinically controllable factors such as antigen dose, the duration of antigen persistence, the presence of immune potentiating agents and the number and timing of any booster immunisations. This is joint work with Dr. Sarah Hook, University of Otago, Dunedin, New Zealand.

2. The Mathematical Model

The model consists of a system of delay differential equations, and is calibrated to experimental data from murine experiments performed specifically for the purpose of the development of the mathematical model.

We model two T-cell populations in the spleen: $CD8^+$ T cells, denoted by the subscript 8, and $CD4^+$ T cells, denoted by the subscript 4. Each T cell population is further sub-divided into four sub-populations: active proliferating cells, Ap, highly apoptotic cells, Aa. normal active cells, An, and memory cells, M. We also include two APC populations: the population in the blood compartment, D_B, and the population in the spleen, D. The T-cell populations are all in the spleen compartment. We assume that there is an average synaptic connection time between APC's and immune cells, τ, required to proved a co-stimulatory response. This introduces a delay into the equations. The synaptic connection time differs for naive and memory cells. Denoting the proliferating, apoptotic, normal and mem-

ory immune cell sub-popluations by A_p, A_a, A_n and M, respectively, the model equations derived from these assumptions are as follows (equations 2-5 are duplicated for CD8$^+$ T-cells, giving 9 equations in all):

$$\begin{aligned}
\frac{dD}{dt} &= \mu_{BS} D_B - \delta_D D \\
\frac{dA_p}{dt} &= \rho \frac{D(t-\tau)A_p(t-\tau)}{\theta + D(t-\tau)} - \delta_A A_p \\
&\quad + \lambda D(t-\tau_M) M(t-\tau_M) - \frac{1}{T} A_p \\
\frac{dA_a}{dt} &= \frac{1}{T} A_p - (r + \alpha + \delta_A) A_a - \frac{1}{\Delta} A_a \\
\frac{dA_n}{dt} &= \frac{1}{\Delta} A_a - (r + \delta_A) A_n \\
&\quad - \left(\mu^*_{SB} + \frac{\Delta_\mu}{1 + D(t)/\theta_{shut}} \right) A_n \\
\frac{dM}{dt} &= r(A_a + A_n) + pM \left(1 - \frac{M}{k} \right)
\end{aligned}$$

3. Simulation Results

After the model is calibrated to the data, simulations are run to validate its behavior. We see that the simulations do, in fact, mimic experimentally observed phenomena, as shown in the Figures 1, 2 and 3.

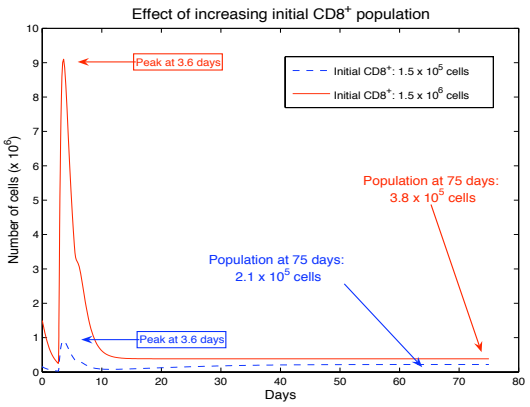

Fig. 1. Different initial CD8$^+$ levels do not affect the timing of the peak, but they do affect the size of the peak as well as the long term population sizes, (1)

4. Vaccination strategies

The size of the system and the introduction of delays makes it difficult to analytically apply control techniques to this problem. However, heuristic methods can be used. We will conclude the talk with a discussion of the results of the application of these methods.

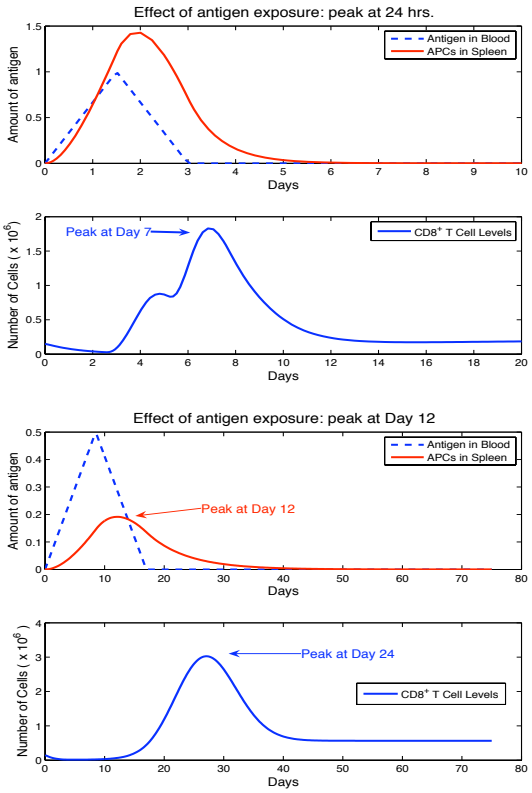

Fig. 2. Antigen exposure affects the timing of the peak response for CD8$^+$ T Cells. These simulations reflect the results discussed in (1)

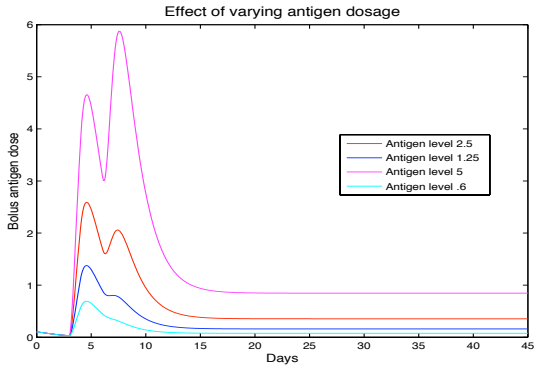

Fig. 3. Changing the antigen dosage changes the size of the peak and the amount of contraction

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SINGULAR ARCS IN THE OPTIMAL ANTIANGIOGENIC PROTOCOLS – ARE THEY OPTIMAL?

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Keywords: Cancer therapy, angiogenesis, optimization.

EXTENDED ABSTRACT

During progression of tumor, molecular factors called activators (stimulators) and inhibitors (blockers) of angiogenesis are released by tumor to develop its own vascular network which enables its growth and in the next stage determines possibility of cancer metastasis. Since this network is necessary for tumor development, in late sixties of the last century a new anticancer therapy called antiangiogenic was proposed target of which was not directly the cancer cells but the new born vasculature (Folkman, 1971). Its main advantage is that it is resistant to the drug resistance (Kerbel., 1997).
The complexity of the process of vascularization results in the complicated models applicable for simulation of the process but completely not useful in synthesis or even analysis of therapy protocols. The exception is a class of models proposed by Hahnfeldt *et al*. (1999) who suggested that the tumor growth with incorporated vascularization mechanism can be described by Gompertz type or logistic type equation with variable carrying capacity which defines the dynamics of the vascular network. D'Onofrio and Gandolfi (2004) proved that using sufficiently high doses of antiangiogenic drugs we are able to annihilate completely the vascular network of the tumor and indirectly eradicate the tumor itself. It can be reached not only using a constant dose of the drug but also by periodic therapy more reasonable from clinical point of view. Nevertheless since the results have an asymptotic character it means that the process of eradication is theoretically infinite and the same the patient once treated by the antiangiogenic therapy should remain under such control to the end of his life. To overcome this difficulty it has been proposed to optimize the therapy in finite horizon (Swierniak *et al*., 2006). The optimization problem for yet another modification of Hahnfeldt model was solved by Ergun *et al*. (2003). Ledzewicz and Schattler (2005) analysed Ergun model and found that optimal trajectories contained singular arcs. Recently they found similar properties for the original Hahnfeldt model. The goal of this presentation is to demonstrate that reasonable modifications of optimal control problems related to all these models lead to optimal solutions which have no singular arcs.
The main idea of Hannfeldt *et al*. (1999) is to treat the carrying capacity which constraints the tumor growth as a varying tumor volume sustainable by the vessels and roughly proportional to the vessel volume *K*. In the case of Gompertz type equation or logistic type equation it implies the following description of dynamics of tumor cells population N (respectively):

$$\dot{N}/N = -\beta \ln N/K, \text{ or } \dot{N}/N = \alpha(1 - N/K) \quad (1)$$

The dynamics of the growth of the vessel volume represented by its *PDT* depends on the stimulators of angiogenesis (*SF*), inhibitory factors secreted by tumor cells (*IF*) and natural mortality of the endothelial cells (*MF*):

$$PDT = f(MF, SF, IF) \quad (2)$$

It may be assumed that the inverse of *PDT* is the sum of these three factors i.e.

$$1 / PDT = MF + SF + IF \tag{3}$$

The spontaneous loss of functional vasculature represented by *MF* is supposed to be negative constant, the stimulatory capacity of the tumor upon inducible vasculature represented by *SF* is found to grow at rate $K^b N^c$ slower than the endogenous inhibition of previously generated vasculature represented by *IF* where:

$$b+c \sim 2/3 \tag{4}$$

From the other hand analysing a diffusion-consumption equation for the concentration of stimulator or inhibitor inside and outside the tumor, Hahnfeld *et al* concluded that inhibitor will impact on target endothelial cells in the tumor in a way that grows ultimately as the area of the active surface between the tumor and the vascular network which in turn is proportional to the square of the tumor diameter. It leads to the conclusion that *IF* is proportional to the tumor volume in power *2/3* since volume is proportional to the cube of the diameter. The expression for *K* suggested in (Hahnfeldt et al., 1999) has therefore the following form:

$$\dot{K} / K = \gamma\, N / K - (\lambda N^{2/3} + \mu) \tag{5}$$

γ, λ, μ being constant parameters. The modification by d'Onofrio and A. Gandolfi (2004) which also satisfies Hahnfeldt's suggestions given by (4) assumes that the effect of *SF* and *MF* on the inverse of *PDT* is constant while the *IF* is proportional to the active surface of the area of tumor:

$$\dot{K} / K = \gamma - (\lambda N^{2/3} + \mu) \tag{6}$$

The reasonable design procedure is to formulate optimal control problem for the system given by the proposed model(s) and the control objective which adequately represents the primary goal of the therapy. We propose to optimize the protocol in the fixed finite time of therapy with the primary goal which is to find the control maximizing *TCP* (treatment cure probability) that leads to the following equivalent form of an optimal control problem:

$$J = N(T_k), \int_0^{T_k} u(t)dt \le \Xi, \qquad 0 \le u(t) \le U_m \tag{7}$$

with known constraining constant parameters. The integral constraints imposed on control variable for antiangiogenic agent represents mostly the shortage in the availability of the agent and only in part the possible side effects of the drugs (not sufficiently recognized yet). Due to isoperimetric form of the problem it could be transformed into the problem with the integral part of the performance index instead of the integral constrain on the control:

$$J = N(T_k) + r\int_0^{T_k} u(t)dt \qquad 0 \le u \le U_m \tag{8}$$

In (Swierniak et al., 2006) we have proved that for model (6) the solution to the optimization problem leads to bang-bang controls and singular arcs are not present. In the case of the original Hahnfeldt we are able to prove that if the cancer population is modeled by logistic type growth than singular solutions are not optimal either. The problem with the Ergun model is slightly different. Since the antiangiogenic therapy is directed towards the vasculature rather than towards tumor itself the reasonable objective is to minimize the volume of the vascular network. If so the dynamics of the tumor may be omitted in the optimization problems and this implies once more the bang–bang optimal solution of the optimization problems.

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MODELLING OF ANGIOGENESIS PROCESS

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Keywords: tumour angiogenesis, stability, global stability

1. INTRODUCTION

Angiogenesis is one of the most important processes in malignant tumours dynamics. It is also recognised as a target for chemotherapy. This possible role of angiogenesis was discovered by Folkman in 1972 (Folkman (1971)), however its implementation is directly connected with anti-angiogenic drugs, which was discovered in nineties by O'Reilly et al. (O'Reilly et.al (1994, 1997)). After more than 30 years after the Folkman discovery, we are able to understand this process much better, compare e.g. Carmeliet et.al (2000); Yangopoulos et.al (2000). In the lack of nutrients, tumour cells secrete growth factors, one of the best known is VEGF (vascular endothelial growth factor), which can stimulate endothelial cells EC to proliferate, migrate and form new blood vessels. However, the newly formed vessels have highly unstable structure and its stabilisation crucially depends on maturation (coverage by pericytes) which is governed by another growth factor — PDGF (platelet-derived growth factor) and the system of angiopoietins Ang1 and Ang2 (compare e.g. Holash et.al (1999)). Therefore, the effective vessel density EVD (namely the total perfused vasculature) can exhibit an oscillatory behaviour.

The considered process is very complicated and therefore, mathematical modelling can bring a better understanding and lead to better treatment protocols, compare Arakelyan et.al (2002). The first mathematical model of angiogenesis was proposed by Hahnfeldt et al. in Hahnfeldt et.al (1999). It is described as a system of two ODEs (ordinary differential equations) based on the Gompertz growth of tumour with carrying capacity equal to endothelial cells volume. This model was studied in d'Onofrio et.al (2004) and it occurs that independently on the parameters there exists exactly one globally stable positive equilibrium. On the basis of the Hahnfeldt et al. model some optimal protocols of anti-angiogenic treatment was proposed, compare, e.g. Ergun et.al (2003); Ledzewicz et.al (2005).

Due to its global stability, the Hahnfeldt et al. model cannot reflect possible instability of the blood vessel formation and structure that is observed in the experiments, e.g. Holash et.al (1999); Gilead et.al (1999). In Arakelyan et.al (2002) much more complicated computer model was proposed to described this dynamics. Next, in Agur et.al (2004) the computer model from Arakelyan et.al (2002) was simplified and described as the system of three (or five) DDE's (delay differential equations) which evolves instable oscillations. This model was also analysed in Foryś et.al (2005) and compared with the experimental data in Arakelyan et.al

(2005). On the other hand, the Arakelyan et al. model cannot exhibit the stable behaviour even in the case without delay, compare Foryś et.al (2005).

Combining the ideas from Hahnfeldt et.al (1999) and Agur et.al (2004) we propose three-variable tumour angiogenesis model with tumour carrying capacity depending on vessel density, similarly to Hahnfeldt et.al (1999). Our model differs from that proposed in Agur et.al (2004) only in the first equation, where carrying capacity was not taken into account.

2. MODEL PRESENTATION

As in Agur et.al (2004); Foryś et.al (2005) we consider three time-dependent variables: tumour size $N(t)$, amount of regulating proteins $P(t)$ and vessel volume. We define effective vessel density as $E(t) = V(t)/N(t)$. We assume that the tumour growth is bounded, but the presence of the vessels enlarge the carrying capacity. Nevertheless, the tumour cannot grow to infinity — after tumour have grown to the proper size, the metastasis process begin — this phenomena is not described by this model. To model behaviour described above, we assume that the tumour growth is governed by the logistic equation with carrying capacity depending on the effective vessel density. The production of regulating proteins is decreasing with increasing vessel density and it is proportional to tumour size. We also consider the natural decay of proteins with the rate coefficient δ. The vessel creation is proportional to the vessel volume with the coefficient depending on the amount of proteins. Finally, we have a system of three ordinary differential equations:

$$\begin{cases} \dot{N} &= \alpha N \left(1 - \dfrac{N}{1+f_1(E)}\right) \\ \dot{P} &= f_2(E)N - \delta P \\ \dot{V} &= f_3(P)V \end{cases} \tag{1}$$

where f_1 is an increasing function with $f_1(0) = 0$ and $f(+\infty) = b_1 > 0$, f_2 is a decreasing convex function with $f_2(0) = a_2 > 0$ and $f(\infty) = 0$, f_3 is an increasing function with $f_3(0) = -a_3 < 0$, $f(c_3) = 0$ and $f_3(\infty) = b_3$.

Substituting V with E in the last equation we obtain

$$\begin{cases} \dot{N} &= \alpha N \left(1 - \dfrac{N}{1+f_1(E)}\right) \\ \dot{P} &= f_2(E)N - \delta P \\ \dot{E} &= \left(f_3(P) - \alpha\left(1 - \dfrac{N}{1+f_1(E)}\right)\right) E\,. \end{cases} \tag{2}$$

3. STEADY STATES

Looking for steady states, from the first equation we see at once that either $N = 0$ or $N = 1 + f_1(E)$. Let consider the first case. From the second equation we immediately obtain that $P = 0$, which implies $E = 0$. Thus the trivial solution $(0, 0, 0)$ is the steady state for the system (2). If $N = 1 = f_1(E)$, from the third equation we have either $E = 0$ or $f_3(P) = 0$. If $E = 0$, from the second equation we obtain $P = a_2/\delta$ and $N = 1$ from the first one. Thus, we got the steady state $(1, a_2/\delta, 0)$. If $E \neq 0$, then $P = c_3$. Using $N = 1 + f_1(E)$ we obtain $f_2(E)(1 + f_1(E)) = \delta c_3$. Depending on the functions f_1 and f_2 there can exist zero, one or more positive steady states $(\bar{N}, c_3, \bar{E})$.

Thus, we have at least two steady states

$$A = (0, 0, 0)\,, \qquad B = (1, a_2/\delta, 0)\,,$$

$$C_i = (\bar{N}_i, c_3, \bar{E}_i)\,.$$

The steady states C_i not necessarily exist.

In order to determine the stability, we calculate the Jacobi matrix for the system (2).

It is easy to see that

$$M(A) = \begin{bmatrix} \alpha & 0 & 0 \\ a_2 & -\delta & 0 \\ 0 & 0 & -a_3 - \alpha \end{bmatrix}$$

and thus the point A is an unstable saddle point.

For the point B we have

$$\begin{bmatrix} -\alpha & 0 & \alpha f_1'(0) \\ a_2 & -\delta & f_2'(0) \\ 0 & 0 & f_3\left(\frac{a_2}{\delta}\right) \end{bmatrix}.$$

Thus, it is stable if $a_2 < c_3\delta$ and unstable for $a_2 > c_3\delta$. We may interpret it biologically in the following way: the stability means that the production of proteins is too small to cause sufficiently fast creation of new vessels. Thus, tumour cannot grow beyond size 1.

For the steady states C_i (if it exists) we have

$$M_C = \begin{bmatrix} -\alpha & 0 & \alpha f_1'(\bar{E}) \\ f_2(\bar{E}) & -\delta & f_2'(\bar{E})\bar{N} \\ \frac{\alpha\bar{E}}{1+f_1(\bar{E})} & f_3'(c_3)\bar{E} & -\frac{\alpha\bar{E}}{1+f_1(\bar{E})} f_1'(\bar{E}) \end{bmatrix}$$

Denoting $\beta = \frac{\bar{E}}{1+f_1(E)}$, $d_1 = f_1'(\bar{E}) > 0$, $-d_2 = f_2'(\bar{E}) < 0$, $c_2 = f_2(\bar{E}) > 0$ and $d_3 = f_3'(c_3) > 0$ we have

$$M_C = \begin{bmatrix} -\alpha & 0 & \alpha d_1 \\ c_2 & -\delta & -d_2\bar{N} \\ \alpha\beta & d_2\bar{V} & -\alpha\beta d_1 \end{bmatrix}$$

Calculating the characteristic polynomial we obtain

$$w(\lambda) = \lambda^3 + (\alpha(1+\beta d_1) + \delta)\lambda^2 +$$

$$+(\alpha\delta(1+\beta d_1) + d_2 d_3 \bar{N}\bar{E})\lambda +$$

$$\alpha d_3 \bar{E}(d_2\bar{N} - c_2 d_1)\,.$$

We would like to determine conditions for negativity of real parts of eigenvalues of M_C. We use Huth-Hurwitz criterion for the polynomial w. We remind that for $w(\lambda) = \lambda^3 + a_2\lambda^2 + a_1\lambda + a_0$, necessary and sufficient condition for having all roots of polynomial w on the left half-plane is: all coefficients a_i has to be positive and $a_1a_2 - a_0 > 0$. By simple but tedious calculations we may check that $a_1a_2 - a_0 > 0$. It is also easy to see that all coefficients except a_0 are positive. Therefore, the steady state C_i is stable if $d_2\bar{N} - c_2d_1 > 0$ and unstable if $d_2\bar{N} - c_2d_1 < 0$. Notice, that for this steady state $\bar{N} = 1 + f_1(\bar{E})$. Using this equality we obtain

$$d_2\bar{N} - c_2 d_1 =$$

$$-f_2'(\bar{E})(1 + f_1(\bar{E})) - f_2(\bar{E})f_1'(\bar{E}) > 0.$$

Then

$$-f_2'(\bar{E})(1 + f_1(\bar{E})) > f_2(\bar{E})f_1'(\bar{E})$$

$$-\frac{f_2'(\bar{E})}{f_2(\bar{E})} > \frac{f_1'(\bar{E})}{1 + f_1(\bar{E})}$$

$$-\left(\ln f_2(\bar{E})\right)' > \left(\ln(1 + f_1(\bar{E}))\right)'$$

$$\left(\ln f_2(\bar{E})(1 + f_1(\bar{E}))\right)' < 0$$

Since logarithm is an increasing function, this implies that the function $g(E) = f_2(\bar{E})(1 + f_1(\bar{E}))$ should be decreasing in the neighbourhood of $\bar{E}$. Notice, that the steady state $\bar{E}$ is a solution to $g(\bar{E}) = c_3\delta$. Since $g(0) > 0$ and $\lim_{E\to\infty} g(E) = 0$ it is easy to see, that the greatest steady state is stable.

The existence of steady state C_i. The positive steady state C_i exists if and only if the function $g(x) = f_2(x)(1 + f_1(x)) - \delta c_3$ has a positive root. Notice, that $g(0) = a_2 - \delta c_3$ and $g(+\infty) = -\delta c_3$. Thus, if $a_2 > \delta c_3$, then there exists at leas one positive root of $g(x) = 0$. Therefore, there exists at least one positive steady state C_1. Notice, that in that case, the steady state B is unstable.

Let differentiate the function g. We obtain

$$g'(x) = f_2'(x)(1 + f_1(x)) + f_2(x)f_1'(x)$$

Notice, that if the function f_1 increases slow enough, then $g'(x) < 0$ and there exist at most one steady state C_1.

4. CONCLUSIONS

In the paper we have proposed the three-variable angiogenesis model which improves the Arakelyan et al. model such that the positive steady state of the system is stable which is impossible in the original model. Our model differs from the original one only in the first equation where we consider the carrying capacity for tumour cells which depends on the effective vessel density. The idea of carrying capacity depending on it comes from **?**, however in our model the dependence is not so simple as in the case of Hahnfeldt et al. model.

We determined conditions under which the unique positive steady state is stable. On the other hand, there can exist more than one positive steady state and in this case at least one of them is unstable. Therefore, such a case can reflect instability described in Arakelyan et.al (2002); Agur et.al (2004). We can also consider the system with delays, as in Agur et.al (2004). Then, destabilisation due to delays occur. Therefore, depending on the parameters, the model proposed in this paper can reflect both types of dynamic — instability of newly formed vessels and stabilisation of it.

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A COMPARISON OF OPTIMAL AND SUB-OPTIMAL STRATEGIES FOR MODELS OF TUMOR ANTI-ANGIOGENSIS

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Invited session: Modelling, control and optimization of dynamical systems: theory and applications to biomedicine

1. INTRODUCTION

The most important limiting factor for the success of cancer chemotherapy treatments lies in both intrinsic and acquired drug resistance. As of today, the search for therapy approaches that would avoid drug resistance still is of a tantamount importance in medicine and two such approaches that are currently being pursued in their experimental stages are immunotherapy and anti-angiogenic treatments. While immunotherapy tries to coax the body's immune system to take action against the cancerous growth, tumor anti-angiogenesis aims at depriving a tumor from developing the necessary blood cells and capillaries that it needs for further growth. Since the treatment does not target cancer cells, but normal cells, no occurrence of drug resistance has been reported in lab studies and for this reason tumor anti-angiogenesis has been called a therapy resistant to resistance which provides a new hope in treatment of tumor type cancers (Kerbel, 1997).

2. MODELLING

There exist several mathematical models for the evolution of tumor anti-angiogenesis as a dynamical system with the one formulated by Hahnfeldt, Panigrahy, Folkman and Hlatky in (Hahnfeldt et al., 1999) probably being the most prominent one. This model was biologically validated in lab experiments and became the basis for several modifications and simplifications (d'Onofrio and Gandolfi, 2004; Ergun et al., 2003) undertaken in an effort to both better understand the dynamical properties of the underlying mechanisms and to make the mathematical model easier and more tractable for analysis. For example, a dynamical systems analysis of the model by Hahnfeldt et al. and of several modifications (with more general growth models for the cancer volume and slightly different dynamics for the evolution related to endothelial cells) is given in the paper by d'Onofrio and Gandolfi (d'Onofrio and Gandolfi, 2004); Ergun, Camphausen and Wein (Ergun et al., 2003) consider an optimal control problem for the scheduling of anti-angiogenic inhibitors both as monotherapy and in combination with radiotherapy. While these models are variations of the specific dynamics proposed by Hahnfeldt et al. in (Hahnfeldt et al., 1999), in the papers by Agur, Arakelyan, Daugulis and Ginosar (Agur et al., 2004) and Forys, Kheifetz and Kogan (Forys et al., 2005) more generally dynamical properties of models for angiogenesis are investigated under minimal assumptions on the form of the growth functions describing the dynamics.

3. MATHEMATICAL FORMULATION

Angiogenesis can be viewed as a complex balance of stimulatory and inhibitory mechanisms regulated through micro-environmental factors. In this talk, following (Hahnfeldt et al., 1999), we will describe the basic principles

of the underlying modelling which are summarized in a two-dimensional dynamical system with the primary tumor volume, p, and the carrying capacity of the vasculature, q, as variables. A growth function describes the size of the tumor dependent on the carrying capacity q and is chosen as Gompertzian in the original model,

$$\dot{p} = -\xi p \ln\left(\frac{p}{q}\right) \tag{1}$$

where ξ denotes a tumor growth parameter. Other models using a different model for the growth function for p are considered in (d'Onofrio and Gandolfi, 2004) or (Forys et al., 2005). The overall dynamics for the carrying capacity is a balance between stimulation and inhibition and its basic structure is of the form

$$\dot{q} = -\mu q + S(p,q) - I(p,q) - Guq \tag{2}$$

where μq describes the loss of endothelial cells due to natural causes (death etc.), I and S denote endogenous inhibition and stimulation terms, respectively, and Guq represents a loss due to additional outside inhibition. The variable u represents the control in the system and corresponds to the angiogenic dose rate while G is a constant that represents the anti-angiogenic killing parameter.

4. OPTIMAL CONTROL

In our papers (Ledzewicz and Schättler, 2005, 2006, 2007) we have considered the optimal control problem of how to administer a given amount of inhibitors to achieve the "best possible" effect in the sense of minimizing the tumor volume both for the model from (Hahnfeldt et al., 1999) and (Ergun et al., 2003). Both optimal solutions contain a singular arc as the center piece of their synthesis. But this corresponds to giving specific time varying dosages and is not practical or even realizable with the current status of medical technologies. In this talk we will compare these optimal solutions with the intuitive and medically commonly used strategy of giving all available inhibitors as one dose initially. Our previous analysis of optimal controls allows to make quantitative judgements as to how good these strategies are relative to the best possible tumor reduction that can be achieved with a limited amount of inhibitors.

5. CONCLUSIONS

For the original model of Hahnfeldt et al. (Hahnfeldt et al., 1999) the achievable tumor reductions are very close to each other if the tumor volume is small - in fact, in some regions of the state space it is optimal to give all available inhibitors in one dose initially - but for larger values of the tumor volume, there is a discernable difference in the reductions that can be achieved by the optimal and suboptimal strategies.

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CONTROL OF HIV AMONGST INJECTING DRUG USERS

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Keywords: Human Immunodeficieny Virus (HIV), Acquired Immune Deficiency Syndrome (AIDS), Injecting Drug Users, Control, Basic Reproductive Ratio, Deterministic Model, Stochastic Model.

1. INTRODUCTION

This talk is concerned with mathematical models for the control of HIV amongst injecting intravenous drug-users (IDUs), particularly needle exchange programs, HIV testing of IDUs and improved cleaning practices. Our model is based on the work of Kaplan and O'Keefe (1993) who developed basic mathematical models for the spread of HIV amongst IDUs using data from Connecticut, New Haven, USA.

2. HOMOGENEOUS MODEL

We start off by outlining a basic existing homogeneous differential equation model for the spread of HIV amongst IDUs incorporating these control strategies. We next describe an improvement of the way in which HIV testing can be treated in this model.

Our model assumes that the total number of drug addicts and the total number of needles remain constant. If π_1, π_2 and β denote the prevalence of HIV amongst untested addicts, tested addicts and needles respectively at time t then the differential equations which describe the spread of the disease are:

$$\begin{aligned}\frac{d\pi_1}{dt} &= (1-\pi_1-\pi_2)\lambda_1\beta\alpha(1-\phi) \\ &\quad -(\mu+\delta_t+\delta)\pi_1; \\ \frac{d\pi_2}{dt} &= \delta_t\pi_1-(\mu+\delta)\pi_2;\end{aligned}$$

and

$$\begin{aligned}\frac{d\beta}{dt} &= (1-\beta)\gamma(\pi_1\lambda_1+\pi_2\lambda_2) \\ &\quad -\beta\lambda\gamma(1-\pi_1-\pi_2)(\theta+\phi-\theta\phi) \\ &\quad -\beta\tau.\end{aligned}$$

Here λ_1 is the sharing injection rate of addicts who do not know that they are infected; λ_2 is the decreased sharing rate of addicts who know that they are infected; α is the transmission probability that when a single uninfected addict makes a single injection with an infected needle the addict is infected and ϕ is the probability that an addict successfully cleans a needle before use. μ is the per capita rate at which addicts leave the sharing, injecting population for reasons other than developing AIDS; δ_t is the per capita HIV testing rate, δ is the per capita rate at which HIV-infected addicts progress to AIDS; γ is the ratio of addicts to needles and θ is the flushing probability that when a single uninfected addict uses an infected needle that needle is left uninfected after use.

For this improved model a key parameter is the basic reproductive ratio. This is the expected number of secondary cases that a single newly infected addict will cause on entering an entirely susceptible addict population. We find that

$$R_0 = \frac{\lambda_1\alpha(1-\phi)}{(\mu+\delta_t+\delta)(\hat{\tau}_1+\lambda_1\hat{\theta})}\left[\lambda_1+\frac{\lambda_2\delta_t}{(\mu+\delta)}\right]$$

where $\hat{\tau}_1 = \tau/\gamma$ and $\hat{\theta} = \theta+\phi-\theta\phi$.

We show that the disease will always die out if $R_0 \leq 1$, whilst if $R_0 > 1$, as well as the disease-free equilibrium (which is always possible) there is a unique endemic equilibrium which is locally asymptotically stable. We verify these analytical results by using deterministic computer simulation using the computer package SOLVER. Our simulations suggest that if $R_0 > 1$ then provided only that disease is initially present in either ad-

dicts or needles then it will eventually tend to the unique endemic equilibrium.

We also look at some simulations for a stochastic version of this model. For the stochastic model some simulations go extinct. In those simulations which do not go extinct the prevalence of infection in both addicts and needles exhibit long term random fluctuations about their respective deterministic endemic equilibrium levels.

3. CONTROL STRATEGIES

For the deterministic model we assess the effect of HIV testing and needle exchange on disease incidence. We use both the basic reproduction number R_0 and the endemic equilibrium level of disease prevalence in addicts as effectiveness measures for differing control strategies. We look at how the equilibrium endemic prevalence varies with the injection sharing rate and HIV testing rate and produce graphs of how R_0 and the endemic equilibrium level of prevalence in addicts vary with different control strategies. We find that HIV testing will be an effective control measure only provided that addicts are both tested regularly and greatly reduce their needle sharing rate. Needle exchange can be an effective control measure provided that needles are exchanged regularly.

4. VARIABLE INFECTIVITY

The model described above assumes that all addicts are equally infectious throughout their entire infectious period. In reality the viral load of an addict has been shown to vary throughout the addict's infectious lifetime, being very high for a relatively short period immediately after the initial infection, then very low for a long period and finally rising to an intermediate level just before the addict develops clinical AIDS (Seitz and Müller (1994)). It seems reasonable to assume that the infectivity of an HIV-infected individual shows a similar variability.

We outline a basic variable infectivity model which divides the addicts into three infectious stages but assumes that all needles have the same infectiousness. This model has been analysed in detail in Greenhalgh and Lewis (2001). We derive an expression for the basic reproduction number R_0 and obtain some equilibrium and stability results. The pattern of results is very similar to those for the single stage infectivity model. Again we perform deterministic simulations to verify the analytical results and then examine the effect of introducing stochasticity into the model.

Finally we graphically examine the effect of needle cleaning and needle exchange on the long term prevalence of disease in needles and addicts. We derive expressions for the critical needle exchange rate to eliminate the disease for a given needle cleaning probability and the critical needle cleaning probability to eliminate the disease for a given needle exchange rate.

5. CONCLUSIONS

By performing an equilibrium and stability analysis on our deterministic needle sharing models we were able to identify suitable performance measures for control interventions such as needle cleaning and needle exchange. These were the basic reproduction number R_0 and the endemic equilibrium prevalence level of HIV amongst addicts. We showed that needle exchange, HIV testing and improved cleaning may all be potentially effective control strategies against the spread of HIV amongst IDUs. Our analysis has provided an empirical justification for introducing the above strategies. These issues are discussed more fully in Lewis and Greenhalgh (1999).

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TWO-SCALE MODEL OF INTERFERON MEDIATED ANTIVIRAL RESPONSE

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Keywords: Biomedical modeling, optimization, multiscale models.

1. INTRODUCTION

Recent advances in experimental techniques have facilitated rapid expansion of knowledge about intracellular processes, intercellular communication, processes that take place during viral infection. On the other hand, mathematical models describing infection dynamics in cell populations have been developed much earlier and are still a subject of research. This paper aims at bridging the gap between models of intracellular processes and population dynamics. It is focused on viral infection dynamics in a cell population, affected by interferon-mediated antiviral response.

Interferons (IFNs) are very important components of the immunodefense system. They are produced by most cell types, and following viral infection are released to intercellular environment, signaling danger to other cells (e.g. Sen, 2001, Kalvakolanu, 2003). Thus they elicit antiviral response by activating cascades of biochemical processes (so called signaling pathways) in other cells. The model includes this release which will be a basis for modeling of processes on population level.

A standard, compartmental model is used to describe dynamics of cell population (see, e.g. Nowak *et al*., 1996, Reynolds *et al*., 2006). Its parameters depend on intracellular biochemical processes, mentioned above. The model is roughly described in the subsequent section.

Taking into account that interferon is not only a *in vivo* produced protein, but also is used as a therapeutic agent (Bekisz *et al.*, 2004), it is possible to use the model presented here to design of treatment protocols. For that aim, an optimization problem can be stated and solved, applying the methodology developed previously for cancer chemotherapy (Swierniak and Smieja 2005; Ledzewicz and Shaettler, 2006).

2. MATHEMATICAL MODEL

At the population level five compartments are considered. Let N_0, N_1, N_2 denote the average number of uninfected and susceptible, virus-resistant and infected cells, respectively. Two compartments are used for describing virus dynamics, P_e and P_i, denoting viral load in extracellular environment and inside cells, accordingly. Then, the system dynamics can be described by the following set of equations:

$$\begin{cases} \dfrac{dN_0}{dt} = k_0 - \lambda_0 N_0 - a_0 P_e N_0 - b_0(U) N_0 \\ \dfrac{dN_1}{dt} = -\lambda_1 N_1 + b_0(U) N_0 \\ \dfrac{dN_2}{dt} = -\lambda_1 N_2 - k_2(U) N_2 + a_0 P_e N_0 \\ \dfrac{dP_e}{dt} = -\lambda_e P_e - k_e P_e N_2 + k_i P_i \\ \dfrac{dP_i}{dt} = k_{prod} N_2 + k_e P_e N_2 - k_i P_i \end{cases}$$

where λ_i correspond to degradation rates of species i, k_0 and k_{prod} are production rates of new

cells and virons, respectively, k_e and k_i denote secretion and internalization rates, correspondingly, a_0 is an infection rate and U represents interferon concentration. Functions $b_0(U)$ and $k_2(U)$ reflect two different antiviral actions of interferon (defense against infection and marking of infected cells for killing by immune system) with U being a control variable.

Two different models are analyzed in the paper. In the first one, interferon is both a product of intracellular signaling pathways and a ligand that activates them. Concentration U is an output of the model describing dynamical processes taking place inside cells. Functions $b_0(U)$ and $k_2(U)$ also result from analysis of signaling pathways. Due to limited space in the extended abstract they cannot be described here. In short, the model consists of more than 20 ODEs (Smieja *et al*. 2006) and only in some cases can be approximated by simple dynamical time-lag elements.

The second model describes behavior of population of cells with damaged immune defense, which do not produce interferon. Then, interferon concentration U is a result of a therapy and is introduced to the extracellular environment as a drug component. Subsequently, a problem of finding optimal therapy arises, addressed in the following section.

3. OPTIMIZATION PROBLEM

The goal of therapy is to minimize the number of infected cells after a given therapy horizon T and reduce side effects of a drug being used. Therefore, the performance index to be minimized can be defined as

$$\min_U \leftarrow J = r_0 N_2(T) + r_1 \int_0^T U(\tau) d\tau$$

The model can be subsequently expanded to include active virus destruction by the cells of immune system and then the performance index would include the term $P_i(T) + P_e(T)$.

To solve the optimization problem Pontryagin maximum principle is used, as in (Kimmel and Swierniak, 2004).

4. CONCLUSIONS

Combining compartmental models of population dynamics with models of signaling pathways is an effective tool to analyze how intracellular processes affect behavior of cell populations. Moreover, it makes it possible to mathematically define problems of optimizing therapy. Though such attempts have been made before, the existing solutions either neglected pharmacodynamics or assumed its simplest possible model. Other approaches concentrated only on intracellular processes, assuming that drug actions are is proportional to concentration of some products inside cells (Ali *et al.*, 2006).

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A mathematical model separates quantitatively the cytostatic and cytotoxic effects of a HER2 tyrosine kinase inhibitor

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Keywords: targeted anti–cancer drugs, cytostatic and cytotoxic effects, mathematical modeling

1. BACKGROUND

Oncogene signaling is known to deregulate cell proliferation resulting in uncontrolled growth and cellular transformation. Gene amplification and/or somatic mutations of the HER2/Neu (ErbB2) proto–oncogene occur in approximately 20% of breast cancers. A therapeutic strategy that has been used to block HER2 function is the small molecule tyrosine kinase inhibitor lapatinib. Using human mammary epithelial cells that overexpress HER2, we determined the anti–proliferative effect of lapatinib through measuring the total cell number and analyzing the cell cycle distribution. A mathematical model was used to interpret the experimental data.

2. RESULTS

The model suggests that lapatinib acts as expected by slowing the transition through G_1 phase. However, the experimental data indicated a previously unreported late cytotoxic effect, which was incorporated into the model. Both effects depend on the dosage of the drug, which shows saturation kinetics.

3. CONCLUSIONS

The model separates quantitatively the cytostatic and cytotoxic effects of lapatinib and may have implications for preclinical studies with other anti–oncogene therapies.

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Multiscale modelling of viral infection of cells and of interferon resistance

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Keywords: viral infection, interferon resistance, mathematical modelling, structured population models, stability analysis

1. Biological background

For a eukaryotic virus to successfully infect and propagate in cultured cells several events must occur: The virion must identify and bind its cellular receptor, become internalised, uncoat, synthesize viral proteins, replicate its genome, assemble progeny virions, and exit the host cell. The virions bud off from the cell, gaining an envelope from the cell membrane as they exit. The new viral particle infects another cell to repeat the cycle. Usually, during the repeated process of self-replication, the virus destroys host's cells.

While these events are taking place, intrinsic host defenses activate in order to defeat the virus. The first-line defense against viruses is based on innate immunity. This includes, among others, activation of the interferon system, induction of apoptosis, and attempted elicitation of immune responses via chemokine and cytokine production. Interferons are a family of active biochemical species, which help to fight viral infections by spreading from infected to uninfected cells and triggering production of effector molecules. The interferons interact with receptors located on the membrane of uninfected cells, which leads to the activation of the reactions cascade in the uninfected cells and production of some proteins. These latter when activated confer on cells resistance from the virus (Rose et al. 2001).

To get a better insight into the dynamics of the processes described above we developed a mathematical model of dynamics of viral infection in vitro, including infection, cell death, production of interferon and development of resistance. The dynamics of the model can be understood as a combat between the invading virus particles and the ability of the immune system to react to the invasion by producing substances conferring resistance to virus. We concentrate on the case, in which the supply of unexposed cells ceases at the moment of infection. This corresponds to conditions prevalent in cell culture experiments.

The model is motivated by experiments involving vesicular stomatitis virus, (Lam et al. 2005; Rose et al. 2001), and respiratory syncytial virus (Rose et al. 2001) including unpublished experimental results performed in Dr. Allan Brasier's laboratory of the University of Texas Medical Branch in Galvestone.

2. Mathematical models

We consider a model for the dynamics of viral infection, which involves wild-type, i.e., unexposed to virus (W), infected (I) and resistant (R) cells, as well as particles of virus (v) outside cells, and molecules of interferon (i), the substance released by infected cells, which boosts the resistance of wild-type cells. The model consists of five ordinary differential equations for variables W, I, R, i and v, each being a function of time,

$$\begin{aligned} W' &= -\alpha_1 v W - \alpha_2 i W, \\ I' &= -\mu_I I + \alpha_1 v W, \\ R' &= \alpha_2 i W, \\ i' &= -\mu_i i + \alpha_i I - \alpha_3 i W, \\ v' &= -\mu_v v + \alpha_v I - \alpha_4 v W, \end{aligned}$$

with initial conditions

$$(W, I, R, i, v)(0) = (W_0, I_0, R_0, i_0, v_0),$$

To understand influence of the intracellular replication process on the observable spread of infection, we differentiate among the intracellular stages of infection for infected cells using an additional variable describing the age of infection. Infected cells of different age produce interferon at different rates and release virions at different rates. Mathematically, this variant requires an additional transport-type partial differential equation to model the infection-age structure in infected cells,

$$\begin{aligned} \frac{\partial I(t,a)}{\partial t} + \frac{\partial I(t,a)}{\partial a} &= -\mu_I(a) I(t,a), \quad a > 0 \\ I(t,0) &= v(t) W(t), \quad t \geq 0 \end{aligned}$$

However, the transport process can be reduced to distributed delay terms in two of the model equations. Therefore, the model with structure can be analysed using local linearised stability results for the functional (delay) type differential equation system (Diekmann et al. 1995).

3. Results

The methods we used to analyse our models involve both global and local methods. As it happens, a conservation law can be derived for the model without structure, application of which guarantees that the solutions of the model converge to limit values as $t \to \infty$. The same conservation law allows to conclude that unexpectedly, in the case with virus mortality, there is always a residual population of wild-type cells. When the virus mortality rate is equal to zero, this is not necessarily the case.

The conservation law can be extended to the structured case, under some additional hypotheses concerning supports of age-dependent mortality and infectivities. This law is mathematically interesting, since it is not a complete law as frequently used in the epidemics theory, however together with nonnegativity, it provides upper bounds, which sufficiently constrain the solutions.

Let us notice that the system, both in the unstructured and structured versions, is somewhat unusual in that it does not have unique equilibrium points. The limits to which the system is converging strongly depend on initial conditions. This property has an impact on the linearised stability. Attracting properties are limited to the subspace spanned by eigenvectors corresponding to nonzero eigenvalues, while the solution slides along the complementary subspace. In the case of the structured model, considerations of linearised stability can be done using a extension of the Mikhailov criterion.

Conditions of stability, which we obtained, seem to have interesting biological interpretations. First of all, the structure can have a stabilising (respectively, destabilising) effect even if the expected lifetime virus production of an infected cell is higher (respectively, lower) in the structured model than in the unstructured model. Also, delaying and shortening the time of new virus synthesis lead to a stabilising effect of structure. These results illustrate the importance of the dynamics of the process of virus proliferation and death of the infected cells. In the ODE system, duration of these processes can be understood as being described by exponentially distributed random variables. Our results indicate that this is not always sufficient and illustrate the need to understand these processes.

One of the important elements of the model is the presence of a mechanism of interferon-induced virus resistance. Interferon can be produced only by infected cells and confers resistance (in our model a complete resistance) on wild-type cells. It is interesting that setting the interferon production rate to zero does not qualitatively change the behaviour of the system. However, it reduces the total number of wild-type and resistant cells.

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HEMOPOIETIC DYNAMICS IN THE BONE MARROW, THE MYELODYSPLASTIC SYNDROMES, AND ISSUES RELATED TO CONTROL OF THIS DISEASE

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Keywords: mathematical modeling, myelodysplastic syndromes, control

1. INTRODUCTION

Hematopoiesis has remained a subject of intense study over the years because it is basically a massive process in the human body that involves various distinct cell lineages and results in the production of billions of different cell types each day. The genesis of this phenomenon is rooted in pluripotent stem cells in the bone marrow (BM) and involves a pool of totipotent stem cells that provide unipotent stem cells to the granulocytic, erythrocytic, thrombocytic and other lines. In each line, unipotent stem cells supply cells to a number of nonproliferating differentiation compartments in the BM before the release of mature neutrophils, erythrocytes, platelets, and other cell types into the blood.

There are a number of disorders such as the myelodysplastic syndromes (MDS) that negatively affect the normal functioning of the hemopoietic system and that are not yet completely understood as is evidenced by the absence of a known cure in certain instances (Anderson *et. al*., 1993; Shimazaki *et. al*., 2000). The myelodysplastic syndromes can be described as a group of acquired hematopoietic disorders with evidence of trilineage dysplasia and an approximately 30% incidence of eventual transformation into acute myeloid leukemia (Raza *et al*., 1995a). These disorders are clonal in nature and involve one or more clones. They evolve from a transformation of the normal hematopoietic state into the precancerous disease state. While some investigations of MDS have led to observations of ineffective hematopoiesis (Raza *et. al*., 1995a, b; Parcharidou *et. al*., 1999) in the BM arising from massive apoptosis of cells in this compartment others have suggested that the precise relationship between increased apoptosis of myeloid precursors and cytopenias should be more precisely explored (Lepelley *et. al*., 1996).

Our aim is to contribute to deepening and enriching the understanding of MDS and its treatment through the use of biomathematical models that give insight into its etiology and evolutionary dynamics. In the process of doing this we hope to address some of the discrepancies arising from the MDS investigations with the view to proposing possible resolutions of such discrepancies. Consequently, we propose to start our investigations by considering hematopoietic dynamics in the peripheral blood and marrow since these compartments understandably form the overwhelming focus of MDS research. We then end up discussing ways in which this disease can be controlled.

2. MODEL DESIGN AND ANALYSES

By relying on information from the literature regarding hematopoiesis (Mackey & Glass, 1977; Kazarinoff & denDriessche, 1979; Lord *et. al*., 1992; Schmitz *et. al*., 1993; Dale *et. al*., 1998; Price *et. al*., 1996; Schrier, 1988; Afenya, 1996; Marer & Skacel, 1999) and drawing upon investigations related to MDS (Anderson *et. al*., 1993; Hellstrom-Lindberg *et. al*., 1997; Shimazaki *et. al*., 2000; Raza *et. al*., 1995a, b; Khan *et. al*., 1991; Parcharidou *et. al*., 1999; Lepelley *et. al*., 1996; Mundle *et. al*., 1996, 2000), it is

appropriate to consider a model that comprises two broad compartments –a BM compartment and a peripheral blood (PB) compartment. Since the BM is said to be surprisingly uniform (Schrier, 1988), it will be assumed to a reasonable first approximation that the cells in this tissue are homogeneously distributed. This assumption is stretched to the PB compartment.

It is well known that cells in the BM spend some time maturing (Lord *et. al*., 1992; Schmitz *et. al*., 1993; Dale *et. al*., 1998) in this tissue before entering the blood to perform various functions during hemopoiesis. This means that a time lag due to cell maturation exists during the movement of cells from the BM compartment to the PB. Also in existence is a feedback mechanism through which cells in the BM are instructed to reproduce to account for shortfalls in the cell population of the PB compartment when situations that entail such developments arise. A schematic description of hemopoietic function is shown in Figure 1. An interpretation of this description that yields the model can be stated in words as follows:

[Rate of Change of the BM Cell Population] = [Growth Rate of Marrow Cells] + [Feedback from the Blood to the BM] –[Rate of BM Cell Apoptosis] – [Release Rate of BM Cells to the Blood].

[Rate of Change of the Blood Cell Population] = [Rate of Influx into and Turnover of Cells in the PB] –[Rate of Efflux of Cells out of the PB].

We note that the rate of influx into and turnover of cells in the PB encompass the rate at which BM cells are released into this compartment and the rate at which PB cells are produced (Lord *et. al*., 1992) in this compartment. The efflux rate of cells out of the PB include the rate of cell loss or cell disappearance (Lord *et. al*., 1992) out of this compartment in addition to the feedback sent from the blood to the BM. In mathematical terms we obtain the following system of equations:

$$\dot{N}_m = \alpha_m(N_m) + F(N_b) - \alpha(N_m(t-T_m))N_m(t-T_m) - \alpha_{md}N_m \quad (1)$$

$$\dot{N}_b = \alpha(N_m(t-T_m))N_m(t-T_m) - \alpha_{bd}N_b \quad (2)$$

with $N_m(0) = N_{m0}$, $N_b(0) = N_{b0}$, and

$$N_m(t) = N_{mc} \text{ when } -T_m \le t < 0 \quad (3)$$

where the parameters and variables in the equations above are described as follows:

$\alpha_m(N_m)$ = state-dependent growth rate of the BM cells per unit time, $F(N_b)$ = state-feedback from the PB to the BM, α_{md} = fractional apoptotic rate of BM cells per unit time, α_{bd} = fractional rate of PB cell loss per unit time, T_m = transit time of cells in the BM due to maturation, $\alpha(N_m(t-T_m))$ = release rate of cells from the BM into the PB, $N_m(t)$ = population of BM cells/liter at time t, and $N_b(t)$ = population of PB cells/liter at time t. The quantity N_{mc} = critical homeostatic level of cells per liter in the BM. In analyzing the model, functional representations are obtained for $\alpha_m(N_m)$ and $F(N_b)$ and system behavior is considered with regards to the parameters. The issues of massive apoptosis and ineffective hematopoiesis are placed within our analytical considerations. Control of MDS is analyzed and simulated by focusing on the mechanisms that could influence maturation delays.

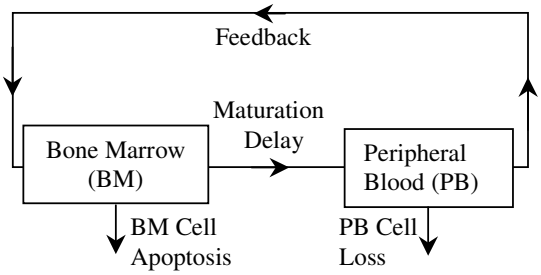

Fig.1. Schematic description of hemopoietic function

3. CONCLUSIONS

Preliminary analysis of the model shows that in normal functioning mode, the hematopoietic system evolves towards a stable state in which feedback mechanisms play an important role in signaling to cells in the marrow to shift to higher levels of production to offset blood cell loss due to various mitigating circumstances. These mechanisms also play the roles of controlling the production of cells when the population of cells in the marrow is at or above a certain critical level. A notable model prediction is the inability of the hematopoietic system to function normally when massive apoptosis occurs in the bone marrow as has been shown to be the case in the myelodysplastic syndromes in a number of clinical investigations (Anderson *et. al*., 1993; Shimazaki *et. al*., 2000; Raza *et. al*., 1995a, b; Parcharidou *et. al*., 1999; Mundle *et. al*., 1996). This prediction is pursued further in simulations of the model to explore how control of MDS could be carried out without causing more massive apoptosis in the marrow.

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Stochastic robustness of NF-κB signaling

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keywords: Stochastic modeling, robustness, innate immunity, NF-κB, TNFα

1. INTRODUCTION

The NF-κB regulatory network controls innate immune response by transducing variety of pathogen and cytokine stimuli into well defined single-cell gene regulatory events. Our analysis of the system is based on the two-feedback loop stochastic model of the NF-κB pathway, which combines the signal transduction cascade that connects cell surface receptors with the core regulatory module we analyzed previously. In the current work we focus on the TNFα signaling, a process initiated by its binding to the surface receptor TNFR1. In short (Fig. 1), the action of regulatory pathway may be summarized as follows: The binding of TNFα trimer initiates formation of an active receptor complex. The active receptors activate the IKKK kinase (transformation from IKKKn to IKKKa), which in turn activates the IKK kinase (transformation from IKKn to IKKa). Active IKKa binds transiently to cytoplasmic (NF-κB|IκBα) complex and phosphorylates IκBα initiating its degradation. Released NF-κB enters the nucleus to induce transcription of its own inhibitors: IκBα and A20 genes. The first negative feedback loop involves the IκBα protein, which is rapidly resynthesized, enters the nucleus and recaptures NF-κB back into the cytoplasm. A second level of negative autoregulation occurs with the synthesis of A20, a which attenuates IKK activity, mostly by converting IKKa into inactive form IKKi, what protects IκBα from continuous degradation.

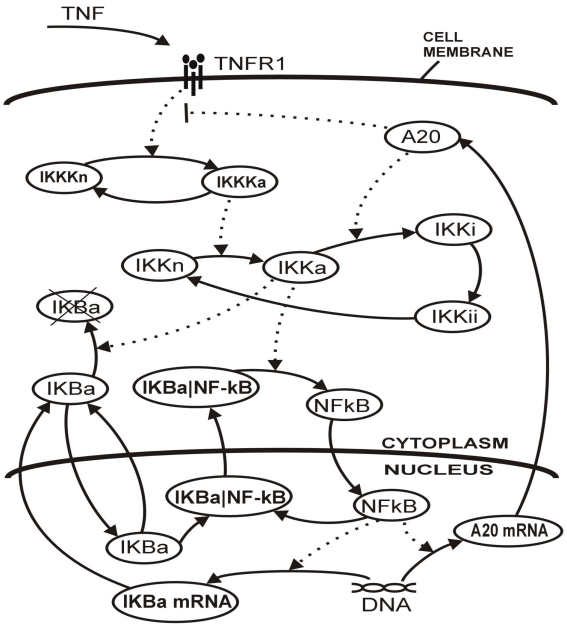

Fig. 1. Schematic of NF-κB regulatory pathway.

2. RESULTS

We identified two stochastic switches key to the functioning of the NF-κB pathway: (1) Activation of A20 and IκBα genes due to binding of NF-κB molecules to the genes promoters and (2) activation of TNFR1 receptors due to binding of TNFα trimers. Both switches are associated with amplification pathways capable of transmitting single molecular events into tens of thousands of synthesized or degraded proteins.

(1) Activation of A20 and IκBα genes results

in synthesis of tens or hundreds of mRNA molecules. In turn, a single mRNA molecule is a template for synthesis of hundreds of protein molecules. In this way the two IκBα gene copies are sufficient to replenish pool of IκBα proteins of about 100,000 molecules, within a half hour.

(2) Binding of a single TNFα trimer leads to formation of a stable active receptor complex with inactivation half time of order of 20min. During this time the single active receptor may activate numerous IKKK kinase molecules. In turn, each active IKKKa activates numerous IKK kinases, and each of IKKa may phosphorylate several IκBα molecules leading to their degradation. This amplification mechanisms enables cells to respond to femtomolar concentrations of TNFα by massive degradation of IκBα and nuclear translocation of NF-κB.

We performed the single cell stochastic numerical simulations of our model to analyze the individual cell responses to persistent stimulation in a broad range of TNFα doses, Fig. 2. At high TNFα dose (above 1ng/ml) the receptor activation rate is high and most of cells are activated in first few minutes after the TNFα stimulation begins. As a result, the first peaks of NF-κB nuclear to cytoplasmic oscillation are well synchronized among cells. Synchronization of subsequent peaks of NF-κB oscillations decreases due to the stochastic processes of activation of TNFR1 receptors and A20 and IκBα genes. For low dose (0.1 and 0.03 ng/ml) the activation of each cell is typically due to the activation of single receptors and thus the first response time varies between cells. As a result, the NF-κB oscillations are not synchronized at all.

3. CONCLUSIONS

Stochastic cell activation leading to the massive NF-κB nuclear translocation and stochastic gene activation leading to the burst of proteins provides a particular "stochastic robustness" in cell regulation. Stochastic robustness assures the minimal response to the signal. Decreasing magnitude of the signal reduces mostly the probability of response, which leads to a smaller fraction of responding cells. This can be a useful strategy: If the TNFα signal is low, some cells respond by a massive NF-κB translocation, whereas some do not respond at all. It helps to avoid ambiguity, such as when a small nuclear concentration of NF-κB leads to activation of an undefined fraction of NF-κB responsive genes. It is natural to expect that such an ambiguous response might do more harm than good. Therefore a better strategy at the tissue level, with a low signal, is to let some cells respond, and let some cells ignore the signal. Stochastic robustness allows cells to respond differently to the same stimulation, but makes their individual responses better defined. Both effects could be crucial in early immune response: Diversity in cell responses causes the tissue defense to be harder to overcome by relatively simple programs coded in viruses and other pathogens. The more focused single cell responses help cells to decide their individual fates such as proliferation or apoptosis.

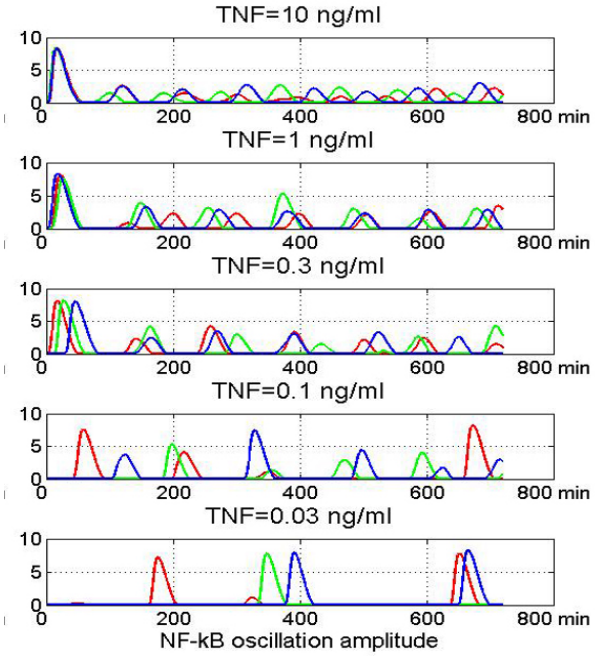

Fig. 2. Amplitude of NF-κB oscillations from single cell simulations for five TNFα doses. Each cell is marked by a different color.

Modelling morphological transformations of multi-cellular systems interacting with local environment

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Keywords: single-cell-based model, multi-cellular growth, tissue development, immersed boundary method

1. Introduction

The proper structure and function of multi-cellular organisms is a result of interactions of the individual cells in the body, and is controlled and guided by various signals interchanged between the neighbouring cells or sensed from the cell local microenvironment. We are interested in building a bio-mechanical model that can be used to investigate cell collaborative or competitive behaviour within the tissue that may lead to the development and maintenance of normal tissues, or to the formation of various tumours.

2. The model

Our computational model of individual cells is based on the immersed boundary method (Peskin, 2002) and couples the continuous description of a viscous incompressible cytoplasm and the extracellular matrix, with the dynamics of separate elastic deformable cells, containing their own elastic plasma membrane, fluid cytoplasm and individually regulated cell processes, such as cell growth, division, epithelial polarisation, apoptosis, and exchange of signals with the surrounding microenvironment.

Due to such interactions with other cells and with the environment cells can undergo certain life processes and acquire specific phenotypes. Every viable cell is constantly inspecting its microenvironment to decide if there is enough of free space for its growth. Cells located inside the cluster may become too crowded to be able to grow and can enter in the resting state. However, the accumulating cells do not simply remain passively stuck together, instead, they actively maintain selective adhesion with other cells and with the extracellular matrix. This results in cell apical-basal orientation (polarity) due to development of a basal-lateral membrane domain composed of membrane receptors in contact with the extracellular matrix and with two other cells, and an apical side facing the hollow lumen. Moreover, a newly formed polarised cells can trigger their neighbours to die by apoptosis that leads to the formation of a lumen.

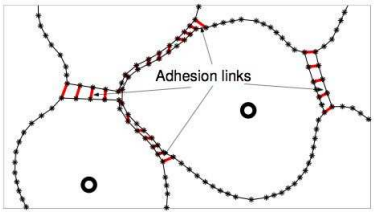

Fig. 1. The cell boundary points (dots) are connected by short linear springs (thin lines); cell nuclei (circles) are located inside the cell; separate cells are connected by the adherent links (thick red lines). The cell cytoplasm enclosed by the plasma membrane is modelled as a viscous incompressible Newtonian fluid.

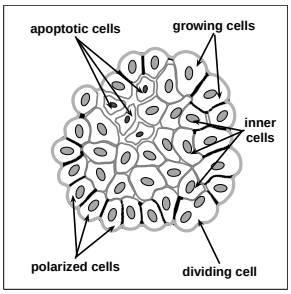

Fig. 2. Morphological alterations in phenotypically different cells—enlargement of growing cells, formation of the contractile furrow between a pair of daughter nuclei in the dividing cell, shrinkage of the area in apoptotic cells, development of distinct membrane domains in polarised cells.

$$\rho\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + (\mathbf{u}(\mathbf{x},t)\cdot\nabla)\mathbf{u}(\mathbf{x},t)\right) = -\nabla p(\mathbf{x},t) + \mu\Delta\mathbf{u}(\mathbf{x},t) + \frac{\mu}{3\rho}\nabla s(\mathbf{x},t) + \mathbf{f}(\mathbf{x},t), \tag{1}$$

$$\rho\nabla\cdot\mathbf{u} = s(\mathbf{x},t), \tag{2}$$

$$\mathbf{f}(\mathbf{x},t) = \int_{\Gamma} \mathbf{F}(l,t)\ \delta(\mathbf{x}-\mathbf{X}(l,t))\ dl, \tag{3}$$

$$s(\mathbf{x},t) = \sum_{k\in\Xi^+} S^+(\mathbf{Y}_k^+,t)\ \delta(\mathbf{x}-\mathbf{Y}_k^+)\ +\ \sum_{k\in\Xi^-} S^-(\mathbf{Y}_k^-,t)\ \delta(\mathbf{x}-\mathbf{Y}_k^-), \tag{4}$$

$$\frac{\partial \mathbf{X}(l,t)}{\partial t} = \mathbf{u}(\mathbf{X}(l,t),t) = \int_{\Omega} \mathbf{u}(\mathbf{x},t)\ \delta(\mathbf{x}-\mathbf{X}(l,t))\ d\mathbf{x}. \tag{5}$$

3. Mathematical formulation

This model is defined on a two-dimensional domain Ω with fixed Cartesian fluid grid $\mathbf{x}$ and the curvilinear grid $\mathbf{X}(l,t)$ for a collection Γ of cell membranes. Eqs.(1)–(2) are the Navier-Stokes equations and the law of mass balance, where $\mathbf{u}(\mathbf{x},t)$ is the fluid velocity, $p(\mathbf{x},t)$ is the pressure, μ is the viscosity, ρ is the density, $s(\mathbf{x},t)$ is the source-sink distribution, and $\mathbf{f}(\mathbf{x},t)$ is the external force density. Eqs.(3)–(5) define interactions between the immersed bodies and the surrounding fluid. Here, $\mathbf{Y}_k^{\pm}$ are the point sources and sinks, and δ is the Dirac delta function.

4. Multicellular growth

This approach allows for modelling various multicellular phenomena by focusing on biomechanical properties of individual cells and on communication between them and between the cell and their microenvironment. It also allows to investigate how individual cells contribute to the formation and maintenance of the whole complex system. We have used this approach to model abnormal tissue bending in the human placental trophoblast (Rejniak et.al, 2004), normal development of epithelial tissues (Rejniak & Anderson, submitted) and various tumours (Rejniak, 2007; Rejniak & Dillon, 2007).

Here, we want to present a specific example of the formation of a hollow epithelial acinus, discuss consecutive steps of its development, specific relations between the neighbouring cells leading to cell epithelial polarisation and cell apoptotic death. We also present, how changes in some model parameters lead to alteration in the final acinar structure, its degeneration and tumour-like behaviour.

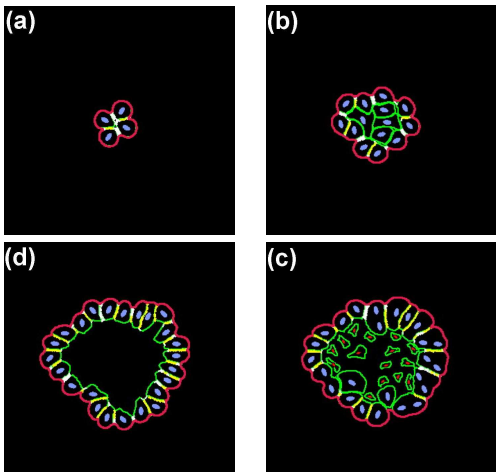

Fig. 3. Formation of a hollow epithelial acinus: (a) a small cluster of cells, (b) two cell subpopulations—inner and outer, (c) emergence of outer polarised cells and inner apoptotic cells, (d) a stable structure composed of one layer of polarised cells surrounding the hollow lumen.

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PLANNING IDENTIFICATION EXPERIMENTS FOR CELL SIGNALING PATHWAYS USING SENSITIVITY ANALYSIS

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Keywords: Cell signaling pathways, sensitivity analysis, experiment design.

1. INTRODUCTION

One of possible approaches to modeling of cell signaling pathways is to use a set of nonlinear ODEs [de Jong 2002]. In order to estimate unknown parameters of such a model several experiments are performed, during which concentrations of part of variables are measured at rare discrete time moments. Usually, a blotting technique is used. In this work we focus on choosing optimal time moments for experiments. This problem has been investigated in the related literature. To solve it a matrix of correlation coefficients between sensitivities of measurements with respect to identified parameters is calculated [Jacquez, Greif 1985], [Jacquez 1998]. Then one tries to choose such time moments for which sensitivities are "less correlated". The standard approach to optimization is the non-gradient Gauss-Seidl technique.
In this work we calculate the gradient of the function of the correlation matrix with respect to times of measurements, then we propose a gradient-based algorithm.

2. PROBLEM FORMULATION

Let us consider a model of a cell signaling pathway in a form of a set of non-linear ODEs:

$$\dot{x} = f(x,u,\theta); \quad x(0) = x_0 \tag{1}$$

where x is a vector of state variables, u is an input signal and $\theta \in R^p$ is a vector of identified parameters.

The output equation is as follows

$$y = g(x,u) \tag{2}$$

For the simplicity of notation let us assume there is only one output variable which is measured at times $t_1, t_2, \ldots, t_n$ giving instantaneous values

$$y(t_i) = g(x(t_i), u(t_i)) = g_i; \quad i = 1,2,\ldots,n \tag{3}$$

After performing experiments one obtains observations

$$z(t_i) = y(t_i) + \varepsilon_i; \quad i = 1,2,\ldots,n \tag{4}$$

where ε_i is an error of zero mean and variance σ_i^2. We assume that we have initial (rough) estimation of parameters $\theta_i^0, \theta_2^0, \ldots, \theta_n^0$ for which measured variable (3) takes values $g_i^0, g_2^0, \ldots, g_n^0$.
We build the sensitivity matrix [Jacquez, Greif 1985], [Jacquez 1998] as follows:

$$G = \begin{bmatrix} \frac{\partial g_i^0}{\partial \theta_1} & \cdots & \frac{\partial g_i^0}{\partial \theta_p} \\ \vdots & \ddots & \vdots \\ \frac{\partial g_n^0}{\partial \theta_1} & \cdots & \frac{\partial g_n^0}{\partial \theta_p} \end{bmatrix} \tag{5}$$

and based on it the Fisher information matrix

$$I = G^T \Sigma^{-1} G \tag{6}$$

where $\Sigma^{-1} = diag[1/\sigma_1, 1/\sigma_2, \ldots, 1/\sigma_n]$.

If the determinant of I is non-zero then I^{-1} is proportional to the covariance matrix of the estimates of θ. We want the covariance matrix to me small. The criterion widely used is to maximize the determinant of I. This is so called *D*-optimal design [Jacquez 1998]. The standard approach is to maximize $\det(I)$ by finding optimal times $t_1, t_2, \ldots, t_n$ using non-gradient Gauss-Seidl technique. To formulate a gradient-based algorithm we formulate following problem:

Problem. Find derivatives

$$\frac{\partial \det(I)}{\partial t_i}; \quad i = 1, 2, \ldots, n \tag{7}$$

3. PROBLEM SOLUTION

Note that $\det(I)$ is a function of the sensitivity matrix G so the problem stated above is to find the "sensitivity function of the function of other sensitivity functions".

For particular time moment t_i one may write

$$\frac{\partial \det(I)}{\partial t_i} = \sum_{j=1}^{p} \frac{\partial \det(I)}{\partial \left(\partial g_i^0 / \partial \theta_j \right)} \cdot \frac{\partial \left(\partial g_i^0 / \partial \theta_j \right)}{\partial t_i} \tag{8}$$

Let us denote the first factor under the sum (8) by q_{ji} and the second factor by r_{ji}. Then let us build matrices $Q = [q_{ji}], R = [r_{ji}], \; Q, R \in R^{n \times p}$.

It can be shown that whole matrix Q may be calculated as follows

$$Q = 2\Sigma^{-1} G \operatorname{adj}(I) \tag{9}$$

The element r_{ji} is the derivative w.r.t. time of the output of the following sensitivity model for the original model (1),(2):

$$\begin{aligned} \dot{\bar{x}} &= f_x(t)\bar{x} + f_u(t)\bar{u} + f_\theta(t)\bar{\theta}; \; \bar{x}(0) = 0 \\ \bar{y} &= g_x(t)\bar{x} + g_u(t)\bar{u} \end{aligned} \tag{10}$$

taken at time t_i where the sensitivity is calculated for θ_j which means the variation $\bar{\theta}$ is a vector of zeros except one element number j which equals 1.

Unfortunately, practical using of (10) requires numerical derivation w.r.t. time. Hopefully, it is possible to derive following formula

$$r_{ji} = \left(g_{xx}(t_i)\bar{x}(t_i) + g_x(t_i) \right) \dot{\bar{x}}(t_i) \tag{11}$$

that does not require any numerical derivation because both $\bar{x}$ and $\dot{\bar{x}}$ appear in the sensitivity model (10).

In order to maximize $\det(I)$ one can combine results (9) with (11) and compute all derivatives (7) and use any gradient-based optimization algorithm.

4. CONCLUSIONS

This work is concerned with the problem of optimal design of experiments in sense of finding optimal times for measurements. The approach has one drawback at first glance. To design the experiment, which is performed in order to estimate parameters, we need initial (rough) estimations of parameters. It may be hard to guess such initial values of parameters and the experiment may be designed for quite different point in the parameter space. However, in practice several experiments for different variables are conducted and it is possible to plan each experiment based on all previous experiments starting with first non-optimally designed experiment.

Having such a tool for experiment planning, two closely related problems may be solved: how many time moments are enough to estimate parameters and what variable (concentration of proteins, protein complexes or mRNA) should be measured.

ACKNOWLEDGEMENT

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Single cell experiments and modeling of p53/Mdm2 pathway

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Keywords: p53, Mdm2, Hopf bifurcation, haploinsufficiency, transfected cells

1. INTRODUCTION

p53 is a transcription factor that regulates cell cycle and functions as a tumor supressor. The concentration of p53 increases in response to stress signal, such as DNA damage or oncogene activation. p53 induces transcription of several hundred genes involved in cell cycle arrest and DNA repair. If the DNA damage proves to be irreparable it initiate apoptosis, the programmed cell death. In normal cells p53 is usually inactive, kept at low level due to Mdm2 induced degradation. The DNA damage leads to p53 phosphorylation enhancing its stability. It results in prolonged oscillations of p53 and Mdm2. Since these oscillations are not synchronized, the only way to observe them, is by means of single cell experiments, (see Geva-Zatorski *et al.*). In all such experiments additional copies of p53 and Mdm2 genes are introduced to the genome (stable transfection). These copies code for fluorescently tagged proteins, which concentration and localization can be analyzed under the microscope.
Since p53/Mdm2 oscillations are induced by elevated stability of p53 protein or lowered stability of Mdm2 protein there is a natural conjecture that a number of p53 and Mdm2 copies may also influence these oscillations. This conjecture is supported by the evidence that the missing p53 copy results in haploinsufficiency and leads to tumor.

2. RESULTS

To verify how the number of gene copies influences the oscillations we constructed the simple model of p53/Mdm2 pathway based on positive and negative feedbacks introduced by Ciliberto *et al.* The model consists of three components: p53, cytoplasmic Mdm2 and nuclear Mdm2.

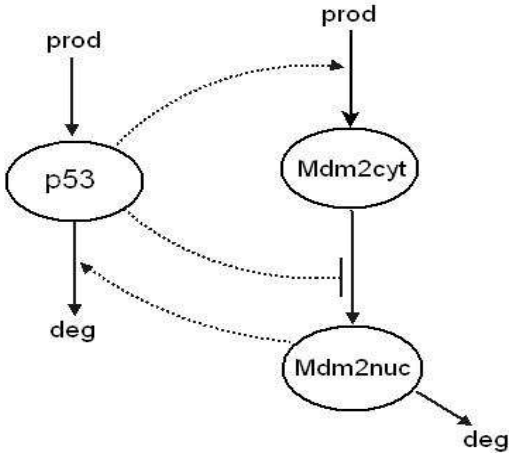

Fig. 1. Diagram of p53/Mdm2 network.

The negative feedback arises since p53 positively regulates production of Mdm2, and in turn Mdm2, when in nucleus, enhances p53 degradation. In addition p53 inhibits nuclear import of Mdm2, and since nuclear Mdm2 induces p53 degradation, this leads to positive feedback.
The pathway can be described by the system of three ordinary differential equations for p53, cytoplasmic and nuclear Mdm2 levels

$$\frac{d(p53)}{dt} = ms_1 - d_1\, p53(Mdm2)^2,$$

$$\frac{d(Mdm2_{cyt})}{dt} = n\left(s_2 + s_3 \frac{(p53)^3}{(p53)^3 + k_3}\right) - \frac{k_1}{p53 + k_2} Mdm2_{cyt},$$

$$\frac{d(Mdm2_{nuc})}{dt} = \frac{k_1}{p53 + k_2} Mdm2_{cyt} - d_2\, Mdm2_{nuc},$$

where m and n are the numbers of p53 and Mdm2 gene copies, respectively.
Since transcription is regulated by p53 tetramers we assumed that p53 induces Mdm2 transcription following a Hill

function, with exponent 3. The nonlinear p53 degradation results from the fact that nuclear Mdm2 must attach several ubiquitines to p53, to initiate its degradation. DNA damage is modeled here by a rapid change in p53 and Mdm2 degradation coefficients. It is known that DNA damage leads to p53 phosphorylation enhancing its stability and increases Mdm2 degradation. As shown in Fig. 2 the model has the required property, i.e. the transition from stable steady point to limit cycle results both due to increased Mdm2 degradation or decreased p53 degradation.

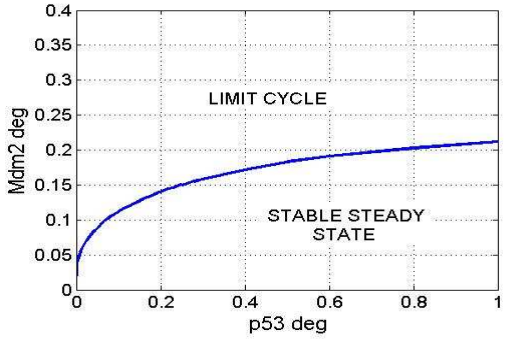

Fig. 2. Regions of stable limit cycles and stable steady states in (d_1 = p53 deg, d_2 = Mdm2 deg) plane for m = n = 2.

Finally, we analyze bifurcation diagrams (Fig. 3) to investigate how the transition from stable point to limit cycle (supercritical Hopf bifurcation) depends on the number of p53 or Mdm2 copies. As shown in Fig. 3 the bifurcation point moves towards higher p53 deg. coefficients as number of p53 gene copies increases. On the other hand the increase in number of Mdm2 copies results in narrowing of oscillatory region (data not shown). It shows that the change in gene copy number due to transfection or missing allele may induce oscillations even when DNA is intact, or it may inhibit oscillations when DNA is damaged.

3. CONCLUSIONS

Our study implies that when one of p53 copies is missing, the system may remain in stable state even when DNA is damaged. This may lead to haploinsufficiency and results in tumor, since the oscillations of p53 and Mdm2 are needed to initiate transcription of p53 dependent genes involved in cell cycle arrest, DNA repair or apoptosis.

The analysis implies also that behavior of transfected cells can be qualitatively different from normal cells and that observed oscillations could be an artifact of experimental setup. Since Mdm2 transfection has the opposite effect to p53 transfection the p53/Mdm2 cotransfection experiments are more reliable (not shown).

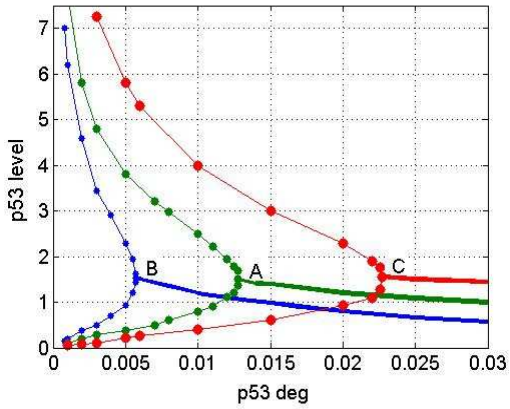

Fig. 3. Bifurcation diagram. A, B and C denote, respectively, diagrams for normal cells (m = n = 2), p53 haploidal cells (m = 1, n = 2) and cells with p53 transfection (m =4, n = 2). Fin, dotted lines represent upper and lower limits of stable limit cycles, the bold lines represent stable steady states.

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Two feedback loop model of p53|Mdm2 signaling pathway

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Keywords: p53, Mdm2, signaling pathways, apoptosis.

1. INTRODUCTION

p53 is a transcriptional factor kept in healthy cells at low level under the control of its inhibitor Mdm2, but activated (phosphorylated) in response to DNA damage. When activated and present in high concentration, it induces the transcription of numerous genes involved in cell cycle arrest and DNA repair. If the last fails p53 final job is to trigger the cell-death program called apoptosis. For this reasons p53 is often called “the guardian of the genome”.

2. RESULTS

In order to analyze the p53|Mdm2 system we expanded and improved the two-feedback loop model introduced by Ciliberto *et al.*

The first feedback is negative and couples Mdm2 with p53. Namely, the phosphorylated p53 triggers production of Mdm2, which is activated, enters the nucleus and ubiquitinates p53 what results in its rapid degradation.

The second feedback is positive in this sense that it blocks the negative loop. Since it involves additional three proteins PTEN, PIP3 and Akt it works on a much slower time scale than the negative feedback. Explicit introduction of PTEN--PIP3--Akt pathway adds time delay (neglected by Ciliberto *et al.*) and results in a novel model with substantially different dynamics. In short; p53 induces transcription of PTEN then PTEN triggers PIP3 deactivation. Active PIP3 is needed to activate Akt, which in turn is activator of Mdm2 enabling its nuclear entry. Thus, deactivation of PIP3 blocks activation (phosphorylation) and nuclear entry of Mdm2 and in turn rescue p53.

The system is activated by DNA damage (or oncogene stimulation), which results in p53 phosphorylation. In turn phosphorylated p53 induces synthesis of proteins responsible for DNA repair.

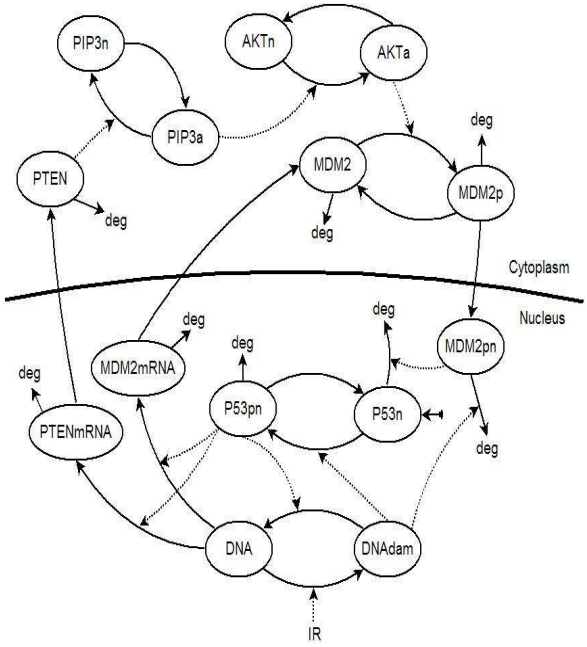

Fig. 1. Diagram of p53|Mdm2 signaling pathway. Notice two feedback loops: negative involving p53 and Mdm2 proteins and positive involving p53, PTEN, PIP3, Akt and Mdm2.

Analysis of the system indicates existence of 3 distinct states; two steady points and limit cycle.

1) Without DNA damage system remains in stable point (healthy cell). The negative feedback loop assures that p53 remains at low level under the control of its inhibitor Mdm2 (see Fig. 2, $t<0$).

2) When DNA is persistently damaged, but the slow positive feedback is blocked (e.g. no PTEN) the system converges to stable limit cycle (Fig. 2A).

3) When DNA is persistently damaged and the slow positive feedback is intact the system after several oscillations converges to second stable point (apoptotic cell), characterized by high p53 level and low Mdm2 level (Fig. 2B). This

second stable point is absent in Ciliberto *et al.* model.

In real situation, there is a competition between DNA repair due to elevated level of p53 and action of the positive feedback. If DNA repair proceeds sufficiently fast, and the DNA damage is removed before Mdm2 phosphorylation is blocked by the slow positive loop, the system converges to the first steady state (healthy cell, Fig. 2D). However, if DNA damage is irreparable (Fig. 2B) or the DNA repair proceeds to slow (Fig. 2C) p53 rises to high level what potentially leads to apoptosis (not modeled explicitly in this work).

3. CONCLUSIONS

Recently, the dynamic of fluorescently tagged p53 and Mdm2 was observed over several days after radiation in living cancer cells. The experiment by Geva-Zatorsky *et al.*, showed irregular oscillations, with period of about 5.5 hours continuing for as long as 72 hours. The fraction of oscillated cells increased with gamma dose reaching 60% following 10Gy. Even at that dose, the analyzed cells proliferated and do not exhibited apoptosis. The prolonged (persistent) oscillations are observed in our model only when the positive feedback loop is at some point blocked, and DNA is irreparable. This supports Geva-Zatorsky *et al.* conjecture that human breast cancer epithelial cells, they studied, “might be deficient in some aspects of p53 regulation and downstream apoptotic responses”.

Based on our analysis we would expect that normal untransformed cells after about 24 hours of unsuccessful DNA repair, would commit to apoptosis.

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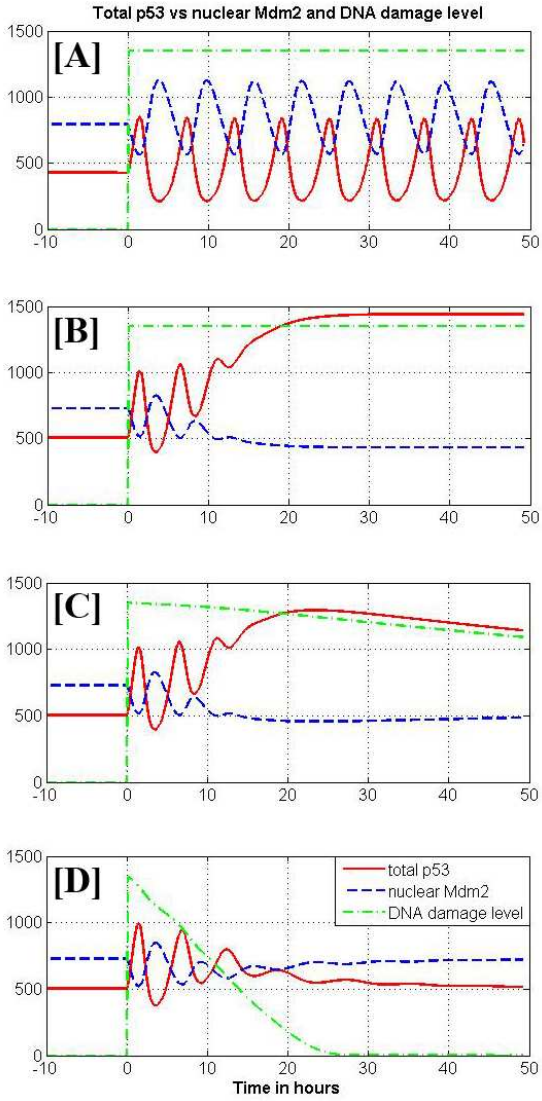

Fig. 2. Model predictions of the cell response to DNA damage. In time T < 0 the system is in first stable point (healthy cell). DNA damage occurs at T = 0. Panel A: without DNA repair and with positive feedback blocked the system converges to limit cycle. Panel B: with positive feedback intact and no DNA repair the system converges to the second stable point (apoptotic cell). Panel C and D: When positive feedback is intact and DNA is repairable then there is a competition between DNA repair and Mdm2 inhibition by a positive feedback. If repair is to slow (panel C) p53 goes high up and the cell commits to suicide. If the DNA repair is fast enough (panel D) p53 converges to the initial level and the cell survives.

Curvature of optimal control: Deformation of classical planar systems

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Keywords: Optimal control, curvature

1. Introduction

Consider the problem of deciding whether a trajectory pair $(u^*(t), x^*(t))$, $t \in [0,T]$ of a generally nonlinear system $\dot{x} = F(x,u)$, $x \in M^n$ is a time-optimal solution connecting the endpoints $x(0)$ and $x(T)$, or whether the system is locally controllable about this trajectory. The classical approach analyzes the endpoint map $u \mapsto x(T,u)$ (for fixed T and $x(0)$) and determine whether or not it is locally an open map. The Pontryagin Maximum Principle and high-order open-mapping theorems provide necessary conditions for a trajectory-control-pair to be optimal. Sufficient conditions for optimality (and necessary conditions for nonlinear controllability) are harder to obtain. Like the Legendre-Clebsch condition, they generally take the form of tests of definiteness for second order derivatives. Recently Agrachev introduced an attractive alternative by developing a notion of curvature of optimal control that generalizes classical Gauss (and Ricci) curvatures. That theory has been developed for systems whose controls take values in a circle or sphere $u \in \mathbb{R}^{n-1}$.

We present initial studies of how this notion of curvature provides insight into the limiting case when the circles become degenerate ellipses in the form of closed intervals or lower dimensional cubes. Of particular interest are well studied accessible, but uncontrollable, nonlinear systems, and systems that exhibit conjugate points. We study how the curvature and conjugate points vary when the set of controlled velocities $S^1 = \{(u_1,u_2)\colon u_1^2+u_2^2=1\}$ is continuously deformed into the interval $I = [-1,1]$. For computational reasons we implement this by adding the parameter ε into the controlled vector field as follows, and leaving the set of control values $U = S^1$ the same.

$$\left\{ \begin{array}{rcll} \dot{x}_1 &=& f_1(x_1,x_2) + u_1 & \text{subject to} \\ \dot{x}_2 &=& f_2(x_1,x_2) + \varepsilon u_2 & u_1^2+u_2^2 = 1 \end{array} \right. \tag{1}$$

Of particular interest are deformations of the well-understood systems (when $\varepsilon = 0$)

$$\left\{ \begin{array}{rcl} \dot{x}_1 &=& u_1 \\ \dot{x}_2 &=& x_1^m + \varepsilon u_2 \end{array} \right. \tag{2}$$

and

$$\left\{ \begin{array}{rcl} \dot{x}_1 &=& -x_2 + u_1 \\ \dot{x}_2 &=& x_1 + \varepsilon u_2 \end{array} \right. \tag{3}$$

with $|u_1| \le 1$.

We are interested in how their properties arise as limits of deformations of the corresponding systems of the form (1). The first family of systems is small-time locally controllable if and only if m is odd. If m is even, the reachable sets exhibit well-known *fold-overs* with consequent appearance of conjugate points.

2. Curvature of optimal control

Unlike the classical Gauss curvature, Agrachëv's curvature is not a function on the state-space, but rather on the cotangent bundle over the state-space. In the case of planar systems, the theory is formulated via a distinguished vertical vector field v on the cotangent bundle which is characterized by the identity $L_v^2 s = -s + bL_v s$ where $s = p_1 dx_1 + p_2 dx_2$ is the tautological one-form on $T^*\mathbb{R}^2$ restricted to the level surface $\mathcal{H}$ of the Hamiltonian (and L denotes Lie

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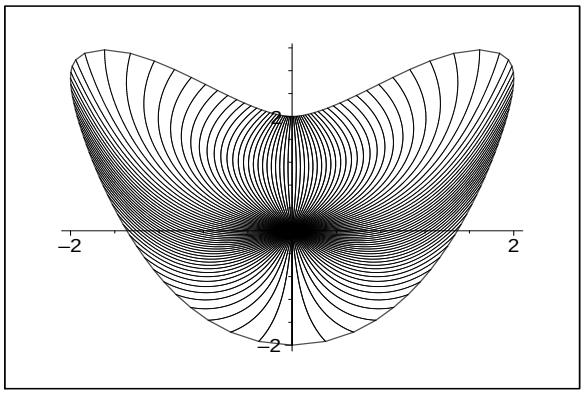

Fig. 1. Reachable set at $T = 2$ of system (2) with $m = 2$, $\varepsilon = 1$

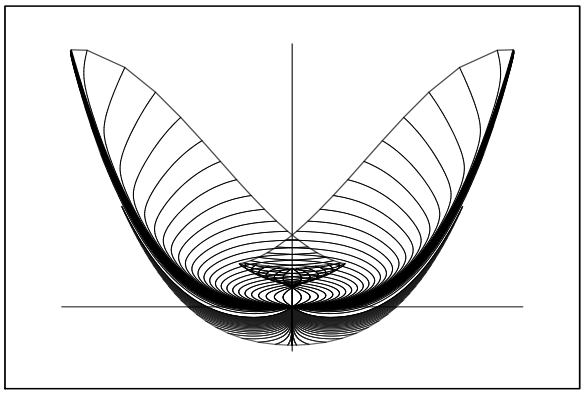

Fig. 2. Reachable set at $T = 2$ of system (2) with $m = 2$, $\varepsilon = 0.2$

derivative). Together with the Hamiltonian field $\vec{h}$ and their Lie bracket one obtains a moving frame

$$V_1 = v, \quad V_2 = [v, \vec{h}], \quad V_3 = \vec{h}$$

on the level surface $H^{-1}(1) \subseteq T^*\mathbb{R}^2$. One readily verifies that the Lie derivatives of this frame satisfy

$$[\vec{h}, V_1] = -V_2, \quad [\vec{h}, V_2] = \kappa V_1, \quad [\vec{h}, V_3] = 0$$

where κ is a scalar function on $\mathcal{H}$ and is called the curvature of the control system (1). Writing the Jacobi equation along an extremal (x_t, p_t) in terms of this moving frame one obtains the time-varying linear differential equation

$$\ddot{y} + \kappa_t y = 0, \;\; y(0) = y(t_c) = 0.$$

which has no nontrivial solutions when $\kappa \leq 0$. In the case on not necessarily negative curvature, standard integral estimates yield lower bounds on the first positive conjugate time t_c.

Notable results for very specific classes of systems were obtained by Serres (4) who studied *Zermelo's navigation problem*, basically the undeformed ($\varepsilon = 1$) system (1). Recent work by Agrachev et. al. (2) extended the theory to higher dimensional systems. Complementary to this is recent work by Chitour and Sigalotti, who investigate the Dubins' car on curved surfaces (3; 5).

3. Deformations and curvature

While most pertinent literature (1; 2; 3; 4; 5), is concerned with the further theoretical development, a main thrust of our work is to explore the boundaries of what is computationally feasible with current technology, suing a combination of symbolic and numeric engines.

While already in the *undeformed* case the formula for the curvature in coordinates fills a whole page, in the case of deformed control sets, the formulae become much too large to be reproduced here. One starts with the Hamiltonian vector field in polar coordinates Next we compute the distinguished vertical vector field v, and the iterated Lie bracket $[\vec{h}, [\vec{h}, v]]$ from which we then obtain both formulae for the curvature, now depending on the deformation parameter $\varepsilon \in [0, 1]$, and numerical simulations of the time evolution of the co-state vector along extremals, as well their projections onto the state-space, as illustrated in figures 1 and 2.

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Geometric Integration for Optimal Control Problems: Application to Underwater Vehicles*

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Keywords: Optimal Control, Geometric Integrator, Submerged Rigid Body

1. INTRODUCTION

Ocean research and exploration has evolved to the point that underwater mechanical systems are a necessity. In order to expand our knowledge base we are pushing to go farther and deeper into the abyss. Among the many technological advances, autonomous underwater vehicles (AUV's) are attracting recent research interests. The ability to reduce or eliminate the human factor in ocean research reduces exploration costs and risk to human life. The ultimate goal is to give the AUV full autonomy and have it do the work for us. With this increasing load of responsibilities, efficiency of movement and energy usage become more important. In this paper, we study the energy minimization problem for a submerged rigid body in a real fluid. For us, a real fluid is a viscous ideal fluid. The equations of motion for a rigid body in a real fluid can be written as a forced affine connection control system on the differentiable configuration manifold $\mathcal{SE}(3)$:

$$\nabla_{\gamma'}\gamma' = \begin{pmatrix} M^{-1}\big(D_\nu(\nu)\nu + R^t\alpha + \varphi_\nu\big) \\ J^{-1}\big(D_\Omega(\Omega)\Omega - r_B \times R^t\alpha + \tau_\Omega\big) \end{pmatrix} \tag{1}$$

where $\alpha = \rho g \mathcal{V} k$. Here, ∇ is the Levi-Civita affine-connection for the Riemannian metric induced by the kinetic energy T. The matrices $D_\nu(\nu), D_\Omega(\Omega)$ represent respectively the drag force and momentum. Finally, we have a restoring force and a restoring moment. The only moment due to the restoring forces is the torque from the buoyancy force $-r_B \times R^t \rho g \mathcal{V} k$ where r_B is the vector from C_G to the center of buoyancy C_B, where ρ is the fluid density, g the acceleration of gravity, $\mathcal{V}$ the volume of fluid displaced by the rigid body and k the unit vector pointing in the direction of gravity. The forces $\varphi_\nu = (\varphi_{\nu_1}, \varphi_{\nu_2}, \varphi_{\nu_3})^t$ and $\tau_\Omega = (\tau_{\Omega_1}, \tau_{\Omega_2}, \tau_{\Omega_3})^t$ account for the control. In the absence of the restoring,drag forces and momentum the equations of motion (1) represent a *left-invariant affine-connection control system* on the Lie group $\mathcal{SE}(3)$. The inherent nonlinear structure of the mechanical system can be exploited through geometric control theory. To begin, we analyze the rigid body submerged in the $xz-$plane. The energy cost we consider is the square of the norm of the control. Pontryagin's Maximum Principle provides information on the structure of the optimal trajectories. Our goal is to apply numerical methods based on these information. Indeed, to numerically solve an optimal control problem (OCP) we have two broad classes of methods: indirect or direct. The indirect methods are based on the application of the maximum principle and are usually called single or multiple shooting methods. The direct methods are based on a rewriting of (OCP) as a finite dimensional optimization problem. The main disadvantage of the direct methods is that they are computationally very demanding since the discretization of (OCP) usually yields a large number of parameters to optimize (we need N large enough so that the discretization make sense with respect to the continuous (OCP)). For this reason we focus here on indirect method. The single shooting method does not usually converge for our problem. However, the multiple shooting method does. In particular, we provide pairs of initial and final configurations at rest for which the single shooting method is unsuccessful but the multiple

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shooting method converges to a solution. Additionally we discuss the use of symplectic integrators and their impact on the solutions.

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REGULARITY PROPERTIES OF OPTIMAL CONTROL FOR SOME MIXED CONSTRAINED PROBLEMS

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Keywords: optimal control, mixed constraints, regularity

1. INTRODUCTION

In this work we investigate regularity properties of optimal control for problems with mixed state-control constraints. To the best of our knowledge, regularity properties of optimal control for such problems have not been studied previously. We consider on a problem (P_{eq}) with equality type constraints:

$$\begin{cases} \text{Minimize } l(x(1)) \\ \quad +\frac{1}{2}\int_0^1 \big(x(t)^*Qx(t)+u(t)^*Ru(t)\big)dt \\ \text{subject to} \\ \dot{x}(t) \;=\; f(t,x(t))+B(t)u(t) \quad \text{a.e.} \\ 0 \;=\; Cx(t)+Eu(t) \quad \text{a.e.} \\ x(0) \;\in\; C_0 \end{cases}$$

and on a problem (P_{in}) with inequality type constraints:

$$\begin{cases} \text{Minimize } l(x(1)) \\ \quad +\frac{1}{2}\int_0^1 \big(x(t)^*Qx(t)+u(t)^*Ru(t)\big)dt \\ \text{subject to} \\ \dot{x}(t) \;=\; f(t,x(t))+B(t)u(t) \quad \text{a.e.} \\ 0 \;\geq\; Cx(t)+Eu(t) \quad \text{a.e.} \\ x(0) \;\in\; C_0 \end{cases}$$

The data for these problems comprise state and control variables $x : [0,1] \to \mathbf{R}^n$, $u : [0,1] \to \mathbf{R}^k$, functions $l : \mathbf{R}^n \to \mathbf{R}$, $f : [0,1] \times \mathbf{R}^n \to \mathbf{R}^n$, $B : [0,1] \to \mathcal{M}_{n\times k}$, matrices $Q \in \mathcal{M}_{n\times n}$, $R \in \mathcal{M}_{k\times k}$, $C \in \mathcal{M}_{m\times n}$, $E \in \mathcal{M}_{m\times k}$ and a closed set $C_0 \subset \mathbf{R}^n$. Here $\mathcal{M}_{p\times q}$ is the set of all $p \times q$ matrices with real entries. We assume that $m < k$, i.e. that the number of constraints is less than the dimension of the control variable.

An important motivation for the study of regularity of optimal control is that prior knowledge of its regularity properties (such as smoothness or Lipschitz continuity) influences the choice of the most effective approximation scheme for numerical solution of optimal control problems. Regularity of optimal control have previously been studied for problems with state constraints or state constraints and pointwise control constraints by, for example, Galbraith et. al (2003); Hager (1979); Malanowski (1978); Shvartsman et. al (2006); Vinter (2000).

In this work we prove that under mild conditions on the data, optimal control is infinitely differentiable in the problem with equality constraints and Lipschitz continuous in the problem with inequality constraints.

We impose the following hypotheses on the data of (P_{eq}) and (P_{in}).

(H1) Function l is locally Lipschitz continuous and f and B are $C^\infty-$ functions.

(H2) The set C_0 is closed.

(H3) The matrices Q and R are symmetric and R is positive definite.

(H4) The matrix E is of full rank, i.e. $\det EE^* \neq 0$.

Crucial to our analysis is the following result from linear algebra.

Proposition 1.1 If $E \in \mathcal{M}_{m\times k}$ with $m < k$ satisfies (H4) then there exist square nonsingular matrices $S \in \mathcal{M}_{m\times m}$ and $T \in \mathcal{M}_{k\times k}$ such that

$$SET = [I \;\; 0],$$

i.e. the left $m \times m$ block in the latter matrix is the identity matrix, and the remaining entries are zeros.

This result follows easily from the Singular Value Decomposition Theorem (see, for e.g., Theorem 7.3.5 in (Horn et. al, 1985)).

2. MAIN RESULTS

Our main results are the following:

Theorem 2.1 Assume (H1)-(H4). Then the optimal control $\bar{u}$ in (P_{eq}) is a C^∞-function.

Theorem 2.2 Assume (H1)-(H4). Then the optimal control $\bar{u}$ to (P_{in}) is Lipschitz continuous.

The idea of the proof of both theorems is to reduce the problem under consideration to a problem without mixed constraints, and then to investigate the implications of the Pontryagin Maximum Principle. We illustrate the aforementioned reduction below.

Let $(\bar{x}, \bar{u})$ be an optimal process to (P_{eq}). Set

$$\bar{v} \equiv \left[\begin{array}{c} \bar{v}_1 \\ \bar{v}_2 \end{array} \right] := T^{-1}\bar{u}, \qquad (1)$$

where $\bar{v}_1 \in \mathbf{R}^m, \bar{v}_2 \in \mathbf{R}^{k-m}$ and T is from Proposition 1.1. It can be shown that there exist functions $\hat{f}$, $\hat{B}$, matrices $\hat{Q}, \hat{S}$ and a positive-definite matrix $\hat{R}$ of corresponding dimensions such that $(\bar{x}, \bar{v}_2)$ is an optimal process to the problem (P_1):

$$\left\{ \begin{array}{ll} \text{Minimize } l(x(1)) & \\ \quad +\frac{1}{2}\int_0^1 \big(x(t)^*\hat{Q}x(t) + 2x(t)^*\hat{S}v_2(t) & \\ \qquad +v_2(t)^*\hat{R}v_2(t)\big)dt & \\ \text{subject to} & \\ \dot{x}(t) &= \hat{f}(t,x(t)) + \hat{B}(t)v_2(t) \text{ a.e.} \\ x(0) &\in C_0 \end{array} \right.$$

Observe that (P_1) is an optimal control problem without mixed constraints.

Similarly, let $(\bar{x}, \bar{u})$ be an optimal process to (P_{in}). Set

$$\bar{w}(t) = \left[\begin{array}{c} -C\bar{x}(t) - E\bar{u}(t) \\ \bar{v}_2(t) \end{array} \right],$$

where $\bar{v}_2$ is defined in (1). It can be shown that $(\bar{x}, \bar{w})$ is an optimal process to problem (P_2)

$$\left\{ \begin{array}{ll} \text{Minimize } l(x(1)) & \\ \quad +\frac{1}{2}\int_0^1 \big(x(t)^*\hat{Q}x(t) + 2x(t)^*\hat{S}w(t) & \\ \qquad +w(t)^*\hat{R}w(t)\big)dt & \\ \dot{x}(t) &= \hat{f}(t,x(t)) + \hat{B}(t)w(t) \text{ a.e.} \\ w(t) &\in \Omega \text{ a.e.} \\ x(0) &\in C_0 \end{array} \right.$$

with

$$\Omega = \Big\{ (w_1, w_2) \in \mathbf{R}^m \times \mathbf{R}^{k-m} : w_1 \geq 0 \Big\}$$

for some functions $\hat{f}$, $\hat{B}$ and matrices $\hat{Q}, \hat{S}$ and $\hat{R}$. Note that problem (P_2) does not contain a mixed constraint, but is a problem with a control constraint of a simple structure.

3. CONCLUSIONS

In this paper we establish regularity properties of the optimal control for a simple class of mixed constrained problems. Proposition 1.1 and the main result in (Shvartsman et. al, 2006) play an important role in the analysis. We hope to extended Theorem 2.1 and 2.2 to cover more general problems.

4. ACKNOWLEDGMENTS

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Minimum time optimality for a single–input affine control system

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Keywords: optimal control, hamiltonian methods, sufficient conditions

We consider the minimum–time problem for a single–input affine control system:

$$\text{minimize} \quad T$$

subject to

$$\dot{\xi}(t) = f_0(\xi(t)) + u f_1(\xi(t)) \quad t \in [0,T]$$
$$\xi(0) = \widehat{x}_0\,, \quad \xi(T) = \widehat{x}_f$$
$$|u| \leq 1$$

The state space is a smooth $n-$dimensional manifold M, $\widehat{x}_0$ and $\widehat{x}_f$ are fixed points and $f_0, f_1 \colon M \to TM$ are smooth vector fields; by smooth we mean C^∞.

The aim of the authors is to give second order conditions for a reference normal Pontryagin extremal $(\widehat{T}, \widehat{\xi}, \widehat{u})$ to be a *local optimizer in the strong topology,* i.e. with respect to all admissible trajectories whose graph belongs to a neighborhood of the graph of $\widehat{\xi}$ in $\mathbb{R} \times M$, independently on the values of the associated control. We call such a strong optimizer a *(time, state)–local optimizer*.

Remark that since we are dealing with a minimum time problem, there is also another kind of strong local optimality, namely if $\widehat{\xi}$ is optimal among all the admissible trajectories whose range lies in a range of the range of $\widehat{\xi}$, $\widehat{\Xi} = \{\widehat{\xi}(t) \colon t \in [0, \widehat{T}]\}$ in M, we say that $\widehat{\xi}$ is a *state–local optimizer*. Remark that any state–local optimizer is a (time, state)–local optimizer but the two notions are not equivalent, see (Stefani Zezza, 2003).

The authors faced the problem of state–local optimality in (Poggiolini Stefani, 2004), when the extremal is bang-bang, and the problem of (time, state)–local optimality in (Stefani, 2004), when the control system is single input and totally singular, and in (Poggiolini Stefani, 2005) when the system is single–input and the reference control is the concatenation of a bang arc and of a singular arc; also we should mention the papers by different authors who considered the problem of local optimality for Pontryagin extremals: (Dmitruk, 1999), (Maurer Osmolovskii, 2002), (Maurer Osmolovskii, 2003), (Sarychev, 1992), (Agrachev et.al, 2002a), (Agrachev et.al, 2002b), (Agrachev Sachkov, 2004).

In this paper we consider a reference control which is a concatenation of bang and singular arcs, for simplicity we assume that there is only one singular arc on the interval $[a,b]$.

The conditions are given through a coordinate-free second variation which is obtained by allowing the switching times of the bang arcs and the singular control to vary. Applying the Gho transformation (integrations by parts on the singular arc) we obtain a quadratic form $J"$ on $\mathbb{R}^r \times \mathbb{R} \times L^2([a,b],\mathbb{R})$, where r is the number of the bang arcs.

The main result of the paper is that, under suitable regularity conditions, the coercivity of $J"$ is sufficient to prove (time, state)–local optimality.

We underline that this sufficient condition is "near" the necessary one in usual sense, while the sufficient condition in (Poggiolini Stefani, 2005) the condition is stronger. Indeed in the bang-singular case we need only regularity conditions on the bang arc and the coercivity of the second variation along the singular arc for the minimum–time problem with end–points fixed and equal to $\widehat{\xi}(a)$ and $\widehat{\xi}(b)$.

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OPTIMAL CONTROL SYSTEMS WITH CONSTRAINTS DEFINED ON UNBOUNDED SETS

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Keywords: optimal control, Lyapunov stability

Let us consider quasilinear control system of the form

$$z''(t) + A(t,u(t))z(t) + \alpha\varphi(t,z(t)) = B(t)u(t), \quad z(0) = v_0 \in \mathbb{R}^N, \quad (1)$$

where $t \in I := [0,\infty)$, $\alpha \in \mathbb{R}$, $z(\cdot) \in H^1\left(I,\mathbb{R}^N\right)$, $u(\cdot) \in L^\infty\left(I,\mathbb{R}^M\right)$, $A(\cdot,\cdot) \in L^\infty\left(I\times U,\mathbb{R}^{N\times N}\right)$, $B(\cdot) \in L^1\left(I,\mathbb{R}^{N\times M}\right)$, $\varphi(\cdot,\cdot) \in C\left(I\times\mathbb{R}^N,\mathbb{R}\right)$, $U \subset \mathbb{R}^N$, $N,M \geq 1$. On trajectories of system (1) we put integral constraint of inequality-type:

$$\int_I \phi(t,z(t)) \leq l, \quad \text{where } \phi(\cdot,\cdot) \in C\left(I\times\mathbb{R}^N,\mathbb{R}\right). \quad (2)$$

We consider control system (1-2) with an integral quality indicator of the form

$$\int_I f((z(t),u(t),t)dt \to \min, \quad (3)$$

where $f : \mathbb{R}^N \times \mathbb{R}^M \times I \to \mathbb{R}$.

We define a space of trajectories as a set of functions which are absolutely continuous on any compact interval $I_0 \subset I$ and which satisfy conditions:

$$\int_I |z(t)|^2 dt < \infty \quad \text{and} \quad \int_I |z'(t)|^2 dt < \infty$$

i.e. $z(\cdot), z'(\cdot) \in L^2\left(I,\mathbb{R}^N\right)$.

The space $H^1(I,\mathbb{R}^N)$ is a Banach space with the norm

$$||z||^2 := \int_I \left(|z'(t)|^2 + |z'(t)|^2\right) dt.$$

One can prove that for a function $z(\cdot) \in H^1(I,\mathbb{R}^N)$ we have

$$z(\infty) := \lim_{t\to\infty} z(t) = 0.$$

Remark 1 *Equation (1) is a second order ordinary differential equation. The problem of existence of solutions to the above equation with conditions $z(0) = v_0$ and $z(\infty) = 0$ is, in fact, two-point boundary value problem.*

As a set of admissible controls we take

$$\mathcal{U} := \{u(\cdot) \in L^\infty\left(I,\mathbb{R}^M\right) : u(t) \in U \text{ for } t \in I\}, \quad (4)$$

where $U \subset \mathbb{R}^M$. The fundamental difference between above optimal control problem (1-4) and classical optimal control problem is that control system (1) and functional (3) are defined on unbounded time interval.

In the sequel, we shall impose the following assumptions:

(A1) the matrix $A(t,u)$ is positively-defined for each $t \in I$ and each $u \in U$,

(A2) the function $\phi(t,\cdot)$ is convex and there are a constant $a_1 > 0$ and a function $a_2(\cdot) \in L^1(I,\mathbb{R})$, such that

$$|\phi(t,z)| \leq a_1|z|^2 + a_2(t)$$

for $t \in I$ and $z \in \mathbb{R}^N$,

(A3) there is a function $\tilde{z}(\cdot) \in H^1(I,\mathbb{R}^N)$ such that $\int_I \phi(t,\tilde{z}(t))dt < l$,

(A4) there are a constant $b_1 > 0$ and a function $b_2(\cdot) \in L^1(I,\mathbb{R})$ such that

$$|f(z,u,t)| \leq b_1|z|^2 + b_2(t)$$

for $z \in \mathbb{R}^N$ and $t \in I$.

We have the following

Theorem 1 *If Assumptions (A1-A3) are satisfies and $\varphi(t,\cdot) = \nabla\phi(t,\cdot)$, then for each initial value v_0 and each control $u_0 \in \mathcal{U}$ there are a constant $\alpha_0 < 0$ and a function $z(\cdot,v_0,u_0) \in$*

$H^1(I,\mathbb{R}^N)$ which is a Caratheodory solution to the equation (1) with condition (2). Moreover, the above solution is asymptotically stable in the sense of Lyapunov i.e. for each sequence $(v_k)_{k\in\mathbb{N}}$ tending to v_0 in $\mathbb{R}^N$ and each sequence $(u_k(\cdot))_{k\in\mathbb{N}}$ of controls tending to $u_0(\cdot)$ in $L^\infty(I,\mathbb{R}^M)$, the sequence of solutions $z_k(\cdot) := z(\cdot,v_k,u_k)$ tends uniformly to $z_0 := z(\cdot,v_0,u_0)$ and $\lim_{t\to\infty} z_0(t) = 0$. If the function $\phi(t,\cdot)$ is positively homogeneous, then $\int_I \phi(t,z_0(t))dt = l$ i.e. equation (1) possesses solution under constraint of the form $\int_I \phi(t,z(t))dt = l$

Applying theorem 1 one can prove that optimal control problem (1-4) possesses a solution.

Theorem 2 *If control system (1-4) satisfies assumptions (A1-A4), then in the set of admissible controls $\mathcal{U}$ (conf. (4)) there exists an optimal control.*

The results presented above can be extended to the case of elliptic systems of the form

$$\triangle z(x) + A(x,u(x))z(x) + \alpha\varphi(x,z(x)) = B(x)u(x), \quad x\in\mathbb{R}^n,\ n\geq 2, \quad (5)$$

with integral constraint

$$\int_{\mathbb{R}^n} \phi(x,z(x))dx \leq l \quad (6)$$

and cost functional

$$\int_{\mathbb{R}^n} f(z(x),u(x),x)dx \to \min. \quad (7)$$

The set of admissible control is of the form

$$\mathcal{U} := \{u(\cdot)\in L^\infty\left(\mathbb{R}^n,\mathbb{R}^N\right) : u(x)\in U\subset\mathbb{R}^M\}. \quad (8)$$

System (5-8) is considered in the Sobolev space $H^1\left(\mathbb{R}^n,\mathbb{R}^N\right)$. For system (5-8) one can prove theorems analogous to the theorems 1 and 2. The most interesting is the case, when $n=3$, $M=N=1$, $A(x,u)=-u$, $\varphi(x,z)=z$, $B=0$ and $\phi(x,z)=|z|^2$. In this case system (5) is reduced to the scalar elliptic equation of the form

$$\triangle z(x) - u(x)z(x) + \alpha z(x) = 0, \quad (9)$$

with integral condition

$$||z||^2_{L^2(\mathbb{R}^3,\mathbb{R})} = \int_{\mathbb{R}^3} |z(x)|^2dx \leq 1, \quad z(\cdot)\in H^1(\mathbb{R}^3,\mathbb{R}). \quad (10)$$

Equation (9) is a well-known stationary Schrödinger equation.

From theorem analogous to theorem 1, it follows that equation (9) possesses a solution $z_u(\cdot)\in H^1(\mathbb{R}^3,\mathbb{R})$ and solution depends continuously on varying potential $u(\cdot)\in L^\infty(\mathbb{R}^3,\mathbb{R})$. Moreover,

$$\int_{\mathbb{R}^3} |z_u(x)|^2dx = 1$$

and

$$\alpha = \min_{z\in S}\int_{\mathbb{R}^3}\left(|\nabla z(x)|^2 + u(x)|z(x)|^2\right)dx,$$

where $S := \{z\in H^1(\mathbb{R}^3,\mathbb{R}) : \int_{\mathbb{R}^3}|z_u(x)|^2dx = 1\}$.

The existence of solution to the Schrödinger equation was proved many years ago by applying direct variational or topological methods. However, as far as we know, the result presented above and concerning continuous dependence of solutions on varying potential is new.

ε-VALUE FUNCTION AND DYNAMIC PROGRAMMING

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Keywords: Dynamic programming, $\epsilon-$optimal control problems, ε-value function, Hamilton-Jacobi inequality

Let us consider the classical optimal control problem of Bolza:

$$\min J(x,u) = \int_a^b L(t,x(t),u(t))dt + l(x(b)), \tag{1}$$

where $a, b \in \mathbb{R}$, $x : [a,b] \to \mathbb{R}^n$ is absolutely continuous function and $u : [a,b] \to \mathbb{R}^m$ is Lebesgue measurable function. Both functions: trajectory $x(\cdot)$ and control $u(\cdot)$ are subject to the following conditions:

$$\dot{x}(t) = f(t,x(t),u(t)) \text{ a.e. in } [a,b], \tag{2}$$

$$u(t) \in U,\ t \in [a,b], \tag{3}$$

$$x(a) = c, \tag{4}$$

where $f : [a,b] \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$, $L : [a,b] \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, $l : \mathbb{R}^n \to \mathbb{R}$ are given, c is point from $\mathbb{R}^n$. We tell that a pair $x(\cdot)$, $u(\cdot)$ is admissible if it satisfies (2), (3) and $t \to L(t,x(t),u(t)$ is summable.

We assume throughout the paper about L, f and l that:

$$(\mathbf{Z}) \begin{cases} (a) & (t,x,u) \to L(t,x,u), \\ & (t,x,u) \to f(t,x,u) \text{ are} \\ & \text{continuous, Lipschitz in } x \\ (b) & \text{and bounded on } [a,b] \times \mathbb{R}^n \times U, \\ & x \to l(x) \text{ is continuous} \\ & \text{and bounded in } \mathbb{R}^n, \\ (c) & U \subset \mathbb{R}^m \text{ is a compact set.} \end{cases}$$

It is well known that in spite of the above strong assumptions (**Z**) the problem (1)-(4) does not have to have a minimizer. However it is also well known (1) that the problem (1)-(4) has the value function $S(t,x) = \inf\left\{\int_t^b L(s,x(s),u(s))ds + l(x(b))\right\}$ (where the inferior is taken w.r.t. all admissible trajectories starting at $(t,x) \in [a,b] \times \mathbb{R}^n$, i.e. $x(t) = x$), which is Lipschitz continuous. Even more, the value function satisfies then the corresponding Hamilton - Jacobi equation

$$S_t(t,x) + \min_{u \in U}\{S_x(t,x)f(t,x,u) \tag{5}$$

$$+L(t,x,u)\} = 0,\ \text{a.e., } S(b,x) = l(x).$$

However, the converse assertion is not true: not each solution to (5) is a value function for the problem (1)-(4). Gonzales (2) proved that $S(t,x)$ is a maximal element of the set

$$W = \left\{ \begin{array}{c} w(t,x) \text{ is lipschitz: } w(b,x) \le l(x), \\ W_t(t,x) + \min_{u \in U}\{W_x(t,x)f(t,x,u) \\ +L(t,x,u)\} \ge 0,\ \text{a.e} \end{array} \right\}$$

The function $(t,x) \to S_\varepsilon(t,x)$ defined in $[a,b] \times \mathbb{R}^n$ we call $\varepsilon-$ value function if:

$$S(t,x) \le S_\varepsilon(t,x) \le S(t,x) + \varepsilon(b-a),$$

$$(t,x) \in [a,b] \times \mathbb{R}^n,\ l(x) \le S_\varepsilon(b,x)$$

$$\le l(x) + \varepsilon(b-a),\ x \in \mathbb{R}^n.$$

It is also well known that there exists a Lipschitz continuous $\varepsilon-$ value function and that it satisfies Hamilton - Jacobi inequality:

$$-\frac{\varepsilon}{2} \le S_{\varepsilon t}(t,x) + \min_{u \in U}\{S_{\varepsilon x}(t,x)f(t,x,u) \tag{6}$$

$$+L(t,x,u)\} \le 0.$$

The question which appears here in a natural way and is very important from numerical point of view is: Lipschiz function $G(t,x)$ satisfying (6) and boundary inequality $l(x) \le G(b,x) \le l(x) + \frac{\varepsilon}{2}(b-a)$, $x \in \mathbb{R}^n$ is an $\varepsilon-$ value function

for problem (1)-(4)? The aim of this note is to answer for that question in affirmative, i.e. we prove the following theorem.

Theorem. Each element of the set W_ε

$$\begin{aligned} W_\varepsilon = \{&w(t,x) \text{ is lipschitz: } l(x) \le w(b,x) \\ &\le l(x) + \frac{\varepsilon}{2}(b-a),\ x \in \mathbb{R}^n; \\ &-\frac{\varepsilon}{2} \le w_t(t,x) + \min_{u\in U}\{w_x(t,x)f(t,x,u) \\ &+L(t,x,u)\} \le 0, \text{ a.a.}(t,x) \in [a,b]\times\mathbb{R}^n\} \end{aligned}$$

is an $\varepsilon-$ value function.

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GENERALIZATION OF THE P–REGULARITY CONCEPT AND OPTIMALITY CONDITIONS FOR DEGENERATE CONSTRAINED OPTIMIZATION PROBLEMS

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Keywords: conditions for optimality, degeneracy, nonregular optimization problems, p-regularity

We consider the nonlinear optimization problem

$$\begin{array}{ll} \underset{x\in X}{\text{minimize}} & f(x) \\ \text{subject to} & F(x)=0, \end{array} \tag{1}$$

where $f : X \to \mathbb{R}$ is a sufficiently smooth function, and $F : X \to Y$ is a sufficiently smooth mapping from a Banach space X to a Banach space Y. The focus is on the case when mapping F is nonregular (degenerate) at the solution x^* of optimization problem (1), that is when the Fréchet derivative $F'(x^*)$ is not onto. In this case, the Euler-Lagrange necessary conditions for optimality,

$$\lambda_0 f'(x^*) + F'(x^*)^* y^* = 0,$$

are trivially satisfied with $\lambda_0 = 0$, and provide no additional information about solutions of (1). The development of optimality conditions for nonregular problems has become an active research topic.

In our previous work, we derived necessary and sufficient conditions for the constrained optimization problems that are p-regular at x^*. Namely, in (1) we derived new optimality conditions for problems with p–regular equality constraints. In (2) and (3) we proposed necessary optimality conditions for p–regular problems with inequality constraints. The main idea of the p-regularity approach is to replace the operator $F'(x^*)$ which is not onto with a linear operator $\Psi_p(x^*)$, related to the pth order Taylor polynomial of F at x^*, which is onto. Moreover, in (1), we introduced a modified (generalized) condition of the p–regularity and derived the corresponding necessary optimality conditions. In this talk, we introduce a new generalization of the definition of the p-regular mappings. The new concept generalizes both the p-regularity definition and the modified p-regularity definition introduced in (1). This generalization allows us to derive optimality conditions for new classes of nonregular optimization problem (1) that satisfies neither p-regular nor introduced in (1) modified condition of p–regularity. To compare our approach with others, we can note that Ledzewicz and Schättler (4; 5) use the terminology p–regular, but in different sense. Furthermore, some problems that satisfy the *generalized* condition of p–regularity could not be treated using the approach presented in (4; 5).

The following theorem gives necessary conditions in the completely degenerate case when $F^{(k)}(x^*) = 0$, $k = 1, \ldots, p-1$, for some $p \geq 2$, but the mapping F is not p-regular at x^*, that is $F^{(p)}(x^*)[h]^{p-1} \cdot X \neq Y$ for some specially chosen vector $h \in X$. To state the theorem, we introduce the generalized definition of p-regularity.

Theorem 1. *Let X and Y be Banach spaces, $f \in C^2(X \to \mathbb{R})$ and $F \in C^{p+1}(X \to Y)$. Let x^* be a solution of optimization problem* (1) *such that $F^{(k)}(x^*) = 0$ for $k = 1, \ldots, p-1$, $p \geq 2$. Assume that there exist elements h_1 and h_2 in X such that $Y = Y_1 \oplus \ldots \oplus Y_p$, where $Y_k = \mathrm{cl}\,(\,\mathrm{Im}(P_k F^{(p)}(x^*)[h_1]^{p-k}[h_2]^{k-1}))$ for $k = 1, \ldots, p$, P_1 is a projector onto Y, and*

for $k = 2, \ldots, p$, P_k is a projector onto $Y \backslash (Y_1 \oplus \ldots \oplus Y_{k-1})$ along $(Y_1 \oplus \ldots \oplus Y_{k-1})$ with respect to Y. Let the mapping $f_k(x)$ be defined by $f_k(x) = P_k F(x)$, $k = 1, \ldots, p$. Assume that for the linear operator $\Psi = \Psi(h_1, h_2)$, defined by

$$\begin{aligned}\Psi &= f_1^{(p)}(x^*)[h_1]^{p-1} + f_2^{(p)}(x^*)[h_1]^{p-2}[h_2] \\ &\quad + \ldots + f_p^{(p)}(x^*)[h_2]^{p-1},\end{aligned}$$

the following generalized p-regularity condition holds:

$$\Psi \cdot X = Y. \tag{2}$$

Assume also that $\Psi \cdot h_1 = 0$ and $\Psi \cdot h_2 = 0$. Then there exists a multiplier $\lambda^* \in Y^*$ such that

$$\begin{aligned}f'(x^*) &+ \Big(f_1^{(p)}(x^*)[h_1]^{p-1} \\ &+ f_2^{(p)}(x^*)[h_1]^{p-2}[h_2] \\ &+ \ldots + f_p^{(p)}(x^*)[h_2]^{p-1}\Big)^* \lambda^* = 0.\end{aligned}$$

In Theorem 1, we use two vectors h_1 and h_2. In the next theorem we use vectors $h_1, \ldots, h_q \in X$ with $q \geq 1$, and consider the case of $p = 2$ with $F'(x^*) = 0$.

We assume again that the space Y is decomposed into the direct sum

$$Y = Y_1 \oplus \ldots \oplus Y_q,$$

but with a different definition of Y_k and a definition of the projector $\bar{P}_k$ similar to definition of P_k given in Theorem 1. Namely, we define $Y_k = \mathrm{cl}\,(\mathrm{Im}\bar{P}_k(F''(x^*)[h_k])$, $k = 1, \ldots, q$.

Theorem 2. *Let X and Y be Banach spaces, $f \in C^2(X \to \mathbb{R})$ and $F \in C^3(X \to Y)$. Let x^* be a solution of optimization problem (1) such that $F'(x^*) = 0$. Assume that there exist vectors $h_1, \ldots, h_q$ in X ($q \geq 1$), such that $h_k \neq 0$, $k = 1, \ldots, q$, and for the mappings $f_k(x) = \bar{P}_k F(x)$ the following generalized 2-regularity condition holds:*

$$(f_1''(x^*)[h_1] + \ldots + f_q''(x^*)[h_q]) \cdot X = Y, \tag{3}$$

where

$$f_k''(x^*)[h_{k+r}, h_{k+p}] = 0,$$

for $k = 1, \ldots, q$, $r = 0, \ldots, (q-k)$, and $p = 0, \ldots, (q-k-r)$. Then there exists a multiplier $\lambda^* \in Y^*$ such that

$$\begin{aligned}f'(x^*) + (f_1''(x^*)[h_1] + f_2''(x^*)[h_2] \\ + \ldots + f_q''(x^*)[h_q])^* \lambda^* = 0.\end{aligned}$$

Remark. Condition (3) with $q = 1$ reduces to the 2-regularity condition in the completely degenerate case $F'(x^*) = 0$.

In addition to necessary conditions given in Theorem 1 and 2, we also present new sufficient conditions of optimality for problem (1) which constraints satisfy a generalized condition of p-regularity (2) or (3).

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WEAK SHARP MINIMA IN MULTIOBJECTIVE OPTIMIZATION

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1. PROBLEMS IN NORMED SPACES

Let X and Y be normed spaces, let Ω be an open subset of X, $S \subset \Omega$, $\bar{x} \in S$, and let $D \subset Y$ be a cone (containing 0). The cone D defines order in Y; we do not suppose D is convex, pointed, or closed. $B(x, \delta)$ denotes the open ball with center $x \in X$ and radius $\delta > 0$, $\mathcal{N}(x)$ is the family of all neighborhoods of x, and $\operatorname{dist}(x, W)$ is the distance from the point x to the set $W \subset X$. The symbols $\operatorname{cl} S$ and $\operatorname{bd} S$ denote, respectively, the closure and the boundary of S.

Given a function $f : \Omega \to Y$, the following abstract multiobjective optimization problem is considered:

$$\min \{f(x) : x \in S\}. \tag{1}$$

Definition 1 *Let $m \geq 1$ be an integer. We say that $\bar{x}$ is a* weak sharp local Pareto minimizer of order m *for (1), denoted $\bar{x} \in \mathrm{WSL}(m, f, S)$, if there exist $\alpha > 0$ and $U \in \mathcal{N}(\bar{x})$ such that*

$$(f(x) + D) \cap B\left(f(\bar{x}), \alpha \operatorname{dist}^m(x, W)\right) = \emptyset \tag{2}$$

for all $x \in S \cap U \backslash W$, where

$$W := \{x \in S : f(x) = f(\bar{x})\}.$$

Under the assumption that D is closed, convex and pointed, Definition 1 is equivalent to Definition 8.2.3 in Bednarczuk (2006). In particular, if $Y = \mathbb{R}$ and $D = [0, +\infty)$, then (2) reduces to

$$f(x) - f(\bar{x}) \geq \alpha \operatorname{dist}^m(x, W),$$

which gives the well-known definition of a *weak sharp local minimizer of order m* for (1); see Studniarski and Ward (1999). On the other hand, if $W = \{\bar{x}\}$ in Definition 1, we obtain the definition of a *strict local Pareto minimizer of order m* for (1); see Jiménez (2002), Definition 3.1.

The following results are generalizations of Proposition 3.4 and 3.5 in Jiménez (2002).

Proposition 1 *$\bar{x} \notin \mathrm{WSL}(m, f, S)$ if and only if there exist sequences $x_k \in S \backslash W$, $d_k \in D$, such that $x_k \to \bar{x}$, $\operatorname{dist}(x_k, W) > 0$ for all k, and*

$$\lim_{k \to \infty} \frac{f(x_k) - f(\bar{x}) + d_k}{\operatorname{dist}^m(x_k, W)} = 0.$$

Proposition 2 *Let $Y = \mathbb{R}^p$ and $D = \mathbb{R}^p_+ = [0, +\infty)^p$. Then the following conditions are equivalent:*

(i) *$\bar{x} \notin \mathrm{WSL}(m, f, S)$;*

(ii) *there exist a vector $\bar{d} \in [-\infty, 0]^p$ and a sequence $x_k \in S \backslash W$ such that $x_k \to \bar{x}$, $\operatorname{dist}(x_k, W) > 0$ for all k, and*

$$\lim_{k \to \infty} \frac{f(x_k) - f(\bar{x})}{\operatorname{dist}^m(x_k, W)} = \bar{d}.$$

2. PROBLEMS IN FINITE-DIMENSIONAL SPACES

In this section we consider problem (1) in the case where $X = \mathbb{R}^n$, $Y = \mathbb{R}^p$ and $D = \mathbb{R}^p_+$. We now introduce a variant of the Mordukhovich normal cone.

Definition 2 (Studniarski, 1999) *Let E and S be subsets of $\mathbb{R}^n$, and let $\bar{x} \in \operatorname{cl} E$. The* normal cone to E at $\bar{x}$ relative to S *is defined by*

$$N_S(E, \bar{x}) := \{y \in \mathbb{R}^n : \exists y_k \to y,\ x_k \to \bar{x},\ t_k \in (0, +\infty),\ w_k \in \mathbb{R}^n \text{ with } x_k \in S,\ w_k \in P(E, x_k) \text{ and } y_k = (x_k - w_k)/t_k\ (\forall k)\},$$

where

$$P(E,x) := \{w \in \operatorname{cl} E : \|x-w\| = \operatorname{dist}(x,E)\}$$

is the metric projection of x onto E.

Remark 1 (i) *If $S = \mathbb{R}^n$, then $N_S(E,\bar{x})$ is equal to to the* Mordukhovich normal cone *to E at $\bar{x}$ (see Mordukhovich, 2006, Vol. I, p. 8):*

$$N(E,\bar{x}) := \{y \in \mathbb{R}^n : \exists y_k \to y,\ x_k \to \bar{x},\ t_k \in (0,+\infty),\ w_k \in \mathbb{R}^n \text{ with } w_k \in P(E,x_k) \text{ and } y_k = (x_k - w_k)/t_k\ (\forall k)\}.$$

(ii) *If $E = \{\bar{x}\}$, then $N_S(E,\bar{x})$ is equal to the well-known* contingent cone *to S at $\bar{x}$:*

$$K(S,\bar{x}) := \{y \in \mathbb{R}^n : \exists y_k \to y,\ x_k \to \bar{x},\ t_k \in (0,+\infty) \text{ with } x_k \in S \text{ and } y_k = (x_k - \bar{x})/t_k\ (\forall k)\}.$$

Definition 3 *Let E be a nonempty closed subset of $\mathbb{R}^n$, and let $\varphi : \mathbb{R}^n \to \mathbb{R}$. For $x \in \operatorname{bd} E$ and $y \in \mathbb{R}^n$, define*

$$\bar{d}_E^m \varphi(x;y) := \limsup_{\substack{\operatorname{bd} E \ni w \to x \\ (t,v) \to (0^+,y)}} \frac{\varphi(w+tv) - \varphi(w)}{t^m}.$$

(In particular, (x,y) is an allowable choice of (w,v).) For $m = 1$, we will write $\bar{d}_E \varphi(x;y)$ instead of $\bar{d}_E^1 \varphi(x;y)$.

Theorem 3 *Suppose that W is closed. If $\bar{x} \in \mathrm{WSL}(m,f,S)$, then, for each $y \in N_S(W,\bar{x})$ with $\|y\| = 1$, there exists $i \in \{1,...,p\}$ such that*

$$\bar{d}_W^m f_i(\bar{x};y) > 0.$$

For weak sharp local Pareto minimizers of order one, a necessary condition can be formulated in terms of *Clarke's generalized directional derivative*; see Clarke (1983). Recall that, for a locally Lipschitzian function $\varphi : \mathbb{R}^n \to \mathbb{R}$, this derivative is defined by

$$\varphi^\circ(x;y) := \limsup_{(t,w) \to (0^+,x)} \frac{\varphi(w+ty) - \varphi(w)}{t}.$$

Proposition 4 *Let E be a nonempty closed subset of $\mathbb{R}^n$, and let $\varphi : \mathbb{R}^n \to \mathbb{R}$ be locally Lipschitzian. Then, for any $x \in \operatorname{bd} E$ and $y \in \mathbb{R}^n$, we have*

$$\varphi^\circ(x;y) \geq \bar{d}_E \varphi(x;y).$$

Corollary 5 *Suppose that W is closed. If $\bar{x} \in \mathrm{WSL}(m,f,S)$, then, for each $y \in N_S(W,\bar{x})$ with $\|y\| = 1$, there exists $i \in \{1,...,p\}$ such that $f_i^\circ(x;y) > 0$.*

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DEVELOPMENT OF A FRAMEWORK FOR EARLY WARNING AND PROACTIVE CONTROL SYSTEM IN FOOD SUPPLY NETWORKS

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Keywords: framework, early warning, proactive control

Food supply networks (FSN) are currently confronted with a lot of challenges. They have to cope with expanding and open international markets with increasing competition, with more demanding customers, retailers and NGO's, with increased legal demands and requirements, with new technologies that 'call' to be used, with increased vulnerability in case of food problems and calamities. The latter is even aggravated by increased transparency. Food problems are published in our media, almost on a daily bases. These problems can jeopardize the very existence of products on the market and of the companies producing them. The nature of these problems may have to with various aspects, such as food quality, operations, or logistics. For example, chickens may die before their arrival at the slaughter house and or have quality attributes that are not in compliance with requirements defined for quality slaughtered products. A similar situation with respect to quality deviations may exist in the pork chain. The weight and quality of pigs arriving at the slaughter house may not satisfy defined requirements. For example the bacon quality of the pigs is of great importance if you want to produce for the British market. Further products may not have the right quality, or even be contaminated with (toxic) substances. These problems thus cause potential losses to the food industry and may cause that the trust in the food system decreases. In order to diminish these losses, it is necessary to predict potential problems in FSN as early as possible and thereafter to take proactive actions to prevent those problems or correct their effects. However, specific characteristics of FSN make it difficult to find out causes and take corrective action in time when problems occur, especially when domain knowledge is missing. Fortunately, the rapid development of information systems in FSN provides us with opportunities to find valuable information from recorded data.

In our research, we are aiming at building early warning and proactive control systems in FSN in order to effectively and efficiently control problems in FSN. They enable managers to exploit recorded data by employing various Data Mining (DM) methods to find causes of problems and predict potential problems based on the status of current FSN. It also collects knowledge obtained in real cases into a knowledge base for managers' reference.

In this paper, we present a framework for early warning and proactive control system in FSN. This framework is built upon our experience in dealing with problems in real cases. It contains knowledge on both content and process aspects for applying DM methods to deal with problems

in FSN. We provide a process model to illustrate the processes for managers to utilize this framework. This process model takes manager's resources into consideration. It helps managers to take advantage of their knowledge and resources while using this framework. For each step of those processes, we also provide information on prerequisites, outcomes, and evaluation criteria in order to ensure that managers arrive at appropriate and usable solutions.

The framework consists of the following components: user interface, knowledge base, task classifier and template approaches, DM method library, and a predictor. The knowledge base is designed to incorporate the knowledge about existing problems in FSN together with their causes, and utilized DM methods. This knowledge base provides essential knowledge sources for managers to deal with real problems in FSN. Managers can either browse the knowledge base for causes of problems or use appropriate Data Mining methods to analyze collected data for causal factors. After that, they can predict potential problems and take timely actions to prevent losses. Since some of those steps require managers to apply specific knowledge on Data Mining, we provide multiple template approaches to guide managers through these steps. For example, in order to do prediction, a manager has to find proper methods, set proper parameters, interpret the outcome of algorithms, and fine-tuning settings in order to get optimal results. Template approaches for prediction are needed here to serve as guidelines for managers executing these steps.

Detailed explanations of each component are given in this paper, together with the relations between them, and how managers cooperate together with them for early warning and proactive control of problems in FSN.

GAME THEORETICAL ASPECTS IN MODELING AND ANALYZING SHIPPING ALLIANCES

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Keywords: Game theory; Non-cooperative; Shipping, Strategic Alliance

Nowadays, there is a trend to establish new business linkages and alliances within the shipping industry together with customers, suppliers, competitors, consultants, and other companies. A number of studies have attempted to explain this phenomenon occuring in the liner shipping industry using a variety of conceptual and theoretical frameworks. This paper focuses on liner shipping´s strategic alliances and their establishment and transformation within the framework of cooperative and non-cooperative game theory. The concepts developed and improved by Nash, Selten and Harsanyi should be considered as effective and capable tools to analyse motivations, competitive structures, strategies and potential pay-offs in a turbulent liner shipping industry.

Not only a liner shipping company could be regarded as a player in shipping alliance, but also a liner shipping strategic alliance itself could be viewed as a player as well when it competes with other alliances. However, in this paper, we pay more attention to the former model assuming those liner companies are unable to make enforceable contracts through outside parties. The aims of this paper are to

1) indicate the motivations of short-run cooperation among several liner carriers;
2) analyse pros and cons of being members in liner shipping strategic alliances;
3) explain the departure of a player when it faces turbulence and unpredictable shipping circumstances
4) advise ways to contain long-run alliance´s stability by increasing benefits while decreasing drawbacks.

Among those four main points, the differences between short term cooperation and long term alliance are the amounts of sub-games and the potential pay-off in future. Consequently, we set up specific models based on non-cooperative games and repeated games to give those differences clear explanations. The outcome of this paper shall be helpful for those liner shipping carriers who attempt to succeed in the shipping industry with greater efficiency, better customer service and lower cost.

PARALLEL DIRECT SEARCH METHODS FOR SIMULATION-BASED OPTIMIZATION

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Keywords: Optimization, distributed computing, computational engineering

In many engineering disciplines, the use of realistic computing models has become an invaluable tool in the design process. Complex simulation codes are able to approximate the behavior of intricate systems or the properties of components without the need for costly physical experimentation. Optimization algorithms can be used to automatically find the set of parameters within the design space for which the simulation promises the most desirable characteristics. However, there are several challenges that must be met to successfully apply this technique to real-world problems.

First, the objective function to be minimized (or maximized) is given only implicitly and a time-consuming simulation is necessary to calculate its value for a given set of parameters. Thus, almost no assumptions can be made about this function, which will often be highly nonlinear and multimodal. Furthermore, there are usually a number of constraints that divide the design space into feasible and infeasible regions of unknown geometry. Derivate information is typically not provided by the simulation codes, and due to numerical noise, the objective function might also be non-smooth. These characteristics make it very hard to apply some classical methods such as gradient-based approaches. A class of optimization algorithms that can be used are so-called direct search methods (1).

Each solution candidate generated by the optimization algorithm must be evaluated, hence necessitating the execution of a time-consuming simulation. Despite the increase of computing power, typical runtimes of a single simulation still span from a few minutes to many hours. This is caused by the demand for larger models, greater accuracy, and the adoption of coupled multiscale and multiphysics simulation codes (2). During the course of the optimization, hundreds or thousands of evaluations are necessary, resulting in very long runtimes. Two common approaches to decrease the time needed are the use of surrogate functions (3) and parallelization. Since the computation time spent within the optimization algorithm itself is several orders of magnitude lower than the time needed for a single simulation, it is useless to introduce parallelism to the internal operations of the algorithm. Instead, the goal is to design the algorithm in a way that allows it to utilize the results of many simulations that can be run simultaneously and independently of each other.

In this paper, eight such parallel direct search methods for simulation-based optimization problems are examined. Most of them are based on well-known sequential search methods and were modified to exploit parallel computing resources:

- Distributed Polytope Search (4) applies geometric operations to a set of points in the search space to generate new solutions. Infeasible solutions are repaired by moving them towards the center of gravity.
- Parallel Scatter Search (5) is a parallel implementation of the well-known scatter search meta-heuristic.
- Asynchronous Parallel Pattern Search (6) is a pattern search method with the unique property of asynchronous parallel operation.
- Simulated Annealing (7) is a parallel variant of the classical SA method which uses a stochastic, temperature-dependant acceptance function to avoid getting stuck in local minima.

- Great Deluge Algorithm (8) is similar to SA but uses a different acceptance function based on a flood level.
- Particle Swarm Optimization (9) simulates a swarm of particles moving through the search space and attracting each other.
- Genetic Algorithm (10), an incarnation of the bioinspired search method for real-valued decision variables.
- Evolution Strategies (11) are closely related to GA but add the concept of so-called strategy parameters, which enable self-adaptation of the search strategy.

Some of the algorithms generate a sufficient number of new solution candidates per iteration in their original, sequential form and are thus easily extended to make use of parallel computation. Others, like Distributed Polytope Search, differ significantly from the algorithm they have been derived from. Furthermore, some of the algorithms can also operate in asynchronous mode, meaning that further operation is not suspended until all pending simulations have finished. This is especially important in a heterogenous computing environment where the runtimes of the simulations vary significantly.

Advances in the area of service-oriented architectures (12) and grid computing (13) make it easier to use resources beyond geographical and organizational boundaries, theoretically enabling even small companies to utilize many thousands of CPUs on demand. However, the problem of licensing still limits the use of commercial simulation software in these environments. Thus, while most of the observations will also apply to large scale computing, the paper focuses on degrees of parallelism of up to a few hundred CPUs – typical of compute clusters or enterprise grids.

The algorithms were used to solve several real-world problems in different engineering disciplines. This includes sheet metal forming and optimization of metal alloy casting processes in the automotive industry, and facility optimization in groundwater management. Results are presented for both a test function as well as two problems from industrial practice. The computational experiments were performed on a 300 CPU Linux Opteron cluster. While the test function allows for an extensive examination of the algorithms' performance over a wide range of utilized CPUs and different problem dimensions, the simulation-based optimization problems indicate the relevance of the contribution to non-academic tasks.

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INTEGRATION OF KNOWLEDGE AND ANALYTICAL MODEL ANALYSIS IN THE FIELD OF FACILITY LOCATION

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ABSTRACT

The focus of "model-related-work" at the Deutsche Post Chair of Optimization of Distribution Networks is the elaboration of optimization models and solution approaches for Distribution Systems in Postal Logistics and Supply Chain Design. There are 4 main classes of optimization problems in this area of application:

facility location,
location routing,
service network design and
vehicle routing and scheduling
problems.

The main characteristics of the models developed in the field of Postal Logistics and SCM are:

- Most of the optimization problems are NP-hard (the exceptions are known of course).
- Problem instances are "large to very large scale".
- Special structures are present (e.g. patterns of constraint types).

Concluding exact methods are successful in special cases or smaller instances only, commercial solvers can not deal with the very large scale real world applications in a reasonable way. Therefore, the world of heuristics and meta-heuristics complemented by high quality lower bounds (for minimization problems) seems to be the only possible approach to solve the real world problems.

It appears that the elaboration of the "appropriate model" is not only science but has also some similarity with art because of the implicit knowledge an expert in the field owns. For example, there are many important design decisions a person who elaborates a model has to make depending on the answers to the following questions:

- Why the model is needed and which are the reasons to use it? (to describe the problem quantitatively and to classify it, to check feasibility of solutions which have been generated without using the model, to prove properties of optimal solutions, to prove properties of algorithmic approaches, to generate solutions model-based?)

- What type of model fits best the respective problem description? (optimization vs. simulation, analytical model, knowledge-model, static or dynamic model, dealing with uncertainty within the model?)

- Which kind of solution methods and respective solvers are available and for which type of instances they can be used successfully (LP, MIP, NLP, heuristics or meta-heuristics, commercial or public domain, available on the web?)

Within the presentation we will propose a modeling environment which helps a human model developer to use the expert knowledge about the respective domain and the expert knowledge about the modeling process as well. Such an modeling environment does not exist today. But, today it seems to be possible to design and to implement such an environment by integrating knowledge based methods (expert systems technology) and techniques dealing with analytical (e.g. algebraic) models of the type "simultan models of Operations Research".There is a need to restrict the domain and therefore we

will focus on the field of "Facility Location" problems which are very important in the strategic planning phase of the applications mentioned above. We will outline the domain knowledge in this field and illustrate why it is so important to implement the experts knowledge about models, their properties, the respective solvers and also external expert knowledge about desired properties of solutions which can not be formulated within the analytical models. Also,we will illustrate our approach using a Facility Location problem in Postal Logistics.

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NEXT GENERATION MODEL MANAGEMENT
MODEL EVOLUTION AS KNOWLEDGE DYNAMICS

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Model management was built upon database theory and the data management paradigm. This was too limiting in many respects and responsible for the eclipse of the discipline, as data management became an increasingly familiar commodity. Yet, modeling is more instrumental in scientific inquiry than even 20 years ago, and more properly belongs in the context of knowledge management. Viewing it from this perspective, we contend that model management research was in many respects ahead of its time and still provides a wealth of important research issues when recast in the contemporary organizational and technological landscape.

We update the static, management control-oriented term *model management* and adopt instead the term *model evolution* to describe the dynamic nature of the modeling lifecycle and its relationship to organizational decision-making. Our objective is to cast model evolution as a pillar of knowledge dynamics in an effort to revitalize this area of information science research. We see the differentiating forces of next generation model management as complexity, distributed computing, and information science.

We note the increased role of modeling and simulation in the role of scientific inquiry, and briefly chart the historical trajectory of model management research. The singular focus on model representation therein tried to parallel the development of database theory, but was not as successful due to the polymorphic and dynamic nature of analytical models, especially simulations. We recognize the continuing relevance of model management research, especially in the fields of Semantic Web and service-oriented architectures, which are grappling with the same ontological semantics and model composition problems that we addressed in studying model integration.

We then view model management through the lens of knowledge management, in particular as an instrument for knowledge flow and dynamics. Modeling is truly much more about knowledge than just data. Modeling, done properly, conveys knowledge that was perhaps previously latent or hidden. For example, conceptual modeling of an information system in the form of Entity-Relationship or UML diagrams facilitates knowledge flow between users and analysts: the users are forced to articulate their mental models, so that analysts may design a computer executable model of those views. A decision model illuminates a larger area of the search space than otherwise would be possible given human cognitive limits, which may, in turn, allow a decision-maker to evaluate more effectively a larger set of alternatives.

We summarize principles and practices of knowledge dynamics such as communities of practice, tacit vs. explicit knowledge (we eschew "tacit" in favor of "hidden" and "latent"), open source knowledge bases, collaborative technology, and people-oriented vs. technology-driven solutions, and set out to establish value propositions and identify relevant research streams in this vein.

Characterizing the next generation model management as knowledge dynamics leads us to consideration of two other phenomena and their impact upon model evolution research:

complexity as an emergent process, and computational modeling and experimentation. The contemporary view of complexity as an emergent process has resulted in a dynamic, bottom up, agent-based approach to modeling that stands in contrast to the more static top down approach historically characteristic of OR/MS analytical modeling. The success of computational modeling and experimentation, particularly in the area of agent-based modeling and simulation, has helped us analyze social phenomena such as organizations, economies, and societies which were previously the bailiwick of primarily qualitative approaches.

We discuss emerging application domains for which next generation model management is well-suited. These include services science, management and engineering (SSME), contemporary supply chain management, alternative energy sources, and emergency response systems. Semantic web and web services are two undertakings of extreme interest which are very amenable to model evolution approaches.

We conclude by suggesting a conceptual framework for model evolution research, and enumerating some dimensions of an associated research agenda.

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MODELING COLLABORATION IN TACTICAL NETWORK-CENTRIC ENVIRONMENTS

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The paper addresses testbed for experimental modeling of decision support and collaborative processes in tactical network-centric operations. This project, supported by partners from Lawrence Livermore National Laboratory, USSOCOM, Sweden, Austria, and Singapore is based on the NPS Tactical Network Topology (TNT) testbed, comprised of long-haul OFDM networks combined with self-forming wireless mesh links to radiation detection sensors, and real-time radiation awareness collaboration with geographically distributed experts. The case-study conducted by the NPS team during the Summer of 2006 included Maritime Interdiction Operation (MIO), High-Value Target (HVT) tracking, and Emergency Response coordination scenarios, in which geographically distributed command centers and subject matter experts collaborate to facilitate situational understanding and course of action selection.

The paper is focused on the findings of the Maritime Interdiction Operation, which is the most representative scenario for exploring globally distributed collaboration between the boarding party taking place in San Francisco Bay area, expert teams on the East Coast, and friendly sites overseas, including Sweden, Austria, and Singapore.

The objective of these experiments is to evaluate the use of networks, advanced sensors, and collaborative technology for conducting rapid MIOs. Specifically, the ability of a boarding party to rapidly set up ship-to-ship communications that permit them to search for radiation and explosive sources while maintaining contact with the mother ship, command and control organizations, and to collaborate with remotely-located sensor experts. The boarding team boards the suspect vessel and establishes a collaborative network and then begins their respective inspections and data collection processes. The boarding officer boards the vessel with his laptop so he can collaborate with all other members of the team. This includes those who are located on the ship, but are physically spread out around different areas of the ship (while searching for contraband material and obtaining fingerprints of crew members), as well as the virtual members of the boarding team – the experts who are located at the different reach back centers. Since there are numerous commercial uses for certain radioactive sources, positive identification of the source in a short time is imperative. There is also pressure to conduct the MIO quickly so as to not detain the ship any longer than necessary.

During the study NPS students observed communication processes of geographically distributed teams and were able to position collaborative process in the decision making space of Simon's problem solving model, Boyd's OODA Loop, and Alberts and Hayes Collaborative C2 model. The results show high fidelity of Alberts and Hayes' Collaborative C2 model and reveal the requirements to collaborative network topology as well as multi-participant team structure.

The results also include observations on the frequency of transactions and the usage patterns of major collaborative tool functions. They are enhanced by the recommendations of how to combine the best elements of the three decision

support models for better mapping of tactical collaborative process.

The described testbed provides several layers of interfaces for integrating new models, tools, and experimentation procedures needed to conduct experimental modeling of decision support and collaboration in tactical network-centric operations.

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A GRID-BASED INFRASTRUCTURE FOR VIRTUAL PRODUCT AND PROCESS OPTIMIZATION IN MANUFACTURING

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Virtual prototyping (concurrent product and process optimization) in manufacturing gains more and more importance, since companies competing on the market noticed the increasing cost pressure alongside higher quality requirements. The utilization of virtual prototyping techniques provides an opportunity to reduce the total development costs and the time to market, while simultaneously innovations of both products and its production processes increase the overall quality of the manufactured parts. The monetary effort and the lack of know-how especially in small and medium sized enterprises (SME) which is required to operate such systems lead to a disadvantage in the more and more globalized market.

The paper states the problem of supporting virtual prototyping processes in the manufacturing industry (by the example of casting and sheet metal forming processes in the German automotive supplier industry) and gives a solution approach by utilizing service-oriented architectures and concepts from grid computing. A pilot implementation of the proposed architecture is introduced and evaluated by case studies (in simulation, optimization and clash-analysis) in both manufacturing (casting and sheet metal forming) domains.

TESTING KNOWLEDGE CREATION THEORIES

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Keywords: Micro-theories of knowledge creation, divergent episteme, falsificationism, paradigmatism, postmodern subjectivism, evolutionary constructive objectivism, testing theories and tools.

ABSTRACT

Motivated by recent emergence of diverse micro-theories of knowledge creation, the paper addresses the question of justification and testing of such theories. Because of the observed divergence of the episteme of three cultural spheres: that of technology, of hard and natural sciences, and of social sciences and humanities, we present a review of the ways of testing tools and theories in these different spheres. Implications concerning testing interdisciplinary and philosophical theories are presented. A review of theoretical results obtained in the 21st Century COE Program *Technology Creation Based on Knowledge Science* is presented. Their testing results and future testing needs conclude the paper.

The necessity of a better, more detailed understanding of knowledge creation processes in the knowledge based economy for the needs of today and tomorrow resulted recently in the emergence of many *micro-theories of knowledge creation,* as opposed to classical concentration of philosophy on *macro-theories of knowledge creation* on a long term historical scale. Historically, we could count the concept of *brainstorming* as first of such micro-theories. However, since 1990 we observe many such new micro-theories originating in systems science, management science and information science, beginning with the *Shinayakana Systems Approach*, the *Knowledge Creating Company* and the *SECI Spiral*, the *Rational Theory of Intuition*, the *I5 (Pentagram) System*, the *OPEC Spiral* and several others. This can be counted as a recent revolution in knowledge creation theories, because all of them take explicitly into account an interplay of *tacit, intuitive, emotive,* and *preverbal* aspects with *explicit* or *rational* aspects of knowledge creation.

Additional results concerning micro-theories of knowledge creation were obtained also in the 21st Century COE Program *Technology Creation Based on Knowledge Science* at the Japan Advanced Institute of Science and Technology (JAIST). For example, the brainstorming process was represented as the *DCCV Spiral* due to the research in this Program. The concept of *Creative Space* developed in this Program tries to provide a synthesis of such diverse micro-theories. The concept of the *Triple Helix* of normal academic knowledge creation combines three spirals: the *Hermeneutic EAIR Spiral* of analysing and interpreting scientific literature, the *Experimental EEIS Spiral* of performing experiments and interpreting their results, and the *Intersubjective EDIS Spiral* of debating and discussing research results; these three spirals characterize main creativity processes at universities and research institutions. The idea of *Nanatsudaki Model of Knowledge Creation Processes* tries to derive pragmatic conclusions from such analysis and synthesis, by combining

seven spirals (objective setting *OPEC,* hermeneutic *EAIR,* socializing *SECI,* brainstorming *DCCV,* debating *EDIS,* roadmapping *I-System,* and experimenting *EEIS*) in an order useful for organizing large research projects.

With all this concentration on describing diverse mechanisms or models of knowledge creation processes, a *critical question arises: how to test, to justify by testing, such micro-theories of knowledge creation?* The standards of testing theories belong to the *episteme* – the prevalent way of creating and justifying knowledge, characteristic for a given historical era or a cultural sphere. However, the episteme of the industrial civilization, called sometimes the *modern* episteme, was subjected to a destruction process, particularly visible in the last fifty years. This has lead to a divergent development of *separate episteme of three cultural spheres:* that of social sciences and humanities, that of hard and natural sciences, and that of technology: they use different languages, but more important is the fact that they use different fundamental epistemic concepts and different ways of constructing and justifying knowledge.

We present here also an attempt to propose a new integration of the episteme, much needed in the beginning era of knowledge civilization. This integration is based on three principles: *evolutionary falsification principle* (an extension of Popperian falsification towards an evolutionary perspective of human development of knowledge in long term historical sense); *emergence principle* (stressing that new properties of a system emerge with increased levels of complexity, and these properties are qualitatively different than and irreducible to the properties of its parts, strengthening and going beyond synergy and holism); and *multimedia principle* (stressing that words are just an approximate code to describe a much more complex reality, visual and preverbal information in general is much more powerful and relates to intuitive knowledge and reasoning; the future records of the intellectual heritage of humanity will have a multimedia character, thus stimulating creativity). Going beyond the concept of a paradigm, we also stress the fundamental role of a *hermeneutical horizon,* an intuitive meta-environment concerning the truth of basic axioms: to have a strictly formal language one needs a formal metalanguage, to have a formal metalanguage one needs a formal meta-metalanguage, and so on – an infinite recursion; thus, the only possible way is to stop and study fundamental assumptions in a non-formal, *intuitive* meta-environment.

However, the issue of testing knowledge creation theories deserves special attention, thus we devote this paper mainly to diverse issues of testing such theories. We conclude that testing of interdisciplinary and philosophical theories, in particular – knowledge creation theories - should thus include:

a) A description and critical review of their relation to the relevant parts of the intellectual heritage of humanity, with logical and hermeneutic tests of the validity of such relation (paradigmatic validity, if applicable, but not necessarily, since interdisciplinary and philosophical theories should be above paradigms);

b) A design of critical experiments, if such are possible, aimed at checking whether the tested theory provides essential new insights;

c) A design of descriptive experiments, if the theory has descriptive character, aimed at checking whether the tested theory describes reality accurately;

d) Cases of applications, if the tested theory allows for prescriptive conclusions, aimed at checking whether applications confirm expected impacts of prescribed actions.

No theory can be fully tested – particularly if it is of social science character; but this should not prevent us from testing theories as diligently as possible. We present in this paper not only recent theories of knowledge creation developed in the 21st Century COE Program *Technology Creation Based on Knowledge Science* and indicated above, but also examples of their testing.

A Hierarchical Multiobjective Routing Model for MPLS Networks

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Keywords: Mutliobjective optimization, multiciteria routing, communication networks, MPLS-Internet

1. INRODUCTION AND MOTIVATION

Modern multiservice network routing functionalities have to deal with multiple, heterogeneous and multifaceted QoS (Quality of Service) requirements. This led to routing models the aim of which is the calculation and selection of one (or more) sequences of network resources (designated as routes, which correspond to loopless paths in the network representation) satisfying certain QoS constraints and the optimisation of route related metrics. Therefore there are potential advantages in formulating important routing problems in these types of networks as multiple objective optimisation problems. These enable the trade-offs among distinct QoS parameters and relevant network cost function(s) to be pursued in a fully consistent manner. It should be noted that the specification of the objective functions and constraints depend strongly on the nature of the considered routing principles, the type of technological platform used by the network and the features of the offered traffic flows associated with different service types.

In the emergent MPLS (Muliprotocol Label Switching) technology for the Internet it is possible the implementation of connection-oriented services from origin to destination. This is feasible by using LSRs (Label Switching Routers) that forward the packets (grouped in Forward Equivalence Classes, FECs), through LSPs (Label Switched Paths) in the network using a specific label switching technique. This in association with other functional capabilities of MPLS enables the implementation of advanced QoS-based routing mechanisms, namely by establishing "explicit routes" (determined at the originating node) for each traffic flow of a given FEC.

Having in mind these features and capabilities of MPLS routing a significant number of routing models have been proposed in the literature in recent years. These approaches often differ in key instances of the modelling framework. In particular such differences are concerned with: i) the scope of the routing optimisation (where we may distinguish network-wide optimisation models and flow-oriented models); ii) the nature of the optimisation model in terms of the objective function(s) and constraints (single/multi-objective, type of QoS-related or other constraints, etc); iii) the level of representation of the traffic flows (representation at the level of micro-flows of packet streams carried on a certain LSP or at the level of the "traffic trunks"-aggregation of traffic flows of the same class placed on the same LSP). Based on

the analysis of the remarkable differences observed in the models proposed in this area, a discussion on key conceptual issues involved in the various modelling approaches and a proposal of a generic hierarchical multi-objective network-wide routing optimisation framework, was presented in [Craveirinha, *et. al*, 05]. The possibility of applying this modeling framework to a MPLS type network, by considering two service classes , namely QoS service (with guaranteed QoS –quality of service levels), treated as a first priority service and Best Effort service (carried on a 'best effort' basis, seeking not to jeopardize the QoS of QoS traffic flows), treated as a second priority service, were the major motivation for this work.

2. CONTENTS OF THE PAPER

This work presents, in detail, a model for multiobjective routing in MPLS networks formulated within the framework developed in [Craveirinha, *et. al*, 05], assuming that there are two classes of services (and different types of traffic flows in each class), namely QoS and Best Effort (BE) services. The flows of QoS type, when accepted by the network, have a guaranteed QoS level, related to the required bandwidth, while BE traffic flows, which are treated in the model as second priority flows, are carried by the network in order to obtain the best possible QoS level for the current network routing solution.

Other feature of the routing model is the use of alternative routing: when a first choice route assigned to a given micro-flow, belonging to a certain traffic flow (corresponding to a "traffic trunk") is blocked a second choice route may be attempted. An important characteristic of this model is the use of hierarchical optimisation typically with two optimisation levels, including fairness objectives: the first priority objective functions refer to the network level objectives of QoS type flows, namely the total expected revenue and the maximal value of the mean blocking of all types of QoS flows; the second priority objective functions refer to performance metrics for the different types of QoS services and the total expected revenue associated with the BE traffic flows. Another important feature of the model is the use of an approximate stochastic representation of the traffic flows in the network, based on the use of the concept of effective bandwidth for macro-flows and on a generalised Erlang model for estimating the blocking probabilities in the arcs, as the one used in [Martins, *et al.*, 2006]. After describing in detail the routing model, including the underlying traffic model, we will present the theoretical foundations of a specialised heuristic strategy for finding "good" compromise solutions to the very complex bi-level routing optimisation problem. This theoretical foundation is based on a conjecture concerning the definition of marginal implied costs for QoS flows and BE flows, which is an extension and adaptation of earlier definitions of implied cost for mono-service networks with alternative routing in [Kelly, 88]. The structure of the heuristic procedure for resolving the problem is analogous to the one described in detail in [Craveirinha, *et. al*, 04] and [Martins *et al.*, 2006] and is based on a constrained bi-objective shortest path model the objective functions of which are QoS or BE marginal path implied costs, depending on the class of the routed traffic, and path blocking probabilities. A description of the main features of a first version of this heuristic will be presented. Also preliminary results obtained with the application of this heuristic to a test network used in a benchmarking study on network-wide routing optimisation with MPLS, will be revealed. Finally conclusions and further work on this model will be outlined.

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Teaching Support System on the Web and Multicriteria Evaluation

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1 Introduction

It is very effective in education to force reports to the students and/or small tests from time to time, and especially so if we check them within a few days and return our comments. However, we usually cannot do that due to our tight schedule. It consumes huge amount of time to check the reports or tests of more than 100 students for one course.

As the PCs and the computer network environment become popular, it becomes realistic to use them for education. We are trying to use a computer network for this kind of educational purpose.

In some problems, private lesson is the best way for education. Actually, some e-learning systems are designed for private lessons. But it is not always useful. The students usually talk over the lessons each other and this seems very effective for them to understand and teach each other. Hence we are developing a teaching support system for mass-education.

Teaching Support System is equipped with real-time processing of the answers entered by students. The students can know the scoring of their respective answers in real time.

We also need to develop a system to grade the students based on the scores obtained by the Teaching Support System. It can treat the elements of the scores from the view-point of multi-criteria decision making (MCDM).

2 Teaching Support System

Our teaching support system consists of the following sub-systems.

*The author wish to express his sincere thanks to S. Adachi for the assist of developing the teaching support system.

- Report System
- Small Test System

The **report system** (RS) accepts free-style text-based sentences, not selection problems. The tutor marks the submitted reports from the web browsers, and the students can see the scores and comments on the PC screen.

The **small-test system** (ST) consists of further sub-systems. The first sub-system (ST-SS1) is based on the selection buttons, and the tutor inputs the problems and their correct answers in advance. The second sub-system (ST-SS2) is also based on the selection buttons, but the problems are not entered. They are spoken in the lecture. This system is expected to increase the attention of the students. The third one (ST-SS3) is free-style description style.

3 Evaluation System

To use the scores of the reports and tests for tutoring purpose, we will extract various indices for multi-criteria evaluation. Our goal is to give students appropriate advices for study as well as deciding the final grade of the course.

The grades of courses of Konan University are the follows; AA (Super Excellent), A, B, C and D (Fail), and K (No attendance). The task of giving one index from many scores is usually done by summing up the scores of small tests with weights (large weights for a large test). This abstraction procedure is largely linked to the multi-criteria decision making problem.

The various variables to be used for decision making are to be computed from the raw data, and the following items will be included in them: attendance times, delay times for submission, average scores for each category (report, and small test), etc.

Our system uses the weighted sum. The objective functions can be designed arbitrary by using the available variables. It is the same for the constraints. The final grading system will be decided by the tutor by various trials of grading.

The obtained system can be used in other ways for other purposes. It will be useful if we can see the difference of the students by their feature of scoring. We will apply Self-Organizing Map (SOM) for this purpose. SOM automatically shows us a map of the data on 2D plane based on the similarity of the high-dimensional data.

The order of the students can be decided by this MCDM setting, but we won't be able to see the difference of their features. Here we will develop a SOM to see the similarity and/or difference between students. SOM will make a link between the ranking by the MCDM framework and grouping of the students.

PREDICTION OF VARIABILITY OF DEMAND BASED ON DOMAIN KNOWLEDGE END EVENT MINING

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Keywords: prediction of demand variability, knowledge, event mining

1. ABSTRACT

The paper presents an approach to support decisions of supermarket managers concerning the preparation of fresh food dishes for current sale. While the real life problem is quite complex – the decisions of preparing fresh food dishes can be made adaptively through entire day of sales, some of fresh food dishes made in the evening can be stored until next day – we analyze here only a simplified problem of preparing beforehand a production plan of fresh food dishes for entire day. However, even such simplified problem has diverse methodological implications. These implications concern: the way of analyzing significant factors for demand prediction, the method of actual demand prediction, as well as the prediction of variability of demand and risk analysis including at least two asymmetric criteria of opportunity losses and for losses of food to be disposed, the method of multiobjective decision support for fresh food dishes production managers. We present in the paper a discussion of several aspects and approaches to address such methodological issues.

Simple demand prediction is not the full answer, because even if the supermarket making fresh food packages prepares a production plan equal to the demand prediction, it can still have losses because of variability of demand. The losses might result either of excess unsold products, or of the unused opportunities and unsatisfied customers that could not buy food because actual demand turned out to be higher than predicted. These losses are each of different character: it is easier to dispose of unsold food than to attract back unsatisfied customers, and the problem is whether the production plan should be slightly higher – and how much higher – than the demand prediction. Therefore, the problem is actually the *prediction of variability of demand* followed by multiple criteria (at least two criteria, but other aspects can be also taken into account) *decision support* of

the *production manager*. There are two parts of support:

- supporting the preparation of the production target or plan (it might include production targets for several products); shortly called *production plan preparation;*
- supporting the modifications of the production targets, if the actual demand differs much from the predicted one; shortly called *production plan modifications*.

We consider the practical case where only "hard" data on production and sales are available. We should thus take into account that data on sales underestimate actual demand if there were no losses due to food disposal (no remaining stocks of food) at the end of the day. We can count as directly relevant for demand and variability predictions only such days when there were food disposal losses (remaining stocks) at the days' end. However, there are diverse ways of unsold food disposal (preserving stocks of fresh food in refrigerators for a limited period of time is usually a viable option) that provide possibilities of adaptive minimization of losses of food to be disposed. Moreover, even if a certain type of fresh food is all sold out, the management can mark the time when it happens and estimate how large was the unsatisfied demand this day. Thus, all sales contain relevant data for demand estimation, they must be only appropriately interpreted, with active involvement of experienced management personnel.

To solve the problem presented above, we propose a new approach based on risk management and estimated probability distributions; we assume the following steps:

- a prediction of the demand,
- a prediction of the variability of demand,
- an application of the data on both, but particularly on variability, for decision support.

In the first step we concentrate on demand prediction. In our approach we support this phase by an analysis of a questionnaire survey aimed at managers of food processing. The goal of this introductory analysis is to explore on which aspects and elements the managers usually focus when making their production decisions. The knowledge from questionnaire survey is extracted by a technique of text mining. This type of analysis helps in finding important factors that should be considered when solving prediction problem. For example, it might be detected that the managers concentrate in their planning process on diverse regional and traditional national events, such as viewing cherry blossoms. Therefore, we can apply event based prediction of the desired level of production.

Concerning the variability, we assume the availability of statistical data on demand (appropriately upgraded if the fresh food was sold out) and the estimation of the probability distribution of demand, either in the form of an empirical histogram or its analytical approximation (by a normal or lognormal probability distribution).

For the decision support, we are considering two criteria:

- the value of lost food (unsold food that must be disposed of due to an overestimation of demand), say, measured as % of sales (either of total sales or of this particular type of food-box) and denoted by s;
- the value of lost opportunity of selling food (food not sold due to underestimation of demand – actually, a better index would be the number of unsatisfied customers, of cases that the customer does not find what she/he wants, but it is difficult to measure the actual number of customers), say, also measured as % of sales and denoted by q.

We assume that practical computations will be based on histograms of data. Let us use the following notation:

$\Delta d = (d_{up} - d_{lo})/n$, where d_{up} is the upper bound, d_{lo} – the lower bound of demand estimation, n is the number of equal size intervals in the histogram, thus Δd is the length of such interval;

$n(pt) = (d_{up} - pt)/\Delta d$ is the number of such intervals *above* the

production target *pt* (in which opportunity losses might occur);

$m(pt) = (pt - d_{lo})/\Delta d$ is the number of such intervals *below* the production target *pt* (in which losses of food to be disposed might occur).

Then the expected loss of opportunity of sales *q* given the production target *pt* can be denoted by $E(q,pt)$ and the expected loss of food to be disposed given the production target *pt* can be denoted by $E(s,pt)$; according to the definition of expected value, they can be computed as:

$$E(q,pt) = \int_0^{dup-pt} qp(q)dq = \sum_{i=0}^{n(pt)-1} \int_{i\Delta d}^{(i+1)\Delta d} p_i q dq = \frac{1}{2}(\Delta d)^2 \sum_{i=0}^{n(pt)-1}(2i+1)p_i$$

and similarly:

$$E(s,pt) = \int_0^{pt-dlo} sp(s)ds = \sum_{i=0}^{m(pt)-1} \int_{i\Delta d}^{(i+1)\Delta d} p_i s ds = \frac{1}{2}(\Delta d)^2 \sum_{i=0}^{m(pt)-1}(2i+1)p_i$$

where $dlo=d_{lo}$, $dup=d_{up}$, and $p_i = p(q_i)$ is the probability density in the interval $[pt+i\Delta d;\ pt+(i+1)\ \Delta d]$ or $p_i = p(s_i)$ is the probability density in the interval $[pt - i\Delta d;\ pt -(i+1)\ \Delta d]$ of the histogram (simply the probability density in the corresponding interval of the histogram).

When using expected values of losses, we can be certain that they are monotone with respect to the changes of *pt:* $E(q,pt)$ monotonically decreases with *pt* and $E(s,pt)$ monotonically increases with *pt.* The larger the interval $d_{up} - d_{lo}$, the higher will be expected losses - of both types, although the essence of the decision support here is first to give the decision maker enough information for making a compromise between these two types of losses.

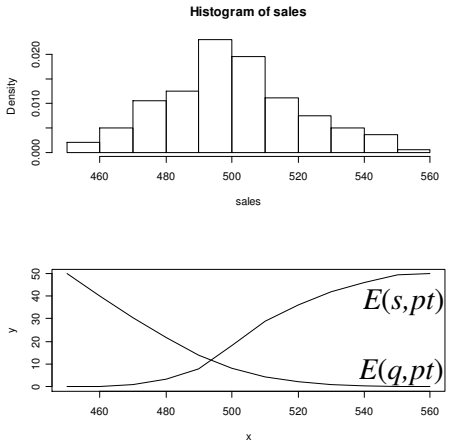

Fig. 1 The graph of the values of losses of opportunity of sales and of losses of disposed unsold food for number of samples equal to 200

Fig. 1 shows an example of the the graph of the *values* of losses of opportunity of sales $E(q,pt)$ (pt – is a production target) and of losses of disposed unsold food $E(s,pt)$. The equal values of $E(q,pt)$ and $E(s,pt)$ are around 495. The presented graph can be considered a tool for decision support. It can be used in two modes: for interactive decision making and in the process of decision automation. In the second case the user can provide additional preferences. It can be observed that such graph can be calculated even if histograms are based on a small amount of data.

MULTICRITERIA DECISION SUPPORT FOR PROBLEMS WITH NUMEROUS AND STRUCTURED CRITERIA

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Keywords: multicriteria optimization, decision support, reference point method, numerous structured criteria

1. PROBLEM

This paper elaborates on how to deal with multicriteria decision problems characterized by structured criteria. This problem is not new but no satisfactory solution procedure is known. For instance, in the case of discrete set alternatives with large number of criteria the AHP approach was utilized but no solution was found which properly addresses numerous criteria of different kinds (Solnes, 2003).

Let a set of decision alternatives $\mathbf{D}$ be known (either finite or infinite given implicitly by constraints) on which there is a defined set $\mathbf{C}$ of criteria numbered by i ($i \in \mathbf{I}$; $\mathbf{I} = \{1, 2, ..., i, ..., I\}$). Each criterion $c_i \in \mathbf{C}$ ($\mathbf{C} = \{c_1, c_2, ..., c_i, ..., c_I\}$) assigns a real value to each of decision alternatives, $c_i : \mathbf{D} \to R$. Criteria are are organized in a multilevel hierarchy $\mathbf{H}$. Values of those c_i which correspond to end nodes in the hierarchy are known. For all other nodes there is a need to define respective c_i functions. Indeed, for each criterion c_i from set of decision alternatives known for each of J_i existing subordinate nodes, that is of the form $c'_i : \mathbf{D} \to R^{J_i}$, where $c'_i(d) = (c_{j_1}(d), c_{j_2}(d), ..., c_{j_{J_i}}(d)),\ d \in \mathbf{D}$, it is necessary to convert to the form $c_i : \mathbf{D} \to R$. Performing the above defined task requires acquiring for each node (those which have subordinate nodes) a solution in "its" multicriteria space and presenting to the stakeholder to obtain guidelines considering preferences of the DM (decision maker).

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2. REFERENCE POINT METHOD

The Reference Point Method (RPM) is an interactive technique implementing the so-called quasi-satisficing approach to multiple criteria decision problems developed mainly by (Wierzbicki, 1982) as the reference point method. The reference point method was later extended to permit additional information from the DM and, eventually, led to efficient implementations of the so-called aspiration/reservation based decision support (ARBDS) approach with many successful applications (Lewandowski and Wierzbicki, 1989). The basic concept of the interactive scheme is as follows. The DM specifies requirements in terms of reference levels, i.e., by introducing reference (target) values for several individual outcomes. Depending on the specified reference levels, a special scalarizing achievement function is built which may be directly interpreted as expressing utility to be maximized. Maximization of the scalarizing achievement function generates an efficient solution to the multiple criteria problem. The computed efficient solution is presented to the DM as the current solution in a form that allows comparison with the previous ones and modification of the reference levels if necessary.

The RPM is based on the so-called augmented max-min aggregation of individual achievements, i.e. the worst individual achievement is essentially maximized but the optimization process is additionally regularized with the term representing the average achievement. This simple scalarization function performs very well for the limited number of criteria while deserving special reconstruction to take into account the multilevel structure of criteria.

3. RPM FOR NUMEROUS AND STRUCTURED CRITERIA

The concept of the solution process gets down to (iterative) execution of following tasks:

Algorithm 3.1: rpmnsc( )

for each $node$
  if $node$ has subordinate nodes
    then mark it as active
    else mark it inactive
repeat
  for each $node$ with all subordinates active
    establish function c_i (based on subordinate criteria, multicriteria methodologies, and interaction with a user)
    mark all subordinate nodes as inactive
    mark processed $node$ as active
until no $node$ with active subordinates exists

Appropriate identification of the preferences of the DM is a critical aspect of an optimization problem. The optimal solution is useless (sometimes even maleficent) if preferences of DM have been badly identified. In case of big number of criteria, the method identifying preferences has to consider limited time and patience of DM. Especially, that it has to be done for every non-end node separately. Free choice of method has to be limited to these, which save the DM a workload. One of such methods might be identification of DM's preferences based on 'sample' of DM preferences and the approximation preferences on set of all possible decision alternatives. In addition 'sample' itself should be prebuilt as much as possible on objective preference points (obtained without DM participation) to allow for a DM to point out his own preferences against the background of these objective ones in a relatively easy way. In other words, the method should define some rational solutions and its criteria values (objective satisfaction levels) and next should identify DMs opinion concerning points between those levels. Based on objective satisfaction levels and DM points, the approximation of preferences on the whole set of decision alternatives is possible to be done. Proposed method suggests usage of typical RPM achievement functions based on aspiration and reservation levels (Granat et.al., 2006) as well as a novel concept of the solidarity point. What is important is that the method can be used on every level of hierarchical structure criteria.

Further, the regularization by the average achievement is easily implementable but it may disturb the basic max-min model in the case of large number of criteria. The only consequent regularization of the max-min aggregation is the lexicographic max-min (nucleolar) solution concept where in addition to the worst achievement, the second worst achievement is also optimized (provided that the worst remains on the optimal level), the third worst is optimized (provided that the two worst remain optimal), and so on (Ogryczak, 2006). Although within the multilevel criteria structure rather an analytic approximation to the nucleolar regularization must be used.

In this work we focus on a case study which deals with alternatives from energy technologies domain characterized by economic, environmental, and social criteria. Two separate sets of alternatives are considered in this work. The first consists of about 50 general technology alternatives. The second one contains ca. 50 so called system expansion scenarios combining these technologies. It also is quite possible that by the way of specifying preferences stakeholder points restrictions which will appear to be a basis for definition of a new scenario. In general case process is iterative not only as it comes to specifying preferences but also in redefining the set of alternatives.

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MULTICRITERIA ANALYSIS FOR PROBLEM SOLVING: OPPORTUNITIES, PITFALLS, CHALLENGES

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Keywords: Multicriteria optimization, model-based decision-making support

1. CONTEXT

In any rational analysis of a complex problem the choice of a method is of critical importance because it predetermines to a large extent the scope (and in most cases the correctness) of analysis. Each analysis method is based on specific assumptions and supports only a certain type of analysis. A selected method must fit to the problem characteristics and the desired scope/features of analysis. This trivial observation is however often forgotten. Hammond, Keeney and Raiffa (2006) summarized the hidden traps in decision making and provided yet another guidelines for decision-making which in turn amplifies the principles of modern decision making discussed e.g., by Wierzbicki and Wessels (2000).

Policy makers and almost all industrial companies, research, educational and other organizations are faced with problems of finding a best compromise between conflicting goals, such as costs versus performance and reliability of products and technologies, and the time to bring them to the market, life-time costs versus environmental impacts, or economic growth versus intergeneration fairness of a pension system, spatial and temporal allocation of costs of climate change mitigation versus ex ante and/or ex post risk management. Making rational decisions for any complex problem requires various analyses of tradeoffs between conflicting goals (objectives, outcomes) that are used for measuring the results of applying various decisions in a wide range of application domains. Therefore multicriteria model analysis is a relevant and powerful tool for supporting rational decision-making. However, every powerful tool can either greatly help or hurt depending on either proper or improper implementation and use. Whether multicriteria analysis will provide opportunities or pitfalls for rational problem solving depends on a proper match between a model representation of the decision problem and the selected method(s) of model analysis.

There are countless successful applications of diverse multicriteria analysis methods, see e.g., (Wierzbicki, Makowski and Wessels, 2000). However, there are new applications, e.g., (Makowski, Granat, Schenler and Hirschberg, 2006), which require developments of new methods.

2. OPEN CHALLENGES

Wierzbicki (1977) proposed one of the most successful methodology for multicriteria analysis, namely scalarizing functions. Actually, as shown by Makowski (1991), basic properties of each of the most commonly used multicriteria methods can be analyzed by examination of the corresponding scalarizing function. We will use this powerful methodology to discuss the challenges of the problem specified by Makowski et al. (2006), to which none of the known methods[1] can be successfully applied, see (Granat and Makowski, 2006) for the justification.

Two key challenges will discussed in more detail. First, is due to the large number (about 50) of criteria organized in a hierarchical structure. It is commonly agreed, see e.g., (Miller, 1956), that humans are able to process only several issues at a time. Therefore a new approach is needed for analysis of problems characterized by large number of criteria. The second challenge is caused by the multimodal distributions of criteria val-

[1] A new approach currently under development will be presented by B. Kozłowski and W. Ogryczak in the same session of the 23rd IFIP TC 7 Conference.

ues which causes many problems with applications of methods successful in analysis of problems having more regular distributions of criteria values, e.g., aspiration-reservation based multicriteria analysis by Granat and Makowski (2000).

3. CONCLUSIONS

Rational decision making is always based on a combination of knowledge, experience, and intuition. Models can represent a relevant part of knowledge, and appropriate methods of model analysis augment experience and intuition in the decision making process. However, one should never forget that there is no simple solution for any problem, which is truly complex. Thus a well organized modeling process can substantially help in finding better solutions but actually the final choice is always made by a decision maker. Development of models for complex problems does, and will, require various elements of science, craftsmanship, and art (see, e.g. (Makowski and Wierzbicki, 2003) for a collection of arguments that supports this statement). This presentation aims at contributing to a better understanding of open challenges that need to be addressed in order to successfully support the new class of decision problems currently analyzed for supporting European energy policy-making.

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OBJECTIVE CLASSIFICATION OF EMPIRICAL PROBABILITY DISTRIBUTIONS AND THE ISSUE OF EVENT DETECTION

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Keywords: objective classification, event detection, multicriteria analysis.

ABSTRACT

While practically all multiple criteria approaches to decision analysis and support concentrate on rationally supporting *subjective* decisions, depending on some form of an elicitation of preferences of the decision maker, there are diverse decision situations where we should suggest decisions that are made *as objectively as possible;* the full objectivity is not attainable for many practical and philosophical reasons, but objectivity can be seen as an useful ideal or goal. Examples of such situations are, on the one hand, managerial decisions influencing many stakeholders, when an aggregation of preferences of stakeholders is impossible. On the other hand, such situations occur also in event detection; e.g., when automatically detecting a case of fire, we should not make decisions based on subjective, personal preferences. We shall call the problem of supporting decisions in such a case the problem of *objective classification* (treating problem of *ranking* as a special case with singleton classes and the problem of *decision selection* and *detection* as special cases with classes *selected – not selected* or *detected – not detected*). We can define objective classification as dependent only on a given set of data, relevant for the decision situation, and independent from any more detailed specification of personal preferences than that given by defining criteria and the partial order in criterion space. Already in this definition, we see the limits to objectivity, because naturally the definition of criteria and their partial order, or of the relevant set of data, can be treated as subjective; however, they are often much more obvious and easy to agree upon than the detailed preferences defined, e.g., by a utility function or a set of weighting coefficients.

Most of classical approaches to multiple criteria decision analysis and support, e.g., based on weighted sum aggregation, are not easily adaptable to the case of objective classification. From known approaches, either the goal programming or the reference point approaches are easily adaptable, because goals or reference points can be defined reasonably objectively from statistics in a given set of data. We concentrate here on reference point approaches, because they have the property of producing always Pareto optimal options (which is not the case in goal programming). The paper reviews the properties of reference point approaches

which make them useful for objective classification.

The paper concentrates on the issue of classification of empirical probability distributions (histograms), which is useful both in management situations and in event detection or event mining. While existing approaches to event detection concentrate on the use of selected moments or other characteristics of empirical probability distributions, we postulate that full empirical distribution preserves more of needed information then selected moments of this distribution, thus multiple criteria classification of distributions can be most effective in event detection. One of advantages of reference point approaches is that they easily deal with so-called *multiobjective trajectory* analysis and optimisation; this can be applied to issues of stochastic dominance and their generalisations needed for multiple criteria event detection based on classification of empirical probability distributions. The paper presents also examples of classes of practical event detection problems in which such formulation is useful.

A COMPUTATIONAL APPROACH TO ESSENTIAL AND NONESSENTIAL OBJECTIVE FUNCTIONS IN LINEAR MULTICRITERIA OPTIMIZATION

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Keywords: optimization, multicriteria programs, efficient (Pareto-optimal) solutions, essential/nonessential objective functions, computer code in Maple

1. INTRODUCTION

In this paper we study the following linear vector optimization problem:

$$\text{Max}\left\{\mathbf{F}^n(\mathbf{x}) = \mathbf{C}\mathbf{x} : \mathbf{x} \in \mathbf{X}\right\}, \qquad \text{(P)}$$

where $\mathbf{X} = \left\{\mathbf{x} \in \mathbf{R}^k : \mathbf{A}\mathbf{x} \leqq \mathbf{b}, \mathbf{x} \geq \mathbf{0}\right\}$ is the feasible set; and

$$F^n(\mathbf{x}) = \left[\left(\mathbf{c}^1\right)^T \mathbf{x}, \ldots, \left(\mathbf{c}^n\right)^T \mathbf{x}\right]^T, \mathbf{c}^i \in \mathbf{R}^k \, (i = 1, \ldots, n)$$

(n>1) is a vector-valued function. Each f_i $(i = 1, \ldots, n)$ is called an objective function. Problem (P) consists to find all the solutions that are efficient in the sense of the following definition.

Definition 1.1. A vector $\mathbf{x}^0 \in X$ is said to be an efficient (Pareto-optimal) solution of problem (P) if and only if there exists no $\mathbf{x} \in X$ such that $\mathbf{F}^n(\mathbf{x}) \geq \mathbf{F}^n(\mathbf{x}^0) \Leftrightarrow$
$\forall i \in \{1, .., n\} f_i(\mathbf{x}) \geq f_i(\mathbf{x}^0) \wedge \exists i \in \{1, .., n\} f_i(\mathbf{x}) > f_i(\mathbf{x}^0)$.
The set of efficient solutions of problem (P) is denoted by X_E^n.

We form a new vector optimization problem (P') adding an objective function f_{n+1} to problem (P). If the set of efficient solutions of problem (P) equals that of (P'), then the objective function f_{n+1} is said to be nonessential.

Information about nonessential objectives gives insights to a decision maker and helps to understand better the problem. This might be a good starting point for further investigations or revision of the mathematical model. Dropping nonessential functions leads to a problem with a smaller number of objectives, which then can be solved more easily. For this reason, the identification of nonessential objectives is an important issue to be used in conditioning and analysis of multiple criteria programs (Gal and Hanne, 1999, 2006; Malinowska, 2002).

In this paper we put together two methods (Gal and Leberling, 1977; Malinowska, 2006) for determining nonessential objective functions. A computational implementation is done using the computer algebra system Maple. The outline of the paper is as follows: in Sec.2 we develop the theory of nonessential objectives. Section 3 is devoted to the main result of the paper: the algorithm to determine if a given objective function of a linear problem is essential or nonessential. Finally, we provide some examples that show the applicability of our methodology and the convenience of the developed computer software. The paper ends with some conclusions.

2. NONESSENTIAL OBJECTIVES

Let X_E^{n+1} denote the set of solutions of the problem

$$\text{Max}\{\mathbf{F}^{n+1}(\mathbf{x}) = \mathbf{C}'\mathbf{x} : \mathbf{x} \in \mathbf{X}\}, \qquad \text{(P')}$$

where $\mathbf{C}' = \left[\left(\mathbf{c}^1\right)^T, ..., \left(\mathbf{c}^{n+1}\right)^T \right]^T$.

Definition 2.1. The objective function f_{n+1} is said to be nonessential in (P') if $X_E^n = X_E^{n+1}$. An objective function which is not nonessential is called essential.

Theorem 2.2. (Gal and Leberling, 1977) The objective function f_{n+1} is nonessential in (P') if the following holds:

$$\mathbf{c}^{n+1} = \sum_{i=1}^{n} \alpha_i \mathbf{c}^i, \alpha_i \geq 0, (i = 1, ..., n).$$

Theorem 2.3. (Malinowska, 2002). Let the set X be nonempty and bounded. The objective function f_{n+1} is nonessential in (P') if, and only if, the following three conditions hold:

(i) $\forall \mathbf{x} \in \mathbf{X} \setminus \mathbf{X}_E^n \; \exists \mathbf{x}' \in \mathbf{X} \;\; \mathbf{F}^{n+1}(\mathbf{x}') \geq \mathbf{F}^{n+1}(\mathbf{x})$;

(ii) $\mathbf{X}_E^n \cap \mathbf{X}_{n+1} \neq \emptyset$, where

$\mathbf{X}_{n+1} = \{\mathbf{x}^0 \in \mathbf{X} : \forall \mathbf{x} \in \mathbf{X} \; f_{n+1}(\mathbf{x}^0) \geq f_{n+1}(\mathbf{x})\}$;

(iii) $\mathbf{X}_E^n \subset \mathbf{X}_E^{n+1}$.

3. MAIN RESULT

The theory in the previous section enables us to work out a computational algorithm to test if an objective function of a linear problem is essential or not. The algorithm can be summarized by the following steps:

Step 0. Is there $\mathbf{c}^{n+1} = \sum_{i=1}^{n} \alpha_i \mathbf{c}^i, (\alpha_i \geq 0)$? If the answer is "TRUE", then the objective function f_{n+1} is nonessential by Theorem 2.2. Otherwise we go to Step 1.

Step 1. Is there $U' = \{\mathbf{u} \in \mathbf{R}^k : \mathbf{C}'\mathbf{u} \geq \mathbf{0}\} = \emptyset$? If the answer is "FALSE", then $X_E^{n+1} = X$ and we go to Step 2. Otherwise we know that condition (i) of Theorem 2.3 holds and we go to Step 5.

Step 2. Does $U = \{\mathbf{u} \in \mathbf{R}^k : \mathbf{C}\mathbf{u} \geq \mathbf{0}\} = \emptyset$? If the answer is "FALSE", then $X_E^n = X$ and function f_{n+1} is nonessential. Otherwise we go to Step 3.

Step 3. Does $\text{int}\mathbf{X} \neq \emptyset$? If the answer is "TRUE", then $X_E^n = X$, and the objective function f_{n+1} is essential. Otherwise we go to Step 4.

Step 4. Does $\mathbf{X}_E^n = \mathbf{X}$? If the answer is "FALSE", objective function f_{n+1} is essential. Otherwise f_{n+1} is nonessential.

Step 5. Does $\mathbf{X}_E^n \cap \mathbf{X}_{n+1} \neq \emptyset$? If the answer is "TRUE", then condition (ii) of Theorem 2.3 holds and we go to Step 6. Otherwise the objective function f_{n+1} is essential.

Step 6. Does $\mathbf{X}_E^n \subset \mathbf{X}_E^{n+1}$? If the answer is "TRUE", then the objective function f_{n+1} is nonessential.

We have implemented each one of the above steps in the computer algebra system Maple. Below we give an example of a simple computer session with our Maple package.

```
>nonessential([x1+x2+x3,
  -x1+x2+x3,x1+x2],{x1<=1,x2<=1,x3<=1});
  Objective x1+x2 is nonessential from step 7.
>nonessential([x1+3*x2,3*x1,
          -3*x1-x2,2*x1+x2],{});
 Objective 2*x1+x2 is nonessential from step 0.
>nonessential([x1+3*x2,2*x1+x2,3*x1,
          -3*x1-x2],{x1<=1,x2<=1});
   Objective -3*x1-x2 is essential from step 3.
```

4. CONCLUSIONS

There are theoretical and practical reasons for developing a method to find if a given objective function is nonessential. In this paper we present such a method and its implementation in Maple. Our algorithm is based on necessary and sufficient conditions for an objective function to be nonessential, and need only to solve a finite number of single objective linear optimization problems.

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INVESTIGATION INTO DEA-ORIENTED PERFORMANCE ASSESSMENT IN THE DOMAIN OF MOLP

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Keywords: Data envelopment analysis, multiple criteria decision analysis, minimax method, efficient frontier, performance assessment

1. INTRODUCTION

MCDA in general and multiple objective linear programming (*MOLP*) in particular can be used for planning future performances. The model structures of *DEA* and *MOLP* have much in common and research on integrating *DEA* and *MOLP* has attracted increasing attentions to support both past performance assessment and future target setting in integrated manners (Cooper, 2004). For instance, Golany (1988) developed an interactive model to allocate a set of input levels as resources and to select the most preferred output levels from a set of alternative points on the efficient frontier. Post and Spronk (1999) combined the use of *DEA* and interactive goal programming to adjust the upper and lower feasible boundaries of the input and output levels. Joro et al (1998, 2003) showed the structural similarity between *DEA* and *MOLP*.

Interactive *MCDA* methods have been investigated to incorporate the *DM*'s preference information into performance assessment and target setting without necessarily requiring *prior* judgments (Yang et al 2006) using the minimax formulations and the gradient projection method (Yang, 1999, 2001; Yang and Li, 2002). Three minimax models have been explored, all equivalent to the output-oriented *CCR* dual model in *DEA* and different from each other in their reference points and weighting schemas, namely the super-ideal point model, the ideal point model and the shortest distance model. The super-ideal point model is shown identical to the output-oriented *CCR* dual model under certain conditions and can be used to conduct efficiency analysis in the same way as the *CCR* model does. Based on the equivalence analysis, a generic *MOLP* formulation is constructed, in which the features of data envelopes, efficient frontiers and efficiency measures can be explored, which is the theme of this paper.

To conduct trade-off analysis along an efficient frontier, it is fundamental to understand its features. Based on our current research and recent literature survey, the graphical illustrations and interpretations of efficient frontiers in *DEA* are limited to simple problems having one input with single multiple outputs, or one output with multiple inputs (Cooper et al, 2000; Joro et al, 2003). There seems to be a lack of means for generating and interpreting data envelopes and efficient frontiers for *DEA* problems with multiple inputs and outputs. Without understanding the features of data envelopes and efficient frontiers, it would difficult to develop appropriate procedures and methods to conduct integrated efficiency and trade-off analyses.

This paper is dedicated to investigating graphical and analytical methods and procedures in *MCDA* for generating and analysing data envelopes and efficient frontiers for *DEA* problems with any numbers of inputs and *DMU*s and with up to three outputs. The investigation is conducted in the dual decision and objective

spaces and provides interesting insight into data envelopes, efficiency measures and efficient frontiers for DEA problems having multiple inputs and outputs, leading to the definitions of efficiency measures including a new technical efficiency score (*TES*) and preferred efficiency score (*PES*). *TES* provides a revised performance measure in situations where the conventional *DEA* efficiency measure seems not appropriate to use. *PES* provides a logical measure between the observed *DMU* and its most preferred efficient solution, showing the extent to which the observed *DMU* needs to improve its performances to achieve the most preferred solution. Several numerical examples are studied to illustrate the findings graphically and to generate analytically data envelopes and efficient frontiers for *DEA* problems of practical size. A case study for UK retail banks is conducted using the investigated methods and procedures.

2. MAIN FINDINGS

The findings reported in this paper show that *DEA*-oriented performance assessment and target setting are in essence MCDA problems and can be dealt with using various *MCDA* methods. This is useful to support the design of pragmatic trade-off analysis processes and performance measures for setting future targets with decision makers' preferences taken into account. As a result of the investigation, the new technical efficiency score (*TES*) and preferred efficiency score (*PES*) were defined. The former provides a revised measure in cases where the conventional *DEA* efficiency measure becomes inappropriate to use; the latter can be used to measure the degree to which the observed *DMU* needs to improve its performance to achieve the most preferred target. The numerical examples and case study demonstrated these findings both graphically and analytically, which can help better understand the efficiency analysis and trade-off analysis for performance management.

3. CONCLUDING REMARKS

In this paper, the graphical and analytical methods and procedures were investigated using concepts, models and techniques in MCDA for generating and analysing data envelopes and efficient frontiers for DEA problems with any numbers of inputs and DMUs and with up to three outputs. The investigation generated interesting insights into the integrated efficiency and trade-off analyses and revealed some features of data envelopes and efficient frontiers which leads to the definition of new efficiency measures. Several numerical examples are studied to illustrate the findings graphically. A case study for UK retail banks is conducted in detail using the methods and procedures investigated in this paper. This study shows that DEA is in essence is a kind of MCDA problem and that DEA-oriented performance assessment and target setting can be interpreted and integrated in the domain of MCDA.

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A Factorization Method for a Singular Perturbation Problem

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Keywords: Elliptic boundary value problem; Factorization; Riccati equation; Invariant embedding; Singular perturbations

1. INTRODUCTION

We want to solve problems on cylinders $\Omega^\varepsilon =]0,a[\times\mathcal{O}^\varepsilon$ in $\mathbb{R}^d$, with $\mathcal{O}^\varepsilon = \varepsilon\mathcal{O}$ and $\mathcal{O}$ a bounded open set in $\mathbb{R}^{d-1}$ ($d = 2$ or 3 in real applications). Parameter ε denotes that the section $\mathcal{O}^\varepsilon$ is much smaller than the length of the axis a. We denote $\Gamma_s^\varepsilon = \{s\} \times \mathcal{O}^\varepsilon$, the lateral boundary of the cylinder $\Sigma^\varepsilon =]0,a[\times\partial\mathcal{O}^\varepsilon$ and a general point $(x_1^\varepsilon, x_2^\varepsilon, \cdots, x_d^\varepsilon) \in \Omega^\varepsilon$ is also denoted by $(x^\varepsilon, y^\varepsilon)$, where $x^\varepsilon = x_1^\varepsilon$ and y^ε denotes the independent variables $(x_2^\varepsilon, ..., x_d^\varepsilon)$. Let $f \in L^2(\Omega^\varepsilon)$, $u_0 \in H^{1/2}(\mathcal{O}^\varepsilon)$, $u_a \in H^{1/2}(\mathcal{O}^\varepsilon)'$ and λ be a positive constant. The problem we want to solve is

$$\begin{cases} -\Delta u + \lambda u = f & \text{in } \Omega^\varepsilon, \\ \dfrac{\partial u}{\partial \nu} = 0 & \text{on } \Sigma^\varepsilon, \\ u = u_0 & \text{on } \Gamma_0^\varepsilon, \\ \dfrac{\partial u}{\partial x} = u_a & \text{on } \Gamma_a^\varepsilon, \end{cases} \tag{1}$$

where ν represents the outward normal vector on the boundary.

The aim of this work is to study the asymptotic behavior of the solution when $\varepsilon \to 0$. We do first a change of variable so that the new domain is the same for all $\varepsilon > 0$. We consider the domain given by the cylinder $\Omega =]0,a[\times\mathcal{O}$ and the change of variable $(x^\varepsilon, y^\varepsilon) = (x, \varepsilon y)$. Therefore, in the new variables (x, y) (1) can be re-written equivalently by

$$\begin{cases} -\dfrac{\partial^2 u}{\partial x^2} - \dfrac{1}{\varepsilon^2}\Delta_y u + \lambda u = f & \text{in } \Omega, \\ \dfrac{\partial u}{\partial \nu} = 0 & \text{on } \Sigma, \\ u = u_0 & \text{on } \Gamma_0, \\ \dfrac{\partial u}{\partial x} = u_a & \text{on } \Gamma_a, \end{cases} \tag{2}$$

2. FACTORIZATION BY INVARIANT EMBEDDING

Factorizing problem (2) by invariant embedding techniques as in Henry et.al (2004b) and Henry et.al (2004a), we arrive to the uncoupled system:

$$\begin{cases} -\dfrac{dQ}{dx} + Q^2 = \lambda I + \dfrac{1}{\varepsilon^2}\mathcal{A}, \\ Q(a) = 0 \end{cases} \tag{3}$$

$$\begin{cases} -\dfrac{dw}{dx} + Qw = -f, \\ w(a) = -u_a \end{cases} \tag{4}$$

$$\begin{cases} \dfrac{du}{dx} + Qu = -w, \\ u(0) = u_0, \end{cases} \tag{5}$$

where $(\mathcal{A}h, \varphi) = (\nabla_y h, \nabla_y \varphi) \ \forall\, h, \varphi \in H^1(\mathcal{O})$. $\mathcal{A}$ is the abstract operator corresponding to Neumann boundary conditions for the laplacian.

3. SINGULAR PERTURBATIONS

Let $e_0, e_1, \ldots, e_n, \ldots$ be an orthonormal basis (with respect to the $L^2(\mathcal{O})$ norm) of eigenvectors of $\mathcal{A}$ in the following sens

$$\begin{cases} -\Delta_y e_i = \lambda_i e_i, & \text{in } \mathcal{O} \\ \frac{\partial e_i}{\partial \nu} = 0, & \text{on } \partial\mathcal{O} \end{cases}$$

Let $\mathcal{W}^r$ be the space defined by

$$u = \sum_{i=1}^{+\infty} u_i\, e_i \in \mathcal{W}^r \leftrightarrow \|u\|^2_{\mathcal{W}^r} = \sum_{i=1}^{+\infty} \lambda_i^r\, |u_i|^2 < +\infty$$

We consider the formal development

$$Q = \varepsilon^{-1} Q_{-1} + Q_0 + \varepsilon Q_1 + \varepsilon^2 Q_2 + \cdots,$$

with Q_i, $i = -1, 0, 1, \cdots$, self-adjoint and non-negative. We also decompose Q_i, fo $i \geq 0$, as

$$Q_i \varphi = \begin{pmatrix} Q_i^{aa} & Q_i^{ab} \\ Q_i^{ba} & Q_i^{bb} \end{pmatrix} \begin{pmatrix} \varphi^a \\ \varphi^b \end{pmatrix},$$

with

$$\begin{aligned} Q_i^{aa} &: \mathcal{W}^1 \to L^2(\mathcal{O})/\mathbb{R} \\ Q_i^{ab} &: \mathbb{R} \to L^2(\mathcal{O})/\mathbb{R} \\ Q_i^{ba} &: \mathcal{W}^1 \to \mathbb{R} \\ Q_i^{bb} &: \mathbb{R} \to \mathbb{R}. \end{aligned}$$

We obtain the following results:

$$\begin{gathered} Q_{-1} = Q_{-1}^{aa} = \mathcal{A}^{1/2}, \\ w_{-1} = 0, \\ Q_0 = Q_0^{bb}(x) = \sqrt{\lambda}\tanh(\sqrt{\lambda}(a-x)), \\ w_0(x) = w_0^b(x) = \\ \frac{u_a^b}{\cosh(\sqrt{\lambda}(a-x))} - \frac{f^b}{\sqrt{\lambda}}\tanh(\sqrt{\lambda}(a-x)), \\ Q_1 = Q_1^{aa} = \tfrac{\lambda}{2}\mathcal{A}^{-1/2}, \\ w_1(x) = w_1^a(x) = -\mathcal{A}^{-1/2} f^a, \\ Q_2 = 0, \\ w_2(x) = w_2^a(x) = -\mathcal{A}^{-1}\tfrac{d}{dx} f^a, \\ Q_3 = Q_3^{aa} = \tfrac{\lambda^2}{8}\mathcal{A}^{-3/2}, \\ w_3(x) = w_3^a(x) = -\mathcal{A}^{-3/2}\tfrac{d^2}{dx^2} f^a + \tfrac{\lambda}{2}\mathcal{A}^{-3/2} f^a. \end{gathered}$$

As one can see, all the tranverse operators Q_i^{ab} and Q_i^{ba} are zero and all the Q_i only dependent on y except Q_0 that only dependent on x.

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FACTORIZATION BY INVARIANT EMBEDDING OF A SECOND ORDER ELLIPTIC OPERATOR

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Keywords: Factorization, Riccati equation, invariant embedding.

1. INTRODUCTION

This work concerns the factorization of elliptic operators, namely the decomposition of a second order elliptic boundary value problem, defined in an open bounded regular domain, in a system of uncoupled first order initial value problems, using the technique of invariant embedding. The method presented here is a return, in a new spatial approach, to the technique of the invariant temporal embedding, defined originally in the context of Dynamic Programming and used in Control Theory for the computation of the optimal feedback.

2. FACTORIZATION BY INVARIANT EMBEDDING

The invariant embedding technique consists in embedding the initial problem in a family of similar problems depending on a parameter, which are solved recursively. In our approach, each problem is defined over a sub-domain limited by a mobile boundary (see Fig 1), depending on the parameter. Defining an operator relating the value of the solution, or its derivative, with the mobile boundary condition, we find a family of operators on functions of the section satisfying a Riccati equation and relating the boundary conditions on the section (Dirichlet-Neumann or Neumann-Dirichlet, for example).

For a given problem, this invariant embedding method is not unique: for instance we can apply the method either to the family of subdomains described above, either to the family of complementary subdomains; also, it is possible to change the type of condition that we impose over the mobile boundary. Without loss of generality, here we particularize the study to a Poisson equation with a Dirichlet boundary condition: $-\Delta u = f$, in Ω, $u_{|\Gamma a} = 0$. We present the case where the family of curves which limits the subdomains defined by the invariant embedding are homothetic to one another and homothetic to a point, and we consider the moving boundary starting on the outside boundary of the domain and shrinking to a point. We show some results dealing with the singularity that will appear at that point.

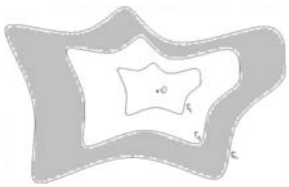

Fig. 1. Invariant embedding in a star shaped domain.

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The computing zoom : method and experimentation

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The invariant embedding technique was devised by R Bellman in the context of optimal control theory to derive the optimal feedback. In many practical situations in the simulation of partial differential equation, we are interested to analyse the solution of the problem more precisely in a particular smaller subdomain of the original domain, so it is desirable to zoom the solution of the problem in a particular region of the domain. Keeping in view this situation, here we apply the same idea of the invariant embedding spacewise for linear elliptic boundary value problems : The original problem in a starlike domain is now embedded in a family of similar problems in smaller domains defined by homothety. Suppose we are interested in the solution only on one of the smaller subdomains : the region of interest. The invariant embedding technique furnishes operators on the boundaries of these homothetic domains (similar to the optimal feedback in the control problem) which relate Dirichlet and Neuman data on the boundary. It provides a boundary condition on the boundary of the region of interest such that the solution of the related problem is exactly the restriction of the solution of the original problem to the domain of interest. The problem solved on the region of interest with the same number of unknowns as the original one will yield a better precision on this domain (region of interest) : this is the zooming effect. Numerical simulations in the framework of P1 finite elements are carried out to demonstrate the method.

QR like factorization for elliptic boundary value problems

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Keywords: Elliptic boundary value problem; Factorization; Riccati equation; Invariant embedding; QR factorization

1. INTRODUCTION

We consider a cylinder $\Omega =]0,1[\times\mathcal{O}$ in $\mathbb{R}^n$, with $\mathcal{O}$ a bounded open set in $\mathbb{R}^{n-1}$. We denote $\Gamma_s = \{s\} \times \mathcal{O}$, the lateral boundary of the cylinder, $\Sigma =]0,1[\times\partial\mathcal{O}$ and a general point $(x, y_1, \cdots, y_{n-1}) \in \Omega$ is also denoted by (x, y), where y denotes the independent variables $(y_1, \cdots, y_{n-1})$. Let $L_y = -\sum_{i,j=1}^{n-1} a_{ij} \frac{\partial^2}{\partial y_i \partial y_j}$ be such that $L = -\frac{\partial^2}{\partial x^2} + L_y$ is a strongly elliptic operator. Let $f \in L^2(\Omega)$, $u_0 \in H^{1/2}(\mathcal{O})$, $u_1 \in H^{1/2}(\mathcal{O})'$. The problem we want to solve is

$$\begin{cases} Lu = f & \text{in } \Omega, \\ u = 0 & \text{on } \Sigma, \\ -\frac{\partial u}{\partial x} = u_0 & \text{on } \Gamma_0, \\ u = u_1 & \text{on } \Gamma_1 \end{cases} \tag{1}$$

We prove that problem (1) can be factorized as

$$-\left(\frac{d}{dx} + Q\right)\left(\frac{d}{dx} - Q\right)u = f \tag{2}$$

each of the first order problems having an initial value at $x = 0$ or $x = 1$. The operator Q satisfies the Riccati equation (3)

2. FACTORIZATION BY INVARIANT EMBEDDING

Factorizing problem (1) by invariant embedding techniques as in Henry et.al (2004), we arrive to the uncoupled system:

$$\frac{dQ}{dx} + Q^2 - L_y = 0, \qquad Q(0) = 0. \tag{3}$$

$$\frac{dw}{dx} + Qw + f = 0, \qquad w(0) = -u_0. \tag{4}$$

$$\frac{du}{dx} = Qu + w, \qquad u(1) = u_1. \tag{5}$$

The present work intends to generalize results obtained by Henry (2003) to some second order strongly elliptic operators not necessarily symetric.

In order to obtain a QR like factorization, we consider the problem

$$\begin{cases} L^2u = Lf & \text{in } \Omega, \\ u = Lu = 0 & \text{on } \Sigma, \\ -\frac{\partial u}{\partial x} = u_0, \quad \frac{\partial (Lu)}{\partial x} = \frac{\partial f}{\partial x}, & \text{on } \Gamma_0, \\ u = u_1, \quad Lu = f & \text{on } \Gamma_1 \end{cases} \tag{6}$$

which we prove to be equivalent to problem (1).

Acting like before, we obtain the uncoupled system:

$$\frac{dQ}{dx} + Q^2 - L_y = 0, \qquad Q(0) = 0. \tag{7}$$

$$\frac{dP}{dx} + PQ + QP + I = 0, \qquad P(0) = 0. \tag{8}$$

$$\frac{dt}{dx} + Qt + Lf = 0, \qquad t(0) = \frac{\partial f}{\partial x}|_{\Gamma_0}. \tag{9}$$

$$\frac{dr}{dx} + Qr + Pt = 0, \qquad r(0) = -u_0. \tag{10}$$

$$\frac{du}{dx} - Qu - PLu - r = 0, \qquad u(1) = u_1. \tag{11}$$

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A robust extension of the Kalman filter for parabolic systems in the deterministic framework

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Keywords: Kalman filtering

We consider the invariant embeding technique for deriving the Kalman filter for parabolic systems in the deterministic framework. We refer to (1) for the description of the filtering problem in a determistic context as a control problem, where the controls are the initial condition and the input perturbation. The invariant embedding technique applied to the optimality system gives rise to the Riccati equation for the gain of the filter and the equation of the state estimate. This can be viewed as a LU factorization of the optimality system. Here we show that a QR like factorization of the optimality system yields a new version of the Kalman filter equations which is more robust in the sense that it is less sensitive to mismodeling.

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Cross Gramians for Nonlinear Systems

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Keywords: gradient systems, cross Gramian, Sylvester equation, Hankel singular values.

1. INTRODUCTION

We aim at extending the approximate balancing method presented in (Sorensen et al., 2002; Aldaheri, 1991). It deals with model reduction for linear symmetric systems in an efficient way, based on solving a Sylvester equation whose solution is the so-called cross-Gramian (e.g. see (Fernando et al., 1983)). The eigenvalues of the cross Gramian are the Hankel singular values of the system. The advantages of this method, in comparison to the usual balancing procedure, are that it requires solving only one Sylvester equation and that it avoids the balancing procedure, being more efficient from computational point of view.
We study the notion of cross Gramians for nonlinear gradient systems, which are the extension of the notion of symmetric systems. We use the prolongation and gradient extension associated to the gradient system, as in (Cortes et al., 2005). The cross Gramian is given for the variational system (part of the prolongation) associated to the original nonlinear gradient system. We obtain linearization results that precisely correspond to the notion of a cross Gramian for symmetric linear systems. Furthermore, starting from the work in (Fujimoto et al., 2005), first steps towards relations with the singular value functions of the nonlinear Hankel operator are studied and yield promising results.

2. LINEAR SYSTEMS CASE

Definition 1 (Sorensen et al., 2002) The cross Gramian X of a linear system $\dot{x} = Ax + Bu,\ y = Cx$, is defined as the solution of the Sylvester equation:

$$AX + XA + BC = 0. \tag{1}$$

If the system is asymptotically stable, then :

$$X = \int_0^\infty e^{At} BC e^{At} dt.$$

□

Definition 2 (Aldaheri, 1991) A linear system is symmetric if and only if $H(s) = H^T(s)$, where $H(s) = C(sI - A)^{-1}B$, or equivalently, there exists T, invertible and symmetric s.t.

$$TA = A^T T,\ TB = C^T.$$

□

The cross Gramian has some interesting properties:

Theorem 3 (Sorensen et al., 2002) If the linear system is symmetric, asymptotically stable and minimal (controllable and observable), then:

$$X = T^{-1}M = WT \text{ and } X^2 = WM,$$

where $M > 0,\ W > 0$ are the observability and controllability Gramians, respectively. □

3. GRADIENT SYSTEMS AND LINEARIZATION

Definition 4 (Cortes et al., 2005) A nonlinear affine system

$$\begin{cases} \dot{x} = f(x) + g(x)u \\ y = h(x) \end{cases}, x \in M,\ u, y \in \mathbb{R}^p \tag{2}$$

is called a gradient system if,

1. there exists a pseudo-Riemannian metric on the manifold M, with the associated matrix $G(x)$, symmetric and invertible for all $x \in M$;
2. there exists a smooth potential function $V : M \to \mathbb{R}$,

such that (2) can be written as:

$$\begin{cases} \dot{x} = -G^{-1}(x)\dfrac{\partial^T V}{\partial x}(x) + G^{-1}(x)\dfrac{\partial^T h}{\partial x}(x)u \\ y = h(x) \end{cases} \tag{3}$$

□

For the nonlinear system two associated systems are defined:

- the prolongation :

$$\begin{cases} \dot{x} = f(x) + g(x)u \\ \dot{v} = \dfrac{\partial f(x)}{\partial x}v + \displaystyle\sum_{j=1}^{m} u_j \frac{\partial g_j(x)}{\partial x}v + g(x)u_p \\ y = h(x),\ y_p = \dfrac{\partial h(x)}{\partial x}v \end{cases}, \tag{4}$$

- the gradient extension:

$$\begin{cases} \dot{x} = f(x) + g(x)u \\ \dot{p} = \dfrac{\partial^T (f(x) + g(x)u)}{\partial x}p \\ +\mathcal{F}(g_{ij}(x), \frac{\partial g_{ij}(x)}{\partial x_k}, f_k(x), p) + \dfrac{\partial h(x)}{\partial x}u_g, \\ y = h(x),\ y_g = g^T(x)p,\ i,j,k = 1...n \end{cases} \tag{5}$$

Theorem 5 (Cortes et al., 2005) Let (2) be locally observable. Assume that (5) exists and is well defined. Then, under additional technical conditions, (2) is a gradient control system, as in (3), if and only if the prolonged system Σ_p and the gradient extension Σ_g have the same input-output behaviour. □

Lemma 6 (Cortes et al., 2005, Lemma 5.5, 5.6) If (2) is a gradient control system, then there exists a diffeomorphism $\phi(x, v) = (x, G(x)v)$, such that $(x, p) = \phi(x, G(x)v)$. □

Linearizing (3), around an equilibrium x_0, a linear gradient (symmetric) system is obtained, whose metric is $T = G(x_0)$. Assume that the observability function and the controllability function of (2), $L_o(x)$ and $L_c(x)$, respectively, exist and are positive definite. Also, suppose that the observability Gramian M and the controllability Gramian W of the linearized system exist and are positive definite. Then $(\partial^2 L_o(x)/\partial x^2) = M$ and $(\partial^2 L_c(x)/\partial x^2) = W^{-1}$. The symmetry of the linearized system, implies, according to Theorem 3, that, near x_0:

$$G^{-1}(x)\frac{\partial^2 L_o}{\partial x^2}(x) = \left(\frac{\partial^2 L_c}{\partial x^2}(x)\right)^{-1} G(x)$$

Moreover, the linearizations of (4) and around an equilibrium $(x_0, 0)$, yield two linear systems dual to each other, in the variables v, p. If (2) is gradient, then $p = Tv$, $T = G(x_0)$. Thus, a study of the variational system (v part of (4)) is motivated.

4. NONLINEAR CROSS GRAMIAN

Denote by Σ'_p, the variational part of (4) and Σ'_g, the p part of (5), of (2) which is assumed gradient. According to Lemma 6, $p = G(x)v$. Assume that $L_o(x, v) = \frac{1}{2}v^T M(x)v$ exists and is positive definite, where the entries of $M(x)$ are smooth functions. Then, $M(x)$ satisfies

$$\begin{aligned} &p^T G^{-1}(x)M(x)\frac{\partial f(x)}{\partial x}v + \frac{1}{2}p^T g(x)g^T(x)p \\ &= \frac{\partial L_o(x,v)}{\partial x}f(x) - v^T\frac{\partial^2 L_o(x,v)}{\partial v \partial x}f(x) \end{aligned} \tag{6}$$

We call $\mathcal{X}(x) = G^{-1}(x)M(x)$ the cross Gramian of Σ'_p.

Remark 7 In the linear case, (6) becomes:

$$T^{-1}M \cdot A + \frac{1}{2}BC = 0,$$

where $X = T^{-1}M$ is the cross Gramian. □

Conjecture 8 For a nonlinear gradient system with the associated variational system Σ'_p, if λ_i, $i = 1, ..., n$ satisfy

$$\frac{\partial L_o}{\partial x}(x(0)) = \lambda \frac{\partial L_c}{\partial x}(x(0)),$$

then they are the squared eigenvalues of $\mathcal{X}(x)$.

Since, the λ's are related to (4), associated to (2), it means that if they are related to the eigenvalues of the cross Gramian, the Hankel singular values can be obtained from solving an eigenvalue problem for $\mathcal{X}(x)$. Then, the metric and the observability function provide the singular values of the system, similar to the linear case.

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Model order reduction for nonlinear IC models

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Keywords: circuit simulation, model order reduction, nonlinear dynamical systems, POD, TPWL

1. INTRODUCTION

Within the design of Integrated Circuits mathematical circuit models play an important role, nowadays. It enables the designer to compute the steady state with a dc analysis or even the complete time-dependent behaviour by a transient analysis. By use of these analyses it is possible to verify or optimize the circuit design. Unfortunately, this becomes a time-consuming task because of the increasing complexity of the real-life applications. Therefore one is interested in much simpler models which still have about the same accuracy for the wanted purpose. Furthermore, these simple models should be constructed from the original models in an automatic way.

2. NONLINEAR MOR

For linear RLC circuits there exist already quite a lot of those techniques. In particular Krylov subspace methods, like PRIMA or SPRIM, appear to be very attractive for large but sparse models. However, many other circuits behave not linearly at all. Proper Orthogonal Decomposition (POD), Empirical Balanced Truncation (EBT) and Trajectory Piecewise Linear (TPWL) still try to use linear techniques for which they require snapshots of the nonlinear system. The first two methods project the original DAE by Galerkin projection. This has the drawback that the model evaluation costs are not reduced at all. Missing Point Estimation (MPE) can help to reduce also the number of function evaluations.

Instead of a global subspace, it is also possible to use a dynamical subspace, e.g. by use of re-cycling Krylov subspaces. Then the size of the model can be much smaller compared to extracted models obtained by projection onto a global subspace. A second option is to allow a more general class of reduced models than only Galerkin projection. The reduced model is a member of a parameterized family of models of fixed size. Model identification techniques can help to get the right model.

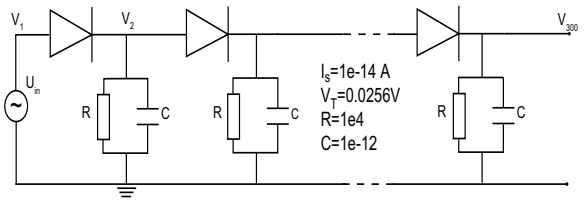

Fig. 1. Structure of the test circuit

3. NUMERICAL RESULTS

We consider the academic diode chain model shown in Figure 1, which is described by the following equations:

$$
\begin{aligned}
V_1 - U_{\text{in}}(10^9 t) &= 0,\\
i_E - g(V_1, V_2) &= 0,\\
g(V_1, V_2) - g(V_2, V_3) - C\dot{V}_2 - \tfrac{1}{R}V_2 &= 0,\\
&\vdots\\
g(V_{N-1}, V_N) - g(V_N, V_{N+1}) - C\dot{V}_N - \tfrac{1}{R}V_N &= 0,\\
g(V_N, V_{N+1}) - C\dot{V}_{N+1} - \tfrac{1}{R}V_{N+1} &= 0,
\end{aligned}
$$

$$
g(V_a, V_b) = \begin{cases} (I_s e^{\frac{V_a - V_b}{V_T}} - 1) & \text{if } V_a - V_b > 0.5 \\ 0 & \text{otherwise} \end{cases}
$$

$$
U_{\text{in}}(t) = \begin{cases} 20 & \text{if } t \le 10 \\ 170 - 15t & \text{if } 10 < t \le 11 \\ 5 & \text{if } t > 11 \end{cases}
$$

Figure 2 shows the numerical solution (nodal voltage in each node) of the original model, computed by the Euler Backward method with fixed step sizes of 0.1 ns. Figure 3 shows the relative errors over all nodes in the time interval $[0,\ 70\text{ns}]$ for the reduced models of different orders constructed by TPWL (top) and POD (down). For TPWL the relative error is most of the time lower then the chosen error bound $\varepsilon = 0.025$. The POD models are, as expected, more accurate, but

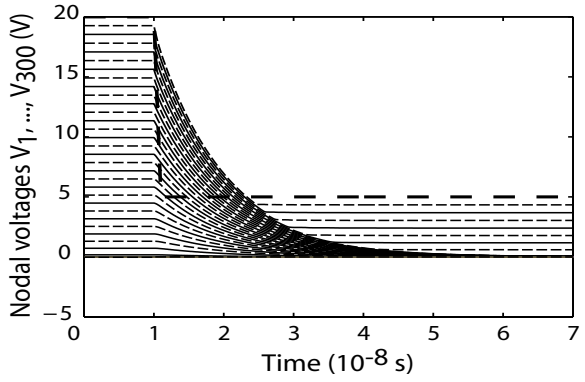

Fig. 2. Numerical solution of the full-scale nonlinear diode chain model.

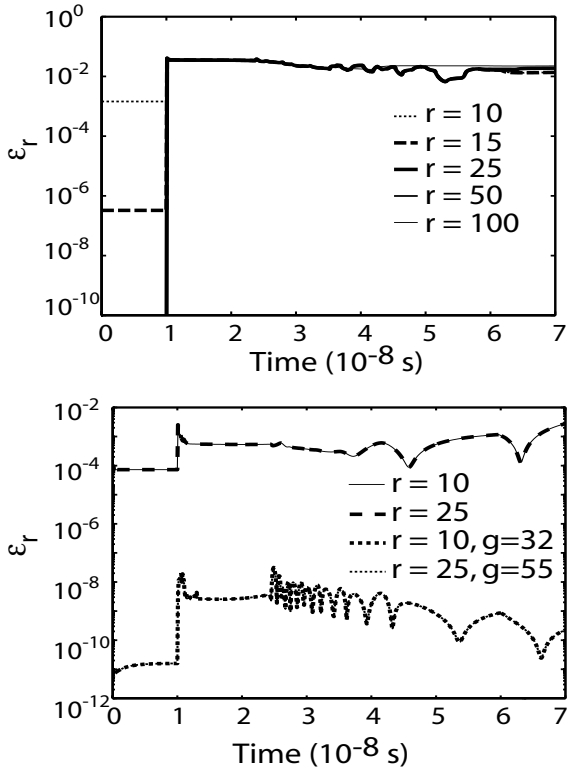

Fig. 3. Relative errors over all nodes for the reduced models created by TPWL (top) and by POD (down).

much slower to simulate than the TPWL models (see the corresponding extraction and simulation times in Table 1). A significant speed up has been achieved by combining the POD with MPE.

4. CONCLUSIONS

The TPWL method seems to be a promising technique to reduce the simulation time for nonlinear DAE systems. It's main advantage is the application of well-developed linear model reduction techniques. The POD method delivers reduced models which are more accurate but also much more expensive to compute. Hence, the missing point estimation is necessary to achieve a reduction of simulation time at all. Both techniques offer a good starting point for further research on MOR of non-linear dynamical systems. For more details about these topics the reader is referred to (1; 2).

Table 1. Comparison of extraction and simulation times in seconds.

Model	r	g	Extr. time	Sim. time
Original	302		0	142
TPWL	10		290	1.1
TPWL	25		285	1.5
TPWL	50		206	2.3
POD	10	302	142	168
POD	25	302	142	182
POD + MPE	10	32	146	74
POD + MPE	25	55	151	123

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PARAMETER ESTIMATION IN NON-LINEAR ELLIPTIC SYSTEMS UTILIZING POD

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Keywords: Proper orthogonal decomposition, elliptic systems, parameter estimation, SQP method

Proper orthogonal decomposition (POD) is a powerful technique for model reduction of linear and nonlinear systems. It is based on a Galerkin type discretization with basis elements created from the system itself. In this work POD is applied to estimate parameters in elliptic partial differential equations (PDEs). The parameter estimation is formulated in terms of an optimal control problem that is solved by an augmented Lagrangian method combined with a sequential quadratic programming (SQP) algorithm. Numerical examples illustrate the efficiency of the proposed approach. In particular, POD is used to estimate the regularization parameters of the identification problem.

POD FOR OPTIMALITY SYSTEMS

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Keywords: Proper orthogonal decomposition, optimal control, partial differential equations, model reduction

Proper orthogonal decomposition (POD) is a powerful technique for model reduction of nonlinear systems. It is based on a Galerkin type discretization with basis elements created from the system itself. In the context of optimal control this approach may suffer from the fact that the basis elements are computed from a reference trajectory containing features which are quite different from those of the optimally controlled trajectory. A method is proposed which avoids this problem of unmodelled dynamics in the POD approach to optimal control. It is referred to as *optimality system proper orthogonal decomposition* (OS-POD).

A fast anti-dissipative method for the minimum time problem. Application to atmospheric re-entry

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Keywords: minimum time problem, Hamilton-Jacobi-Bellman equation, anti-dissipative scheme, atmospheric reentry

We deal with a minimum time problem with state constraints that we study via a finite horizon target problem. The theoretical study of this latter problem shows that the value function satisfies an evolutive HJB equation. We focus here on the numerical approximation of this discontinuous value function by discretization of the HJB equation.

There is a large litterature on the numerical approximation of HJB equations. It concerns essentially the case when the function to approach is continuous. In this case classical schemes give quite good approximations. Nevertheless, as these schemes involve finite differences, they produce a lot of numerical diffusion especially around discontinuities and for long horizons. Hence they are no more efficient when approximating discontinuous functions.

The anti-dissipative UltraBee scheme has been developed to study compressible gas dynamics [4], and more precisely to solve the transport equation. A generalization to HJB equations and many academic tests have been done to evaluate the behaviour of the scheme when dealing with discontinuities. Its comparison with the viability algorithm was encouraging to study more deeply the scheme. We recently proved the convergence of this explicit non monotone scheme for general piece wise continuous functions with compact support [2].

On the other side, a sparse storage of the data allows to achieve a better precision and an important gain of time. The storage capacity is also more efficiently managed by this technique.

The combination of the anti-dissipative UltraBee scheme with the sparse storage technique allows to develop a fast method that we are presenting.

Besides the minimum time problem, we apply our method to several academic examples in 2D and 3D coming from various domains (viability, fronts propagation, ...). A particular application consists in a simplified model of atmospheric reentry in minimum time under a thermal state constraint. The main model that we consider is proposed by Betts [1]. This problem has been deeply studied by Bonnard and Trelat [3] from the theoretical point of view. They also proposed a trajectory reconstruction using the multiple shooting method. We treat here the problem by our anti-dissipative method. We are also interested in the optimal trajectory reconstruction starting from the numerical value function.

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MEMORY-EFFICIENT IMPLEMENTATION OF STABLE NONSMOOTH NEWTON'S METHOD: APPLICATION TO CONTROL-STATE CONSTRAINED OPTIMAL CONTROL PROBLEMS

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Keywords: optimal control, nonsmooth Newton's method, control-state constraints, stable multiple shooting method, checkpointing

We consider the following optimal control problem (OCP) subject to mixed control-state constraints:

$$\begin{aligned} \text{Minimize} \quad & \int_0^1 f_0(x(t),u(t))dt \\ \text{s.t.} \quad & x'(t) = f(x(t),u(t)) \text{ a.e. in } [0,1], \\ & \psi(x(0),x(1)) = 0, \\ & c(x(t),u(t)) \leq 0 \text{ a.e. in } [0,1], \end{aligned}$$

where $x \in W^{1,\infty}([0,1],\mathbb{R}^{n_x}), u \in L^\infty([0,1],\mathbb{R}^{n_u})$. Without loss of generality we consider only autonomous problems on the fixed time interval $[0,1]$. The functions $f_0 : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}$, $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$, $\psi : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_\psi}$, $c : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_c}$, are supposed to be at least twice continuously differentiable w.r.t. to all arguments.

Several approaches towards the numerical solution of OCP have been investigated in the literature. The so-called direct discretization method is based on a discretization of the infinite dimensional optimal control problem and leads to a finite dimensional nonlinear program. The latter can be solved numerically by suitable programming methods such as, e.g., sequential quadratic programming. The direct discretization method turns out to be very robust in practice. Nevertheless, the computational effort grows at a nonlinear rate with the number of grid points used for discretization.

The so-called indirect method for optimal control problems attempts to satisfy the necessary conditions that are provided by the well-known minimum principle numerically. The exploitation of the minimum principle leads to a nonlinear multi-point boundary value problem that has to be solved. Although the indirect method usually leads to the most accurate solutions, it suffers from the drawback that it requires a good initial guess in order to convergence. One crucial task is to estimate the sequence of active and inactive intervals of the control-state constraint.

In our talk we consider the indirect approach, which avoids the latter drawback, and apply the nonsmooth Newton's method for its realization. The method is based on a nonsmooth reformulation of the necessary optimality conditions. A brief outline of the essential ideas of the algorithm is as follows. The necessary conditions are stated in terms of a local minimum principle. By use of the Fischer-Burmeister function the local minimum principle is transformed into an equivalent nonlinear and nonsmooth equation in appropriate Banach spaces:

$$F(z) = 0, \qquad F : Z \to Y,$$

where Z and Y are appropriate Banach spaces. Application of the globalized nonsmooth Newton's method generates sequences $\{z^k\}$, $\{d^k\}$ and $\{\alpha_k\}$ related by the iteration

$$z^{k+1} = z^k + \alpha_k d^k, \qquad k = 0,1,2,\ldots.$$

Herein, the search direction d^k is the solution of the linear operator equation $V_k(d^k) = -F(z^k)$ and the step length $\alpha_k > 0$ is determined by a line-search procedure of Armijo's type for a suitably defined merit function. The linear operator V_k is chosen from an appropriately defined generalized Jacobian $\partial_* F(z^k)$ (for details see (1)).

In our talk we describe how the search direction d^k can be computed by the multiple shooting approach. We particularly consider the dichotomy case, so that the linear operator V_k contains both fast growing and fast decaying modes. Utilizing this fact, we can successfully solve the linear system $V_k(d^k) = -F(z^k)$ combining compactification and decoupling, where the decoupling corresponds to the splitting of growing and decaying modes, which results in a stable version of the nonsmooth Newton's method.

Each iteration of the Newton's method contains three alternative sweeps through a time horizon, so that the information evaluated within each sweep is required to integrate the others two. To reduce the huge memory requirement, resulting by the straightforwardly storing all information evaluated during each sweep, we apply checkpointing techniques. As developed in (2; 3), checkpointing means that not all intermediate states are saved but only a small subset of them is stored as checkpoints. Because of the triple sweep within each Newton iteration, we are faced here with a nested checkpointing, where checkpoints from various sweeps must be kept simultaneously. In our talk we describe some heuristics to construct appropriate nested reversal schedules.

Finally we present some numerical examples.

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Fast Computation of the Hessian of the Lagrangian in the Sequential Approach for Optimal Control

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Keywords: optimal control, single shooting, multiple shooting, Hessian, Lagrangian, adjoints

1. INTRODUCTION

Direct methods have been proven to efficiently solve large scale optimal control and nonlinear model predictive control problems. A comprehensive overview of the different solution techniques is given in the book of Grötschel et al. [1]. For notational simplicity this contribution focuses on single shooting though the results are also applicable for the multiple shooting approach.

In single shooting typically medium size dense NLPs have to be solved. State of the art nonlinear programming solvers employ either interior point methods or sequential quadratic programming (SQP). In both cases either the exact or an approximate Hessian of the Lagrangian is required by the nonlinear programming solver. The contribution of this paper is a new methodology for the fast computation of this Hessian for path-constrained optimal control problems.

2. PROBLEM STATEMENT

We consider Mayer-type optimal control problems involving linear-implicit DAE systems of index less than or equal to one. Single shooting is one approach to solve such optimal control problems. The discretization of the optimal control problem leads to the following nonlinear program:

$$\min_{p} \quad \Phi(t_f, x(t_f), p) \tag{1}$$

$$\text{s. t.} \quad B\,\dot{x}(t) = f(t, x(t), p)\,, \tag{2}$$

$$x(t_0) = x_0(p)\,, \tag{3}$$

$$g(t_i, x(t_i), p) \le 0, \quad i = 0, \ldots, N\,, \tag{4}$$

$$h(t_f, x(t_f), p) \le 0\,, \tag{5}$$

$$t \in [t_0, t_f]\,. \tag{6}$$

Here, $x(t) \in \mathbb{R}^{n_x}$ is the state vector including algebraic variables, $p \in \mathbb{R}^{n_p}$ is a time-invariant parameter vector including discretized control variables. $B \in \mathbb{R}^{n_x \times n_x}$ is the mass, $f(t, x(t), p) \in \mathbb{R}^{n_x}$. $g(t_i, x(t_i), p) \le 0 \in \mathbb{R}^{n_g}$, $i = 0, \ldots, N$ are the relaxed path constraints on a grid $t_0 < t_1 < \cdots < t_N = t_f$, and $h(t_f, x(t_f), p) \le 0 \in \mathbb{R}^{n_h}$ are the endpoint constraints. Note that equation (2) is solved by an underlying integration.

The Lagrangian of the nonlinear program can be stated as

$$\begin{aligned}\mathcal{L}(p, \mu, \nu) =& \Phi(t_f, x(t_f), p) + \nu^T\, h(t_f, x(t_f), p) \\ &+ \sum_{i=0}^{N} \mu_i^T\, g(t_i, x(t_i), p)\end{aligned} \tag{7}$$

with Lagrange multipliers $\mu_i \in \mathbb{R}^{n_g}, i = 0, \ldots, N$ and $\nu \in \mathbb{R}^{n_h}$. This contribution focuses on the computation of the Hessian of the Lagrangian with respect to p namely $\mathcal{L}_{pp}$.

3. ADJOINT EQUATIONS

If no path constraints are present, the computation of (7) is reduced to the computation of

$$\frac{d^2}{dp^2}\left(\Phi(t_f, x(t_f), p) + \nu^T\, h(t_f, x(t_f), p)\right).$$

In this situation second-order adjoint sensitivity analysis can efficiently provide the Hessian.

Haug and Ehle [2] employ second-order adjoint equations for the sensitivity analysis of mechanical systems. Özyurt and Barton [3] investigate the combination of directional second-order adjoint equations with automatic differentiation techniques.

The main idea in second-order adjoint sensitivity analysis is to introduce adjoint variables $\lambda(t) \in \mathbb{R}^{n_x}$ and $\lambda_p(t) \in \mathbb{R}^{n_x \times n_p}$ for the states and first-order sensitivities, respectively. First-order sensitivities $x_p(t)$ can be computed by an integration of first-order sensitivity equations e.g. Schlegel et al. [4]. While the state and first-order systems have to be integrated forward in time, the first-order and second-order adjoint systems have to be integrated backwards. During this backward integration the states and first-order sensitivities have to be present for example, by interpolation. After solving the adjoint systems, the Hessian can essentially be obtained by solving a quadrature problem of dimension $n_p(n_p+1)/2$ [3].

If path constraints are involved, second-order adjoint sensitivity analysis cannot be applied without additional considerations. In this case, second-order derivatives of DAE-embedded functionals evaluated at different points in time are involved:

$$\frac{d^2}{dp^2}\left(\mu_i^T\, g(t_i, x(t_i), p)\right), \quad i = 0, \ldots, N\,.$$

Thus, in a primitive approach, $N-1$ additional second-order adjoint systems have to be integrated.

The contribution of the authors is the introduction of so called composite adjoints. Using the approach of composite adjoints, only one adjoint system has to be solved. The computation of the Hessian of the Lagrangian with composite adjoints essentially comprises

- the forward integration of the combined state and first-order sensitivity system of dimension $\mathbb{R}^{n_x \times (n_p+1)}$,
- the backward integration of the combined first-order and second-order adjoint system of dimension $\mathbb{R}^{n_x \times (n_p+1)}$,
- the solution of a quadrature problem of dimension $n_p(n_p+1)/2$.

4. OTHER APPROACHES

In comparison, the computation of the Hessian with a primitive adjoint sensitivity approach comprises

- the forward integration of the combined state and first-order sensitivity system of dimension $\mathbb{R}^{n_x \times (n_p+1)}$,
- the backward integration of N combined first-order and second-order adjoint system of dimension $\mathbb{R}^{n_x \times (n_p+1)}$,
- the solution of N quadrature problems of dimension $n_p(n_p+1)/2$.

Employing second-order forward sensitivity equations e.g. Vassiliadis [5] comprises

- the forward integration of the combined state, first-order and second-order sensitivity system of dimension $\mathbb{R}^{n_x \times (n_p(n_p+1)/2+n_p+1)}$.

5. NUMERICAL CASE STUDY

A numerical case study will be provided.

6. CONCLUSIONS

A new methodology to efficiently provide the Hessian of the Lagrangian of in single shooting has been proposed. The algorithm employs the novel concept of composite adjoints to reduce the computational effort of a Hessian evaluation. Although not an topic of this contribution the algorithm can easily be adapted for multiple shooting.

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ADAPTIVE PARAMETERIZATION FOR DIRECT OPTIMAL CONTROL COMPUTATIONS

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Keywords: optimal control, numerical approximation

1. INTRODUCTION

The direct computational methods of optimal control use finite-dimensional parameterizations of control and, possibly, state trajectories. Interval polynomials are used, with the coefficients and sometimes the nodes being decision variables. In the *adaptive direct methods* (Cervantes, Biegler 2001, Schlegel *et al.* 2005), the decision space is systematically reconstructed by mesh refinement to improve the approximation.

In this paper, the adaptation is based on the monotone structural evolution (MSE) (Szymkat, Korytowski 2003, 2006). The adjustment of the decision space proceeds in a series of *structural changes*, separated by periods of gradient optimization. The changes, based on *efficiency* analysis speed up optimization and are continued until the maximum principle conditions are met with sufficient accuracy.

Consider a control system $\dot{x} = f(x,u), 0 \le t \le T$, $x(0) = x^0$ with the state $x(t) \in \boldsymbol{R}^n$. The piecewise continuous controls u take values in $\boldsymbol{U} \subset \boldsymbol{R}^m$. The horizon $T > 0$ is fixed or free. The cost $S(u,T) = \varphi(x(T),T)$ is minimized subject to $h(x(T)) = 0_r$. To treat this constraint by penalty method, define an auxiliary cost $S_\rho(u,T) = \varphi(x(T),T) + \frac{1}{2}\rho \| h(x(T)) \|^2$, $\rho > 0$.

Let $H(\psi,x,u) = \psi^{\mathsf{T}} f(x,u)$. The adjoint vector ψ is a solution of $\dot{\psi} = -H'_x(\psi,x,u)$, $t \in [0,T]$, $\psi(T) = -\varphi'_x(x(T),T) - \rho\, h'(x(T))^{\mathsf{T}} h(x(T))$.

2. BASICS OF MSE

Define the nodes $0 = t_0 \le t_1 \le \ldots \le t_N = T$. The *control structure* is a sequence of procedures P_i, $i = 1,2,\ldots,N$ that determine the control, $u(t) = P_i(x(t),t,p_i)$ in $[t_{i-1},t_i[$ where p_i is a parameter. The procedures (taken from a fixed, finite set), their number, order and parameters, the nodes $t_1,\ldots,t_{N-1}$ and, possibly, t_N are decision variables. The restrictions of control to $[t_{i-1},t_i[$ are called *arcs*. For the *boundary* arcs define constant procedures taking values at expected hamiltonian maximizers. On the *interior* arcs $u(t) = P(t,p)$ where P is an Hermite interpolation polynomial with the coefficient vector p.

The *approximation mapping* $A : \boldsymbol{D} \supset \boldsymbol{D}_a \to \boldsymbol{\mathcal{U}}$, from an admissible set in a finite-dimensional decision space into a functional control space, allows the cost to be redefined as a function of the decision vector, $\Sigma(d) = S_\rho(A(d),T)$. In MSE, the decision space is adapted to the accumulated knowledge on optimal solution by structural changes, determined by mappings of the form $(\boldsymbol{D},d) \mapsto (\overline{\boldsymbol{D}},\overline{d})$ where $d \in \boldsymbol{D}_a \subset \boldsymbol{D}$, $\overline{d} \in \overline{\boldsymbol{D}}_a \subset \overline{\boldsymbol{D}}$. Let A be assigned to $\boldsymbol{D}$ and $\overline{A}$ to $\overline{\boldsymbol{D}}$. The *condition of control preservation* $\overline{A}(\overline{d}) = A(d)$, $d \in \boldsymbol{D}_a$, $\overline{d} \in \overline{\boldsymbol{D}}_a$ guarantees monotonicity of the cost. Two kinds of structural changes are used in MSE: the dimension of the decision space increases in a *generation*, and is diminished in a *reduction*. To define the *efficiency* E of a generation, let $d_0 \in \boldsymbol{D}$ be the

decision vector before and $\bar{d}_0 \in \overline{\boldsymbol{D}}$, after it. Let $\overline{\Sigma}(\bar{d}) = S_\rho(\bar{A}(\bar{d}), T)$. If $\gamma = -\Sigma'(d_0)$ points to int $\boldsymbol{D}_a$ and $\bar{\gamma} = -\overline{\Sigma}'(\bar{d}_0)$ to int $\overline{\boldsymbol{D}}_a$, then the efficiency $E = \|\bar{\gamma}\|^2 - \|\gamma\|^2$. Otherwise, appropriate projections are used. A *driving* generation occurs if $E/\|\gamma\|^2$ exceeds a given threshold. The number of simultaneously generated nodes is limited by additional rules.

The basic algorithm of MSE is as follows.

1^0 Selection of initial decision space and starting point.
2^0 Termination, if optimality conditions in $\boldsymbol{\mathcal{U}}$ are satisfied.
3^0 Generation, if promising or needed.
4^0 Iteration of gradient optimization.
5^0 Reduction, if necessary.
6^0 Return to 2^0.

The optimality conditions in step 2^0 are based on the *maximum principle conditions*. Step 3^0 is distinctive for MSE and crucial for convergence. The gradient and efficiency computations use adjoint solutions. While the gradients can be found differently, the adjoints are indispensable for verifying the MP conditions, and for choosing generations with satisfactory efficiency.

3. POLYNOMIAL REPRESENTATION

Every interior control arc is an Hermite interpolation polynomial (Sharma, Mathur 1979)

$$u(t) = \sum_{i=0}^{k_s} \left(p_{s-1}^i V_{k_s i}(t, t_{s-1}, t_s) + p_{s-}^i V_{k_s i}(t, t_s, t_{s-1}) \right)$$

where $t \in [t_{s-1}, t_s[$, $s \in \{1,...,N\}$,

$$V_{ki}(t,a,b) = \frac{(t-a)^i}{i!} \left(\frac{b-t}{b-a} \right)^{k+1} \sum_{j=0}^{k-i} C_{k+j}^k \left(\frac{t-a}{b-a} \right)^j$$

$$p_{s-1}^i = u^{(i)}(t_{s-1}+), \; p_{s-}^i = u^{(i)}(t_s-), \; 0 \le i \le k_s .$$

In such a representation, all decision variables have clear geometric interpretations, and it is easy to impose regularity requirements.

The admissible decision variables satisfy p_{s-1}^0, $p_{s-}^0 \in \boldsymbol{U}$, $s = 1,...,N$, and the condition of proper arrangement of nodes (including the implicit non-saturation condition). The control regularity conditions at the nodes read $p_s^i = p_{s-}^i \quad \forall s \in K_i$ where $K_i \subset \{1,...,N-1\}$, $i = 0,1,...$ Special rules apply to the nodes adjacent to boundary arcs.

Let $J_{ki}(a,b) = -\int_a^b \nabla_u H(\psi, x, u) V_{ki}(t,a,b)\,\mathrm{d}t$.

The cost derivatives w.r.t. decision variables are expressed by (Szymkat, Korytowski 2007)

$$\Sigma'_{p_s^i} = J_{k_s i}(t_s, t_{s+1}), \; \Sigma'_{p_{s-}^i} = -J_{k_s i}(t_s, t_{s-1}) \text{ if } s \notin K_i,$$

$$\Sigma'_{p_s^i} = J_{k_s i}(t_s, t_{s+1}) - J_{k_s i}(t_s, t_{s-1}) \text{ if } s \in K_i,$$

$$\Sigma'_{t_s} = H(\psi(t_s), x(t_s), p_s^0) - H(\psi(t_s), x(t_s), p_{s-}^0) + \sum_{i=0}^{k_s} \left(u^{(i+1)}(t_s+) J_{k_s i}(t_s, t_{s+1}) - u^{(i+1)}(t_s-) J_{k_s i}(t_s, t_{s-1}) \right)$$

4. IMPLEMENTATION

The method is illustrated with two computational examples. In the first, an inverted pendulum on a car with scalar control and quadratic cost is considered. The second example deals with a non-isothermal semi-batch reactor with two controls. We use 'driving' generations of two types: *nodal*, which consist in inserting one or two new nodes (in the latter case at the same point), and *degree* generations where the polynomial order is increased.

The efficiency of generations of these types is nonnegative at stationary points of the optimization algorithm in constant decision space. If the efficiency identically vanishes, the corresponding control fulfils the necessary optimality conditions of the maximum principle. Apart from the driving generations, there are 'forced' generations resulting from control saturation. The choice of the type and parameters of a driving generation is based on a comparison of the respective relative efficiencies.

The numerical experiments show that a moderate increase of the amount of analytical work may result in a substantial improvement of convergence rate.

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A CROSS-ROAD OF CONTROL THEORY AND ROBOTICS: THE METHOD OF ENDOGENOUS CONFIGURATION SPACE

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Keywords: Mobile manipulator, control system, continuation method, inverse kinematics, performance

1. INTRODUCTION

This paper presents a control theoretic approach that provides a uniform theory of stationary and mobile robotic manipulators. A mobile manipulator is a robotic device composed of a mobile platform and a stationary onboard manipulator. A synergy of mobility and manipulation capabilities makes these devices of paramount usability in personal and service robotics. In the paper we concentrate on the kinematics of a mobile manipulator that consists of a noholonomic mobile platform and a holonomic onboard manipulator. As an example of such a robot Figure 1 presents a 4 wheel mobile platform carrying a 3 degree of freedom manipulator. We

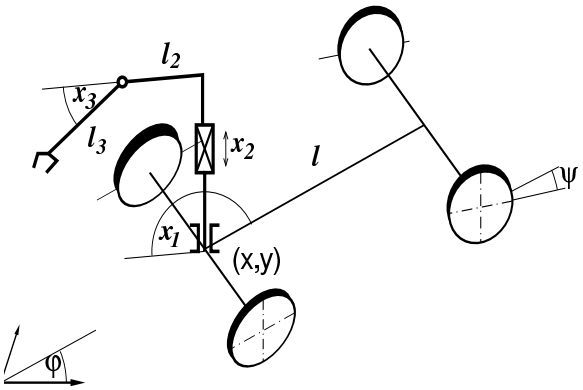

Fig. 1. Mobile Manipulator

let $q = (\mathsf{x}, \mathsf{y}, \varphi, \psi) \in R^4$ describe the position, orientation and the heading angle of the platform, while $x = (x_1, x_2, x_3) \in R^3$ denotes joint positions of the onboard manipulator. Cartesian positions of the end effector are denoted as $y = (y_1, y_2, y_3) \in R^3$. Under assumption of no side-slip of the platform wheels the kinematics of this mobile manipulator become a driftless control system

$$\dot{q}_1 = u_1 \cos q_3 \cos q_4,\ \dot{q}_2 = u_1 \sin q_3 \cos q_4,$$
$$\dot{q}_3 = u_1 \sin q_4,\ \dot{q}_4 = u_2,$$

with output function

$$y = (q_1 + (l_2 + l_3 \cos x_3)\cos(q_3 + x_1),$$
$$q_2 + (l_2 + l_3 \cos x_3)\sin(q_3 + x_1), x_2 + l_3 \sin x_3)\,.$$

2. METHODOLOGY

In the general case the control system representation of kinematics of the mobile manipulator assumes the following form

$$\begin{cases} \dot{q} = G(q)u = \sum_{i=1}^{m} g_i(q)u_i, \\ y = k(q, x). \end{cases} \tag{1}$$

Above, the vector $q \in R^n$ refers to platform generalized coordinates. The controls $(u(\cdot), x)$ driving the system (1) include instantaneous platform speeds $u(t) \in R^m$ and joint positions $x \in R^p$ of the manipulator. The set of control functions, equipped with inner product

$$\langle (u_1(\cdot), x_1), (u_2(\cdot), x_2) \rangle_{RW} = \int_0^T u_1^T(t) R(t) u_2(t) dt + x_1^T W x_2,$$

forms a Hilbert space $\mathcal{X} = L^2_m[0, T] \times R^p$ called the *endogenous configuration space* of the mobile manipulator (Tchoń and Jakubiak, 2003). The vector $y \in R^r$ collects taskspace coordinates. The end point map

$$K_{q_0,T}(u(\cdot), x) = y(T) = k(\varphi_{q_0,T}(u(\cdot)), x), \tag{2}$$

where $q(t) = \varphi_{q_0,t}(u(\cdot))$ stands for the platform trajectory, defines the kinematics of the mobile manipulator. The Jacobian operator is a derivative of the kinematics

$$J_{q_0,T}(u(\cdot),x)(v(\cdot),w) = \frac{d}{d\alpha}\Big|_{\alpha=0} K_{q_0,T}(u(\cdot)+\alpha v(\cdot), x+\alpha w) = C(T,x)\int_0^T \Phi(T,s)B(s)v(s)ds + D(T,x)w.$$

The computation of the Jacobian utilizes the variational system

$$\begin{cases} \dot{\xi} = A(t)\xi + B(t)v, \\ \eta = C(t,x)\xi + D(t,x)w \end{cases}$$

associated with (1), where matrices

$$A(t) = \frac{\partial(G(q(t))u(t))}{\partial q}, \quad B(t) = G(q(t)),$$
$$C(t,x) = \frac{\partial k(q(t),x)}{\partial q}, \quad D(t,x) = \frac{\partial k(q(t),x)}{\partial x},$$

come from the linear approximation of system (1) along the control-trajectory pair $(u(t), x, q(t))$. An endogenous configuration $(u(\cdot), x) \in \mathcal{X}$ is regular, if the Jacobian is surjective, otherwise the configuration is singular. A necessary and sufficient condition of regularity is the full rankness of the Gram matrix

$$\mathcal{D}_{q_0,T}(u(\cdot),x) = D(T,x)W^{-1}D^T(T,x) + C(T,x)\int_0^T \Phi(T,s)B(s)R^{-1}(s)\times B^T(s)\Phi^T(T,s)ds\, C^T(T,x) \quad (3)$$

of the linear approximation to (1). At regular configurations the system (1) is locally output controllable. The singular configurations correspond to singular controls of this system.

3. INVERSE KINEMATICS

A fundamental problem of robotics is the inverse kinematics problem: Given the kinematics (2) and a desirable taskspace point $y_d \in R^r$, find a configuration $(u(\cdot), x) \in \mathcal{X}$ such that $K_{q_0,T}(u(\cdot), x) = y_d$. An application of the continuation method yields a dynamic system in $\mathcal{X}$

$$\frac{d}{d\theta}\begin{pmatrix} u_\theta(t) \\ x(\theta) \end{pmatrix} = -\gamma J^{\#}_{q_0,T}(u_\theta(\cdot), x(\theta))\times (K_{q_0,T}(u_\theta(\cdot), x(\theta)) - y_d)(t), \quad (4)$$

underlying the Jacobian inverse kinematics algorithms. Above, the operator $J^{\#}_{q_0,T}(u(\cdot),x)$ denotes a right inverse of the Jacobian. The most often used is the Jacobian pseudoinverse operator

$$\Big(J^{\#}_{q_0,T}(u(\cdot),x)\eta\Big)(t) = \begin{bmatrix} R^{-1}(t)B^T(t)\Phi^T(T,t)C^T(T,x) \\ W^{-1}D^T(T,x) \end{bmatrix} \mathcal{D}^{-1}_{q_0,T}(u(\cdot),x)\eta.$$

4. PERFORMANCE

The Jacobian operator $J_{q_0,T}(u(\cdot),x)$ transforms the motion from the endogenous configuration space into the taskspace. A quality of this transformation can be assessed by looking at the taskspace image

$$E_{q_0,T}(u(\cdot),x) = J_{q_0,T}(u(\cdot),x)S_{q_0,T} = \{\eta \in R^r \mid \eta^T \mathcal{D}^{-1}_{q_0,T}(u(\cdot),x)\eta = 1\}.$$

of the unit sphere $S_{q_0,T} \subset \mathcal{X}$, called the dexterity ellipsoid of the mobile manipulator. Functions of eigenvalues of the dexterity matrix $\mathcal{D}_{q_0,T}(u(\cdot),x)$ may be used as dexterity measures of the configuration $(u(\cdot),x)$. Averaged configuration dexterities provide performance measures of the mobile manipulator as a whole.

5. CONCLUSION

In the paper we shall derive a collection of Jacobian algorithims (Tchoń and Jakubiak, 2003), (Tchoń, 2006), discuss their convergence and repeatability, as well as introduce specific performance measures of mobile manipulators. The performance optimization will result in providing motion patterns and design objectives for mobile manipulators.

6. ACKNOWLEDGMENTS

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Implementations of control laws for motion camouflage in a pursuit-evasion system

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Keywords: optimization and control; nonlinear systems; scalar and vector Lyapunov function

1. Introduction

Motion camouflage is a sly technique found in nature and employed by bats and hoverflies. We analyze the pursuit-evader system by introducing strategies for both players for capturing its prey and escaping its predator. Analytical bounds for feedback laws and sufficient conditions for initial cost and intial conditions are found to guarantee either capture or evasion in finite time. We also have numerical implementation satisfying the inequalities. Moreover, the steering laws are implemented in a testbed to check feasibility in a real environment.

Motion camouflage is a sly technique that allows a pursuer to approach a prey while appearing to remain stationary from the viewpoint of the prey. To accomplish this, the pursuer follows a path in which a line connecting the pursuer and the evader at each time step retains the same slope; see fig. 1. In this way, the evader identifies no movement from the pursuer. The motion camouflage strategy has been observed in nature. For instance, it has been suggested that bats use motion camouflage to minimize the time to capture of a moving prey. In (9)-(1), the experimental data suggests motion camouflage interactions between hoverflies.

In this work, we extend the work of Justh and Krishnaprasad (4) on steering laws for motion camouflage. An earlier study of the mathematics of motion camoulfage was done by Glendinning (2). We analyze the interaction of both the pursuer and evader when the strategies are present. In (4), feedback laws are derived from a cost function based on the ratio of change of the baseline vector corresponding on the positions of the pursuer and evader. In addition, analytical studies show bounds on the gain to guarantee capture at some time. Here we analyze the bounds on the gains for both the strategies of the players in the pursuit and evasion cases. Moreover, we also have numerical simulations to verify the analytical bounds as well as testbed simulations for the steering laws to demonstrate its feasibility in a real environment.

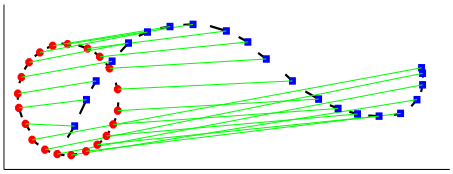

Fig. 1. The round dots represent the evader as the square dots represent the pursuer.

2. Modeling Equations

The equations of motion for the players are the following (4),(8), and the references therein:

$$\dot{r}_p = x_p,$$
$$\dot{x}_p = y_p u_p,$$
$$\dot{y}_p = -x_p u_p.$$

and

$$\dot{r}_e = \nu x_e,$$
$$\dot{x}_e = \nu y_e u_e,$$
$$\dot{y}_e = -\nu x_e u_e$$

where r_p and r_e are the position of the pursuer and evader, respectively. The corresponding unit tangent vectors are x_p and x_e while the unit normal vectors are denoted y_p and y_e. In addition, the controls u_p and u_e are the curvatures of r_p and r_e, respectively. These systems of equations are so-called Frenet-Serret equations. The derivation of these equations can be found in (5).

In the work of Justh and Krishnaprasad (4), the control law u_p is a motion camouflage feedback which forces the *pursuer to be in the same constant bearing as the evader*.

Definition 2.1 *Motion camouflage with respect to the point at infinity is*

$$r = \lambda \bar{r}$$

where

$$r = r_p - r_e,$$

$\bar{r}$ is a unit vector, and $\lambda \in \mathbb{R}$.

The cost function associated with the motion camouflage is

$$\Gamma(t) = \frac{\frac{d}{dt}|r|}{|\frac{dr}{dt}|},$$

which is the ratio of the rate of change of the baseline vector r and the absolute rate of change of the baseline vector. Moreover,

$$\begin{aligned}\dot{\Gamma} &= \frac{|\dot{r}|}{|r|}\left[\frac{1}{|\dot{r}|^2}\left(\frac{r}{|r|}\cdot\dot{r}^{\perp}\right)^2\right] \\ &+ \frac{|\dot{r}|}{|r|}\left[\frac{1}{|\dot{r}|^2}\left(\frac{r}{|r|}\cdot\dot{r}^{\perp}\right)\right](1-\nu\,(x_p\cdot x_e))\,u_p \\ &+ \frac{|\dot{r}|}{|r|}\left[\frac{1}{|\dot{r}|^2}\left(\frac{r}{|r|}\cdot\dot{r}^{\perp}\right)\right](\nu-(x_p\cdot x_e))\,\nu^2 u_e\end{aligned}$$

3. Results

We study the interaction of the players in a pursuit-evasion game, that is, when both control feedback strategies are present. Let the strategies be

$$u_p = -\mu\left(\frac{r}{|r|}\cdot\dot{r}^{\perp}\right)$$

and

$$u_e = \beta\left(\frac{r}{|r|}\cdot\dot{r}^{\perp}\right)$$

where $\beta, \mu \geq 0$. In addition, we have proven some sufficient conditions for the pursuer to capture the evader while maintaining motion camouflage.

In order to demonstrate its feasibility in a real environment, we implement the steering laws introduced in (4) and control laws above onto the UCLA Applied Math Lab micro-car testbed (3). The testbed is comprised of two major components, a tracking system and car-like vehicles. See the paper (7) for more details on the construction of the testbed.

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On the identification of time-varying systems in Reproducing Kernel Hilbert Spaces

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Keywords: Bayes estimation; Tikhonov regularization; Gaussian processes; nonparametric identification; time-varying parameters; compactness in infinite dimensional spaces;

1. Introduction

During recent years much attention has been devoted to the problem of identification of time-varying systems. To cite some examples, in [9, 17] Kalman filter based algorithms for estimation of time-varying parameters are presented and stability and convergence results are derived. A discussion about performance of recursive least squares identification and related adaptive control can be found in [5, 6] while in [19] identification of time-varying systems is investigated in the framework of information-based complexity. Neural networks and Markov chain Monte Carlo based identification strategies are proposed in [20, 10]. A more recent topic includes also the study of the so called linear parameter-varying models, originally introduced in [13], where the system coefficients are rational functions of the parameters. Applications of such models to robust gain scheduling problems can be found in [14, 1]. In [11] an instance of the problem with state measurements and one parameter is shown to be equivalent to a linear regression while in [3] the identification problem is solved in terms of input/output and parameter trajectory data.

While all the papers mentioned above are concerned with discrete-time models, this paper considers a class of linear state space systems with parameters evolving according to a continuous-time Gauss Markov process. We also assume that such stochastic process admits a state-space representation and that the parameter trajectory is not accessible to direct measurements. Our problem is to reconstruct such trajectory from a finite set of nonlinearly related output data. The novelty of the paper is first to show how this continuous-time identification problem can be embedded under the framework of Tikhonov regularization and reproducing kernel Hilbert space (RKHS) theory [2, 18]. Next, we exploit such theoretical connections to derive a novel identification algorithm which may exhibit significant computational advantages with respect to those procedures that rely upon discretizations of the temporal axis. The current work can also be seen as an extension to state-space models and general RKHSs of that presented in [4].

Recent papers in control literature have studied function estimation problems from the perspective of regularization by assuming a linear relationship between the unknown map and the measurements, see e.g. [8, 12, 15, 16]. In this work we instead consider a nonlinear function estimation problem in an infinite-dimensional context and this naturally raises additional and delicate issues. For instance, establishing existence of the optimal trajectory of the time-varying parameters is far from trivial. To overcome these difficulties, the first part of our work will be devoted to the development of a new compactness result related to RKHSs embedded in spaces of continuous functions. Recent work on this subject has lead to results that show pre-compactness of unit balls of RKHSs in the sup-norm (uniform) topology, see e.g. Section 5 in Chapter 3 of [7]. In this paper, we will demonstrate that every scalar Gaussian process that admits a state-space

representation is isometrically isomorphic to a RKHS whose unit ball is compact in the uniform topology. This result is key since it will allow first to derive conditions on the system to be identified which ensure existence of the solution to the problem. Next, it will exploited to design an efficient numerical procedure for system identification. Our algorithm reconstructs the optimal parameter trajectory by generating a sequence of finite-dimensional Tikhonov-type regularization problems whose solutions converge in the sup-norm topology to that of the original infinite-dimensional problem. In particular, the compactness result guarantees that an accurate approximation of the continuous-time trajectory can be captured by subspaces whose dimension may turn out to be small with respect to the size of observed data. This may thus render the proposed numerical scheme extremely efficient.

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ON CONVERGENCE FOR ELLIPTIC SHAPE OPTIMIZATION PROBLEMS

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After an introduction to elliptic shape optimisation problems, a nonlinear Galerkin approach is investigated for the approximate solution of shape problems. The main focus of the talk is on the behaviour of optimal solutions Ω_N^* of finite dimensional auxiliary optimization problems related to Ω^*, the optimal solution of the original problem. Based on sufficient second order conditions, a complete convergence analysis for a sequence of semidiscretized problems can be provided **in case of well-posed problems**. For extension to fully discretized problems, a lemma of Strang type is presented for estimating the consistency error. Numerical results confirm the theoretical results.

A SHAPE OPTIMIZATION PROBLEM IN FISHWAYS: MODELING AND NUMERICAL RESOLUTION

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Keywords: Optimal shape design, Fishway, River, Shallow water

1. INTRODUCTION

From the end of last century to the present times, it has been growing the interest to solve the ecological problems appearing when the hand of man acts on the nature. One of these problems is the necessity to preserve and enhance stocks of diadromous (fish that migrate between freshwater to saltwater) and resident fish in our rivers. When a dam or a weir is constructed in a river, it is necessary to build a hydraulic structure that enables fish to overcome the dam to their spawning and other migrations. This hydraulic structure is known as a fishway (also fish ladder or fish pass). There are several types of fishways, but the vertical slot type (1) is generally used. It consists of a rectangular channel with a sloping floor that is divided into a number of pools. Water runs downstream in this channel, through a series of vertical slots from one pool to the next one below. The water flow forms a jet at the slot, and the energy is dissipated by mixing in the pool. Fish ascends, using its burst speed, to get past the slot, then it rests in the pool till the next slot is tried (see Fig. 1).

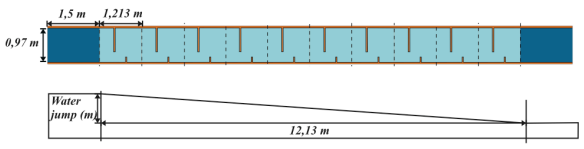

Fig. 1. Ground and plant for the fishway.

In this work, we take interest in the optimal design of these river fishways. We look for the location and length of the baffles separating the pools, in order to obtain a suitable water velocity. In the zone of the channel near the slots, we look for a velocity suitable for fish leaping and swimming capabilities. In the remaining of the fishway, we look for a velocity close to zero for making possible the rest of the fish. Moreover, in all the channel, we try to minimize the flow vorticity.

2. MATHEMATICAL FORMULATION

We consider a fishway $\omega \subset \mathbb{R}^2$ consisting of several pools (separated by dashed lines in Fig. 1) built in a rectangular channel. We also consider two transition pools, one at the beginning and other at the end of the channel. The baffles separating the pools are made vertical to a flume bed slope that ranges from 2 to 20%. Water enters by the left side and runs downstream to the right side, and fish ascend in the opposite direction.

Water flow in the channel along the time interval $(0,T)$ is governed by the shallow water (Saint Venant) equations:

$$\left.\begin{array}{l} \dfrac{\partial H}{\partial t} + \vec{\nabla}.\vec{Q} = 0 \\ \dfrac{\partial \vec{Q}}{\partial t} + \vec{\nabla}.(\vec{u} \otimes \vec{Q}) + gH\vec{\nabla}(H-\eta) = \vec{f} \end{array}\right\} \quad (1)$$

in $\omega \times (0,T)$ and where $H(x,t)$ is the height of water at point $x = (x_1, x_2) \in \omega$ at time $t \in (0,T)$, $\vec{u}(x,t) = (u_1, u_2)$ is the averaged horizontal velocity of water, $\vec{Q}(x,t) = (Q_1, Q_2) = \vec{u}H$ is the flux, g is the gravity acceleration, $\eta(x)$ represents the bottom geometry of the fishway, and the second member $\vec{f}$ collects all the effects of bottom friction, atmospheric pressure and so on. These equations must be completed with a suitable set of initial and boundary conditions.

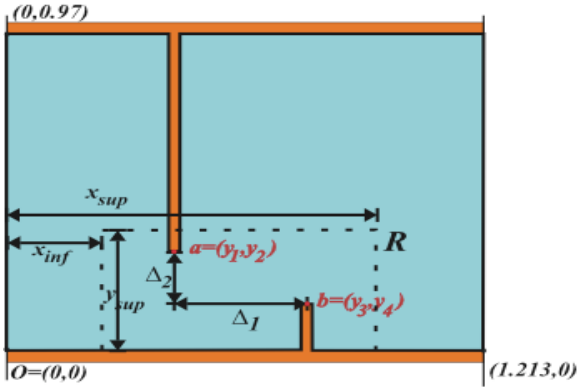

Fig. 2. Scheme of the first pool.

The design variables will be the two midpoints corresponding to the ends of the baffles (points $a = (y_1, y_2)$ and $b = (y_3, y_4)$ in Fig. 2). These two points will configure the shape of the complete fishway ω, since we assume that the structure of the ten pools is the same. We will impose several constraints on the design variables: first, we will assume that point a and b are inside the dashed rectangle of Fig. 2, that is, the following eight relations must be satisfied:

$$\left.\begin{array}{l} x_{inf} \leq y_1, y_3 \leq x_{sup} \\ 0 \leq y_2, y_4 \leq y_{sup} \end{array}\right\} \tag{2}$$

The second type of constraints are related to the fact that the vertical slot must be large enough so that fish can pass comfortably through it. This translates into the two additional relations:

$$\left.\begin{array}{l} y_3 - y_1 \geq \Delta_1 \\ y_2 - y_4 \geq \Delta_2 \end{array}\right\} \tag{3}$$

Finally, we introduce the objective function which is intended for obtaining an optimal velocity of water in such a way that in the zone of the channel near the slots (say the lower third) the velocity be as close as possible to a desired velocity $(c, 0)$ suitable for fish leaping and swimming capabilities (and depending on the species of fish). In the remaining of the fishway, the velocity must be very small for making possible the rest of the fish. Moreover, in all the channel, we must minimize the existence of flow turbulence. Thus, if we define the target velocity $\vec{v}$ by:

$$\vec{v}(x_1, x_2) = \left\{ \begin{array}{ll} (c, 0), & \text{if } \; x_2 \leq \frac{1}{3} 0.97 \\ (0, 0), & \text{otherwise} \end{array}\right. \tag{4}$$

the objective function is given by:

$$\begin{aligned} j(\omega) = \; & \frac{1}{2} \int_0^T \int_\omega \|\vec{u}^\omega - \vec{v}\|^2 dx\, dt \\ & + \frac{\alpha}{2} \int_0^T \int_\omega |curl(\vec{u}^\omega)|^2 dx\, dt \end{aligned} \tag{5}$$

where $\alpha \geq 0$ is a weight parameter for the role of the vorticity in the whole cost function, and $\vec{u}^\omega = \dfrac{\vec{Q}^\omega}{H^\omega}$ for $(H^\omega, \vec{Q}^\omega)$ the solution of the state system (1).

Then, the optimization problem consists of finding the optimal shape ω of the fishway (that is, the optimal points a and b, satisfying the constraints (2) and (3)) such that minimizes the objective function given by (5).

We also obtain an expression for the gradient of the objective function *via* the adjoint system.

3. NUMERICAL SOLUTION

We propose a characteristics-Galerkin method for solving the state system, and two algorithms to solve the optimization problem: (i) a derivative-free algorithm (Nelder-Mead), and (ii) a gradient-type method computing the cost gradient by solving the adjoint system with the characteristics-Galerkin method.

Finally, we show numerical results obtained for a standard fishway.

4. CONCLUSIONS

We formulate, analyze and solve an optimal shape problem related to the design of fishways in rivers. Once the ecological problem is mathematically posed and discretized, a gradient-type algorithm and a direct search method are proposed for solving the discrete optimization problem. Finally, the efficiency is confirmed by the numerical experiments developed by the authors.

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WITH DISCRETE ADJOINT BASED OPTIMISATION TOWARDS ANISOTROPIC ADAPTIVE FEM

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Keywords: anisotropic refinement, adaptive FEM, discrete adjoint, optimisation

1. INTRODUCTION

The modelling of many technological processes involves strongly anisotropic features in the solutions of PDEs, e.g. boundary or interior layers in many fluid flow problems. Efficient numerical approximation of such solution features by means of the finite element method requires the use of anisotropically adapted meshes, like for example Shishkin meshes. However, application of this approach relies on *a priori* analysis on the thickness, position and stretching direction of the anisotropic solution feature. If it is impossible to obtain this information *a priori*, as it is often the case for problems with interior layers of unknown position for example, automatic mesh adaptation based on *a posteriori* error estimates or error indicators is essential in order to obtain efficient numerical approximations.

Historically the majority of work on automatic mesh adaptation used locally uniform refinement, splitting each element into smaller elements of similar shape. This procedure is clearly not suitable to produce anisotropically refined meshes. The resulting meshes are over-refined in at least one spatial direction, rendering the approach far less efficient than that of the anisotropic meshes based on *a priori* analysis.

Automatic anisotropic mesh adaptation is an area of active research, e.g. [2, 1]. Here we present a recent approach to this problem [3], which draws upon techniques from control theory and optimisation. The core of the idea is to use not only an *a posteriori* error estimate to guide the mesh refinement, but its sensitivities with respect to the positions of the nodes in the mesh as well.

2. OUTLINE

The underlying idea is to use techniques from mathematical optimisation to minimise the estimated error by moving the positions of the nodes in the mesh appropriately. This basic idea is of course not new, but the approach taken to realise it is.

A key ingredient is the utilisation of the discrete adjoint technique to evaluate the sensitivities of an error estimate $J = J(u_h(s), s)$ with respect to the node positions s, where $u_h = u_h(s)$ denotes the solution of the discretised PDE, $R(u_h, s) = 0$, which depends upon the node positions s. The sensitivities

$$\begin{aligned} \frac{DJ}{Ds} &= \frac{\partial J}{\partial u_h}\frac{\partial u_h}{\partial s} + \frac{\partial J}{\partial s} \\ &= \frac{\partial J}{\partial s} - \Psi^T \frac{\partial R}{\partial s}, \qquad (1) \end{aligned}$$

$$\left[\frac{\partial R}{\partial u_h}\right]^T \Psi = \frac{\partial J}{\partial u_h}, \qquad (2)$$

are thereby evaluated according to (1), utilising the adjoint solution Ψ which is defined by (2). This way, DJ/Ds can be evaluated without computing $\partial u_h/\partial s$ first, reducing the number of equation systems to be solved from $\mathcal{O}(\dim(s))$ to just two, independent of $\dim(s)$. As the number of nodes can easily be larger than one hundred even in extremely coarse meshes (if the domain geometry is complicated), this approach is of fundamental importance to make gradient based optimisation methods feasible for this type of problem. Fast optimisation algorithms like BFGS-type methods can be applied to obtain significant reductions in the error estimate J after a few optimisation steps. The aim of this procedure is to provide a mesh with problem adapted anisotropic

elements, which may then be used as a good basis for further locally uniform adaptive mesh refinement.

3. NUMERICAL EXAMPLE

To demonstrate feasibility of the approach it is applied to a number of model problems. For the purpose of this abstract we consider a reaction diffusion equation,

$$-\Delta u + \tfrac{1}{\varepsilon^2} u = \tfrac{1}{\varepsilon^2} \quad \text{in} \quad \Omega$$

subject to

$$u = 0 \quad \text{on} \quad \Gamma_D$$
$$\tfrac{\partial u}{\partial n} = 0 \quad \text{on} \quad \Gamma_N,$$

where

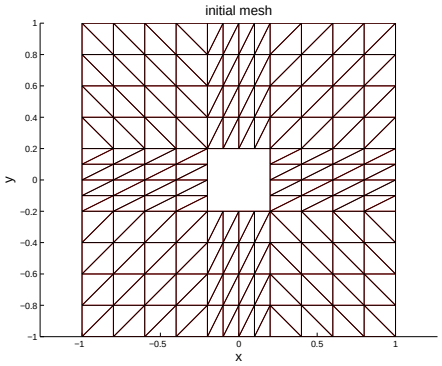
$$\Omega := (-1,1)^2 \setminus (-\tfrac{1}{5}, \tfrac{1}{5})^2$$
$$\Gamma_D := \left[-\tfrac{1}{5}, \tfrac{1}{5}\right]^2 \setminus \left(-\tfrac{1}{5}, \tfrac{1}{5}\right)^2$$
$$\Gamma_N := [-1,1]^2 \setminus (-1,1)^2$$

Figure 1 shows an initial mesh for this problem and an adapted one for $\varepsilon = 10^{-3}$. Concentration of the elements in the boundary layer which forms around the hole at the centre of the domain is clearly visible, and significantly increased aspect ratios in the boundary layer may be observed. For more detail on the approach and the example we refer to [3].

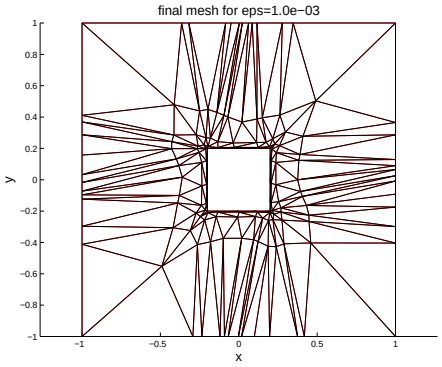
4. CONCLUSIONS

The approach has first been presented in [3], where it has been applied to reaction diffusion test problems. The simplicity and generality of the underlying ideas imply that it should be applicable to a wide range of problems with anisotropic solution features. The only requirement is that an *a posteriori* error estimate is available which is sufficiently robust with respect to mesh deformations. In [3] convection diffusion problems were proposed as a further class of test problems. These tests have since been carried out with the expected positive results, which we will presented here as well.

In all strongly anisotropic test cases the proposed approach resulted in a significantly more accurate solution when compared to a standard adaptive h-refinement strategy with the same fixed maximum number of degrees of freedom in the discretisation. This demonstrates that a clear advantage is obtained by introducing the node movement step which allows to generate suitable anisotropy in the mesh.



(a)



(b)

Fig. 1. Initial (a) and adapted (b) meshes for the reaction-diffusion model problem with a boundary layer around the square hole

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A NOTE ON NONSMOOTH OPTIMAL CONTROL PROBLEMS

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Keywords: nonsmooth optimal control, necessary conditions, singular state subarcs

1. INTRODUCTION

The lecture is concerned with general optimal control problems (OCP) which are characterized by a nonsmooth ordinary state differential equation. More precisely, we assume that the right-hand side of the state equation is piecewise smooth and that the switching points, which separate these pieces, are determined as roots of a state- and control-dependent (smooth) switching function.

Nonsmooth optimal control problems of this type rarely have been mentioned in the literature. Of course, they are special examples for the rather general theory of Clarke, Ref. (1).

For this kind of nonsmooth OPC new necessary conditions are derived. These conditions depend on the order of the switching function with respect to the control variable and of certain regularity assumptions concerning the occurence of subarcs where the switching function vanishes identically, so called singular subarcs. Examples of order zero and of order one are considered.

2. NONSMOOTH OCPs

The general nonsmooth OCP is given as follows.
Problem (OCP). Determine a piecewise continuous control function $u : [a,b] \to \mathbb{R}^m$, such that

$$I \;=\; g(x(b)) \tag{1}$$

is minimized subject to the following constraints (state equations, boundary conditions, and control constraints)

$$\begin{aligned} &x'(t) \;=\; f(x(t),u(t)),\;\; t\in[a,b],\;\; x(t)\in\mathbb{R}^n,\\ &r(x(a),x(b)) \;=\; 0\,,\\ &u(t)\in U=\Pi_i[u_{i,\min},u_{i,\max}]\subset\mathbb{R}^m. \end{aligned} \tag{2}$$

The right-hand side of the state equation is of the form

$$f(x,u) \;=\; \begin{cases} f_1(x,u), & \text{if } S(x,u)\le 0,\\ f_2(x,u), & \text{if } S(x,u)>0, \end{cases} \tag{3}$$

where the functions S, f_k $(k=1,2)$, and r are assumed to be sufficiently smooth.

3. NECESSARY CONDITIONS

Let (x^0,u^0) denotes a solution of OCP which satisfies the order-zero condition, i.e. $S_u(x^0(t),u^0(t))\neq 0$. Further, the following regularity assumption may hold. There exists a finite grid $a =: t_0 < t_1 < \ldots < t_s < t_{s+1} := b$ such that the optimal switching function $S[t]$ is either positive or negative in each open subinterval $]t_{j-1},t_j[,\;\; j=1,\ldots,s+1$. Then the following necessary conditions hold

Theorem 1 There exist an adjoint variable $\lambda : [a,b]\to\mathbb{R}^n$, which is a piecewise C^1–function, and Lagrange multipliers $\nu_0\in\{0,1\},\;\; \nu\in\mathbb{R}^\ell$, such that

$$\begin{aligned} \lambda'(t) \;&=\; -H_x(x^0(t),u^0(t),\lambda(t)),\\ u^0(t) \;&=\; \text{argmin}\{H(x^0(t),u,\lambda(t)) :\; u\in U\},\\ \lambda(a) \;&=\; -\frac{\partial}{\partial x^0(a)}\,[\nu^T r(x^0(a),x^0(b))],\\ \lambda(b) \;&=\; \frac{\partial}{\partial x^0(b)}\,[\nu_0\, g(x^0(b)) + \nu^T r(x^0(a),x^0(b))],\\ \lambda(t_j^+) \;&=\; \lambda(t_j^-),\quad j=1,\ldots,s,\\ H[t_j^+] \;&=\; H[t_j^-],\;\; j=1,\ldots,s. \end{aligned}$$

Here, the Hamiltonian is given by $H := H_k := \lambda^T f(x,u)$, where $k\in\{1,2\}$ is chosen according to the sign of S in the corresponding subinterval.

If one allows a *singular state subarc*, say $[t_1,t_2]$, which is characterized by $S(x,u)=0$,

$\forall t \in [t_1, t_2]$, on this subarc the minimum principle has to be modified as a constrained minimum principle

$$u^0(t) \;=\; \text{argmin}\{H :\; u \in U,\; S(x^0(t), u) = 0\}.$$

Further, if the order-zero condition is substituted by the *order-one assumption* $S = S(x)$ and

$$S_u^{(1)}(x^0(t), u^0(t)) \neq 0,$$

where $S^{(1)} := S_x(x)^{\mathrm{T}} f_1(x, u)$, the continuity of the adjoint variable is lost. Instead the following jump condition of the adjoints has to be satisfied

$$\lambda(t_j^+) \;=\; \lambda(t_j^-) + \kappa_j S_x(x^0(t_j)),\; j \in J_{\text{reg}} \cup J_{\text{entry}},$$

Here, $j \in J_{\text{reg}}$ are the indices of isolated roots t_j of the switching function, and J_{entry} denotes the indices of the entry points of singular state subarcs.

4. APPLICATIONS

We consider two examples. The first one is taken from the well-known book of Clarke, Ref. (1). It describes the control of an electronic circuit which encludes a diode and a condensor. The control u is the initializing voltage, the state variable x denotes the voltage at the condensor. The problem is given in form of a nonsmooth OCP of the order zero. Depending on the parameters of the model, the solution may contain a singular state subarc.

The second example is an economic optimal control model due to Pohmer, Ref. (2),(3), which describes the personal income distribution of a typical consumer, who wants to maximize the total utility of his lifetime by controling the consumption, the rate of the total time used for working, and the rate of working time used for education and extended professional training. The state variables are the human capital and the capital itself. The utility function contains different parts which represent the influence of consumption, time of recreation, and human capital. Into this problem a parameter enters which describes the interest rate of capital. It is obvious that this parameter in general will differ for positive and negative values of the capital. Thus, the resulting problem in a natural way becomes a nonsmooth OCP of the order one. For this, the necessary conditions are derived and numerical solutions are presented. Again, it turns out that for a certain distance of the positive and negative interest rate, the optimal solution contains a singular state subarc.

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Second Order Sufficient Conditions for Space-Travel Optimal Control Problems

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Keywords: Optimal Control Theory, Second Order Sufficient Conditions, Space-Travel Problems, Re-Entry, Orbit Transfer

1. INTRODUCTION

Dependent and independent control functions are often found in space-travel problems, vehicle models or economic problems. We treat optimal control problems governed by an ordinary differential equation. Into this state equation control components enter by multiplication. If the factor vanishes on a subinterval, the dependent controls can be chosen freely. We call dependent controls on these subintervals *free control subarcs*. The solution of the optimal control problem is no longer unique.

Known second order sufficient conditions (2) cannot be applied to problems with free control subarcs. We develop new sufficient conditions and verify these conditions for solution candidates of an orbit transfer problem.

Our first focus lies on sufficient conditions for regular optimal control problems with free final time. The appearing Riccati differential equation has a special structure, which recurs in the treatment of optimal control problems with free control subarcs. New sufficiency results are established for the Re-entry problem.

2. RE-ENTRY PROBLEM

The Re-entry optimal control problem (4) describes the flight of an Apollo-type vehicle through the atmosphere of the earth. The aim is to minimize the heating-up of the vehicle while entering the atmosphere.

We are able to show sufficiency for the well-known solution candidate obtained by the application of necessary conditions. The calculated solution candidate is a weak local minimum.

3. ORBIT TRANSFER PROBLEM

Typical examples for optimal control problems with free control subarcs are space-travel problems. Sufficient conditions have only been shown for problems with minimal flight time (1). In that work no free control subarcs exist.

We follow the example of a fuel optimal Earth-Mars orbit transfer problem treated in (3). The independent control function is the thrust β, whereas the thrust angle ψ is a dependent control function. If β vanishes on a subinterval, the problem does not depend on the control ψ any more. A free control subarc exists.

We treat solution candidates with a bang-bang control function β and a continuous control function ψ. The solution candidate is compared with other functions having the same switching structure depending on free control subarcs. We are able to show second order sufficient conditions for these solution candidates.

4. CONCLUSIONS

New second order sufficient conditions are developed for optimal control problems with free control subarcs. In a first step, we show sufficient conditions for the Re-entry problem with free final time. If we compare solution candidates with same switching structures, we can show sufficiency for a solution candidate of an orbit transfer problem.

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ON EXISTENCE RESULTS FOR INFINITE HORIZON OPTIMAL CONTROL PROBLEMS

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Keywords: optimal control, infinite horizon, weighted Sobolev spaces, existence results

1. INTRODUCTION

Still at the beginning of the previous century the optimal control problems with infinite horizon became very important with regards to applications in economics and biology, where an infinite horizon seems to be a very natural phenomenon, (5), (3), (10). Since then these problems were treated by many authors and various necessary, sufficient as well as transversality conditions were obtained, see for instance (6), (9). The question of existence of optimal solution was investigated among others by (1), (2), (4), (11) and (12).

2. THE MAIN PROBLEM CONSIDERED

The main problem we consider in this talk is formulated as follows. Minimize the functional

$$J(x,u) = \int_0^\infty r(t,x(t),u(t))\tilde{\nu}(t)dt$$

subject to all pairs

$$(x,u) \in\in W_p^{1,n}(\mathbb{R}^+,\nu) \times L_p^r(\mathbb{R}^+,\nu) \ ,$$

satisfying almost everywhere on $\mathbb{R}^+$
the state equations

$$\dot{x}(t) = f(t,x(t),u(t))\,,$$

the control restrictions

$$u(t) \in U, \quad U \in Comp\,(R^r) \setminus \{\,\emptyset\,\},$$

the initial conditions

$$x(0) = x_0.$$

The integral in the functional J is understood in Lebesgue sense. The remarkable on this statement is the choice of the weighted Sobolev- and weighted Lebesgue spaces as state and control spaces respectively. The idea of considering the state trajectories in weighted Sobolev spaces was firstly mentioned in (8). The functions ν and $\tilde{\nu}$ are assumed to be continuously differentiable, integrable over $\mathbb{R}^+$ having its values in $(0,1]$. We call such functions weights. These considerations give us the possibility to extend the admissible set and simultaneously to be sure that the adjoint variable belongs to a reflexive Banach space.

3. THE MAIN RESULT AND CONCLUSIONS

As the main result we formulate an existence theorem for the formulated problem for concrete classes of function f. The good imbedding properties of the weighted Sobolev space, convexity of the integrand function in control variable and some growth conditions which are assumed to be satisfied by the functions r and its derivative allow us to ensure the weak lower semicontinuity of the integral functional involved in the problem statement. This in turn is important in order to use the generalized Weierstrass theorem for the proof of the existence result. Verification of the weak compactness of the feasible set frames the second part of the proof.
Finally we formulate several examples, such as Resource Allocation Model, demonstrating the applicability of the theorem.

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NONOCCURRENCE OF THE LAVRENTIEV PHENOMENON IN NONCONVEX OPTIMAL CONTROL

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Keywords: Banach space, integrand, Lavrentiev phenomenon, optimal control problem

In this talk we discuss nonoccurrence of the Lavrentiev phenomenon for a large class of nonconvex optimal control problems with a state variable and a control variable belonging to Banach spaces. We say that the Lavrentiev phenomenon occurs for an optimal control problem if its infimum on the full admissible class of trajectory-control pairs is less than its infimum on a subclass of trajectory-control pairs with bounded controls.

The Lavrentiev phenomenon in the calculus of variations was discovered in 1926 by M. Lavrentiev in [3]. There it was shown that it is possible for the variational integral of a two-point Lagrange problem, which is sequentially weakly lower semicontinuous on the admissible class of absolutely continuous functions, to possess an infimum on the dense subclass of C^1 admissible functions that is strictly greater than its minimum value on the admissible class. Since this seminal work, the Lavrentiev phenomenon is of great interest in the calculus of variations [1-8]. The original example of Lavrentiev was simplified by Mania in [4]. In [1] Ball and Mizel demonstrated that the Lavrentiev phenomenon can occur with fully regular integrands. Sarychev [5] constructed a broad class of integrands that exhibit the Lavrentiev phenomenon. Nonoccurrence of the Lavrentiev phenomenon was studied in [2, 6-8]. Clarke and Vinter [2] showed that the Lavrentiev phenomenon cannot occur when a variational integrand $f(t, x, u)$ is independent of t. Sychev and Mizel [7] considered a class of integrands $f(t, x, u)$ which are convex with respect to the last variable. For this class of integrands they established that the Lavrentiev phenomenon does not occur. Sarychev and Torres [6] studied a class of optimal control problems with control-affine dynamics and with continuously differentiable integrands $f(t, x, u)$. For this class of problems they established Lipschitzian regularity of minimizers which implies nonoccurrence of the Lavrentiev phenomenon. In our talk we consider a class of optimal control problems identified with the corresponding complete metric space of integrands $\mathcal{M}$ which satisfy a growth condition common in the literature and satisfy a Lipschitz condition on bounded sets [8]. We show that for most elements of $\mathcal{M}$ (in the sense of Baire category) the infimum on the full admissible class of trajectory-control pairs is equal to the infimum on a subclass of trajectory-control pairs whose controls are bounded by a certain constant.

When we say that a property of elements of a complete metric space Z holds for most elements in Z we mean that the set of all elements of Z which possess this property contains an everywhere dense G_δ subset of Z. In this case we also say that the property holds for a generic (typical) element of Z or that a generic (typical) element of Z possesses the property.

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REGULARIZED INCOMPLETE OBLIQUE PROJECTIONS METHOD FOR SOLVING LEAST-SQUARES PROBLEMS IN IMAGE RECONSTRUCTION

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Keywords: Rank-deficient least-squares problems, minimal norm solution, incomplete projections, regularization

1. INTRODUCTION

Large and sparse systems of linear equations arise in many important applications [1] as radiation therapy treatments planning, computational mechanics, optimization and in image processing problems like electromagnetic geotomography [2].

In practice, problems coming from the tomographic image reconstruction are in general inconsistent and of deficient rank. Those characteristics imply projection methods are particularly useful for solving them [1].

Many problems in the field of tomographic image reconstruction are modeled by the linear least-squares problem, that is : find $x^* \in \Re^n$ such that $\min_x \|Ax-b\|^2_{D_m}$, where A is an $m \times n$ matrix and $b \in \Re^m$, where $\|.\|_{D_m}$ denotes a weighted norm, and D_m is a positive definite matrix.

C. Popa has developed an extension of ART (Algebraic Reconstruction Technique) [1], called KERP [2], which converges for inconsistent systems, and more recently in [3] the authors showed its efficiency in the case of rank-deficient systems. Within the framework of the Projected Aggregation Methods (PAM) we have developed acceleration schemes based on projecting the search directions onto the aggregated hyperplanes, with excellent results in both consistent and inconsistent systems [4,5]. In particular, the IOP algorithm [5] uses a scheme of incomplete oblique projections onto the solution set of the augmented system $Ax - r = b$, which converges to a weighted least squares solution of the system $Ax = b$. It is known that not always the minimum norm solution turns out to be the closest to the true image. In this paper, as other authors like [3], we consider the regularized weighted least squares problem

$$\min_{x\in\Re^n} \frac{1}{2}\|Ax-b\|^2_{D_m} + \beta R(x) \qquad (1)$$

where D_m is a matrix of weights of data, and the second term is a function that penalizes the image roughness. The discrete smoothing norm in the previous problem can be defined (see [3]) as $R(x) = 2U(x)$, where

$$U(x) = \sum_{j=1}^{n} \sum_{i\in S_j} w_{ji} V(x_j - x_i, \delta),$$

S_j is a set of indices of the nearest neighborhood of pixel j, w_{ji} is a factor of weight, and $V(x_j - x_i, \delta)$ is a potential function. As it can be seen in the literature [3], there are several proposals aiming at the same objective. We have adopted $V(x_j - x_i, \delta) = (\frac{x_j - x_i}{\delta})^2$. This gives raise to the problem

$$\min_{x\in\Re^n} \frac{1}{2}\|Ax-b\|^2_{D_m} + \frac{1}{2}x^T M x, \qquad (2)$$

where the matrix M is positive definite, depending upon the weights w_{ji} and the S_j sets of indices of the nearest neighborhood of each pixel j.

As in [5], we define two convex sets in the $(2n+m)$- dimensional space $\Re^{2n+m}$, denoting by $[u;v]$ the vertical concatenation of $u \in \Re^n$, with $v \in \Re^{m+n}$,

$$\mathcal{P} = \{p : p = [x;r], x \in \Re^n, r \in \Re^{m+n}\} \qquad (3)$$

being $r = [r_1; r_2] \in \Re^{m+n}$, such that satisfy $Ax - r_1 = b$, $M^{\frac{1}{2}}x - r_2 = 0$, and

$$\mathcal{Q} = \{q : q = [x; 0], x \in \Re^n, 0 \in \Re^{m+n}\}, \quad (4)$$

adopting the distance $d(p, q) = \|p - q\|_D$, for all $p \in \mathcal{P}$, $q \in \mathcal{Q}$. D is a diagonal matrix of order $2n + m$, whose n first elements are 1's, and the next m coincide with those of D_m, and the last n elements are 1's.

By means of a direct application of the Karush-Kuhn-Tucker (KKT) conditions [1] to the problem

$$\min\{\|p - q\|_D^2 : \forall p \in \mathcal{P}, \forall q \in \mathcal{Q}\} \quad (5)$$

it is possible to prove (see [5]) that this is equivalent to (2). This observation led us to use the IOP algorithm for solving (2), applying an alternate projections scheme between the sets $\mathcal{P}$ and $\mathcal{Q}$, similar to the original development in [5].

In the following sections we will present the RIOP algorithm based on the same scheme of the IOP algorithm, together with some related results needed for defining it and the corresponding convergence theory. In the last Section we will report numerical experiences for comparing the performance of the RIOP algorithm with the version of Kaczmarz Extended (KERP)[3] using simulated reconstruction problems in borebole electromagnetic geotomography.

2. INCOMPLETE OBLIQUE PROJECTION ALGORITHM

In order to solve the regularized weighted least squares problem (2) we consider its equivalence with (5). This observation led us to apply an alternate projections scheme between the sets $\mathcal{P}$ and $\mathcal{Q}$, but replacing the computation of the exact projections onto $\mathcal{P}$ by suitable incomplete or approximate projections, according to IOP algorithm in [5]. In order to compute the incomplete projections onto $\mathcal{P}$ we apply our ACCIM algorithm [4,5], which uses simultaneous projections onto the hyperplanes of the augmented system $Ax - r_1 = b_1$ and $Mx - \tilde{r}_2 = 0$, and is very efficient for solving consistent problems and convenient for computing approximate projections with some required properties, as explained in [5].

The diagonal matrix $D_{m+n} \in \Re^{m+n,m+n}$ is defined in such a way of allowing us to modify the weights of the residuals r_1 and $\tilde{r}_2$. The idea is to strongly penalize r_1, and to use the Euclidean norm in regard to $\tilde{r}_2$ for diminishing its influence in the general procedure.

3. NUMERICAL RESULTS AND CONCLUSIONS

In the full paper we will present a comparison of the results obtained with RIOP, IOP [5],KERP [2], RKERP [3], for several image reconstruction problems. As it will be seen the RIOP efectiveness is remarkable in several problems. In forthcoming papers we will analyze alternative functions for penalizing the least squares problem, aiming at smoothing the image. Likewise, in regard to the same $R(x)$ used in this paper we will study the effect of adding neighboring pixels using a wider radius, and also what suitable weights are from a practical viewpoint.

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CONVERGENCE OF RELAXED ALTERNATING PROJECTION METHODS

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Key words: alternating projection method, Fejér monotonicity, weak convergence

Abstract

Let $\mathcal{H}$ be a real Hilbert space equipped with a scalar product $\langle\cdot,\cdot\rangle$ and with the norm $\|\cdot\|$ induced by $\langle\cdot,\cdot\rangle$. Further, let $A, B \subset \mathcal{H}$ be nonempty, convex and closed subsets. In the practical considerations one often needs to find an element of the intersection $A \cap B$ or, more general, to solve the following problem

$$\begin{aligned} &\text{find } a^* \in A \text{ and } b^* \in B \text{ such that} \\ &\|a^* - b^*\| = \inf_{a\in A, b\in B} \|a - b\|. \end{aligned} \tag{1}$$

We suppose that this infimum is attained. Several optimization problems, e.g. the convex feasibility problem can be reduce to problem (1) (see, e.g., [SY98, Section 2.9] for details). Problems of this kind have many practical applications, e.g. in signal reconstruction (see, e.g. [CB99] or [SY98, Chapter 6]), in image reconstruction or in intensity modulated radiation therapy (see, e.g. [CZ97, SY98, HK02]), where the convex subsets are described by a large and sparse system linear equalities or inequalities.

An important method generating sequences converging weakly to a solution of problem (1) is the von Neumann alternating projection method (AP-method) (see, e.g. [BB94, Section 4]). In the method, there are evaluated the metric projections successively onto A and B. It is known that $a^* \in A$ and $b^* \in B$ realizes the distance between A and B if and only if $a^* = P_A b^*$ and $b^* = P_B a^*$, i.e. $a^* \in \operatorname{Fix} P_A P_B$ or $b^* \in \operatorname{Fix} P_B P_A$ (see, e.g. [BB94, Lemma 2.2(i)]). Therefore, it is enough to find an element of $\operatorname{Fix} P_A P_B$ in order to find a solution of problem (1). In this lecture we construct a generalization of the AP-method and prove the weak convergence of the method to a solution. Consider a sequence $(x_k) \subset \mathcal{H}$ generated by the following iterative scheme

$$\begin{aligned} &x_1 \in A \text{ – arbitrary} \\ &x_{k+1} = P_A(x_k + \mu_k \lambda_k (P_A P_B x_k - x_k)), \end{aligned} \tag{2}$$

where the *relaxation parameter* $\mu_k \in [0, 2]$ and the *step size* $\lambda_k \geq 0$. We call the method (2) the *relaxed alternating projection method* (RAP-method). If we set $\mu_k = \lambda_k = 1$ in (2) we obtain the AP-method. One can show that any sequence (x_k) generated by the AP-method converges weakly to an element $x^* \in \operatorname{Fix} P_A P_B$ (see, e.g. [BB94, Theorem 4.8 and Lemma 2.2]). If $A \cap B \neq \varnothing$ then any sequence (x_k) generated by the RAP-method (2) converges weakly to an element $x^* \in \operatorname{Fix} P_A P_B = A \cap B$ if $\lambda_k = 1$ and $\mu_k \in [\varepsilon, 2 - \varepsilon]$, where $\varepsilon > 0$ (see, e.g. [BB96, Corollary 3.2.2] for more general

result). Gurin et al. have proposed the step size

$$\lambda_k = \frac{\|P_B x_k - x_k\|^2}{\langle P_B x_k - x_k, P_A P_B x_k - x_k\rangle} \qquad (3)$$

in order to accelerate the convergence of the RAP-method in the case $A \cap B \neq \varnothing$ (see, [GPR67, Theorem 4]). Recently, Bauschke et al. have applied this idea in the case A and B are subspaces of $\mathcal{H}$ (see [BDHP03, Theorem 3.23]). Unfortunately, the weak convergence of the RAP-method is not guaranteed for the step size (3) proposed by Gurin et al. if $A \cap B = \varnothing$.

We show the weak convergence of two RAP-methods to a fixed point of the operator $P_A P_B$, in the general case and in the case A is a closed affine subspace, without assumption $A \cap B \neq \varnothing$. In the case $A \cap B \neq \varnothing$ the proposed step sizes are not less than the proposed by Gurin et al.

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APPROXIMATE SUBGRADIENT METHODS OVER LAGRANGIAN RELAXATIONS ON NETWORKS

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Keywords: Nonlinear Programming, Approximate Subgradient Methods, Network Flows

Consider the nonlinearly constrained network flow problem **(NCNFP)**

$$\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to} & x \in \mathcal{F} \\ & c(x) \leq 0, \end{array}$$

where:

- The set $\mathcal{F}$ is

$$\mathcal{F} = \{x \in \Re^n \mid Ax = b,\ 0 \leq x \leq \overline{x}\},$$

  where A is a node-arc incidence $m \times n$-matrix, b is the production/demand m-vector, x are the flows on the arcs of the network represented by A, and $\overline{x}$ are the capacity bounds imposed on the flows of each arc.
- The side constraints $c(x) \leq 0$ are defined by $c : \Re^n \rightarrow \Re^r$, such that $c = [c_1, \cdots, c_r]^t$, where $c_i(x)$ is either linear, or nonlinear and twice continuously differentiable on the feasible set $\mathcal{F}$ for all $i = 1, \cdots, r$.
- $f : \Re^n \rightarrow \Re$ is nonlinear and twice continuously differentiable on $\mathcal{F}$.

We focus on the primal problem **NCNFP** and its dual problem

$$\begin{array}{ll} \text{maximize} & q(\mu) = \min\limits_{x \in \mathcal{F}}\ l(x, \mu) \\ \text{subject to:} & \mu \in \mathcal{M}, \end{array}$$

where the Lagrangian function is

$$l(x, \mu) = f(x) + \mu^t c(x)$$

and $\mathcal{M} = \{\mu \mid \mu \geq 0,\ q(\mu) > -\infty\}$. We assume throughout this paper that the constraint set $\mathcal{M}$ is closed and convex, q is continuous on $\mathcal{M}$, and for every $\mu \in \mathcal{M}$ some vector $x(\mu)$ that minimizes $l(x, \mu)$ over $x \in \mathcal{F}$ can be calculated, yielding a subgradient $c(x(\mu))$ of q at μ. We propose to solve **NCNFP** by using primal-dual methods (1).

The minimization of the Lagrangian function $l(x, \mu)$ over $\mathcal{F}$ can be performed by means of efficient techniques specialized for networks (10).

Since $q(\mu)$ is approximately computed, we consider *approximate subgradient methods* (4; 5; 6) in the solution of this problem. The basic difference between these methods and the classical subgradient methods is that they replace the subgradients with inexact subgradients.

An approximate subgradient method is defined by

$$\mu^{k+1} = [\mu^k + s_k c^k]^+,$$

where c^k is an approximate subgradient at μ^k, $[\cdot]^+$ denotes the projection on the closed convex set $\mathcal{M}$, and s_k is a positive scalar stepsize.

Different ways of computing the stepsize have been considered:

(a) Constant step rule (CSR) with Shor-type scaling (9).

(b) A variant of the constant step rule (VCSR) of Shor.

(c) Diminishing stepsize rule with scaling (DSRS) (8; 3; 9).

(d) The diminishing stepsize rule without scaling (DSR) suggested by Correa and Lemaréchal in (2).

(e) A dynamically chosen stepsize rule based on an estimation of the optimal value of the dual function by means of an adjustment procedure (DSAP) similar to that suggested by Nedić and Bertsekas in (7) for incremental subgradient methods.

The convergence of these methods was studied in the cited papers for the case of exact subgradients. The convergence of some of these approximate subgradient methods has been analyzed in (5; 6) (see also (4)).

In this work we put forward some basic convergence results when c^k is an approximate subgradient, which extend similar results obtained by Shor (9) for exact subgradients. Moreover, we compare the quality of the computed solution and the efficiency of the approximate subgradient methods when using CSR, VCSR, DSRS, DSR, and DSAP over **NCNFP** problems.

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Green Function and its Role in the Optimal Control of Infinite Dimensional Neutral Systems

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Abstract: In this talk, we shall deal with standard optimal control problems of linear neutral functional differential equations in Banach spaces. For the basis of the system theory of neutral models, the fundamental solution (Green function) is constructed and a variation of constants formula of the mild solution is established. We introduce a class of neutral resolvents of operators and prove that the Laplace transform of fundamental solution is just its neutral resolvent. Necessary conditions handling the fixed time integral convex cost problem of optimality are characterized in terms of the solutions of associated neutral adjoint systems. The maximum principle for time varying control domain is derived from optimality conditions. Also, the time optimal control problem to a target set for linear neutral systems is investigated.

LEVEL SET METHOD FOR SHAPE AND TOPOLOGY OPTIMIZATION OF CONTACT PROBLEMS

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Keywords: contact problem, structural optimization, level set method

1. INTRODUCTION

This paper deals with topology and shape optimization of an elastic contact problems. The shape optimization problem for elastic contact problem is formulated. Shape as well as topological derivatives formulae of the cost functional are provided using material derivative and asymptotic expansion methods, respectively. These derivatives are employed to formulate necessary optimality condition for simultaneous shape and topology optimization. Level set based numerical algorithm for the solution of the shape optimization problem is proposed. Numerical examples are provided and discussed.

2. PROBLEM FORMULATION

Consider deformations of an elastic body occupying two – dimensional domain Ω with the smooth boundary Γ. Assume $\Omega \subset D$ where D is a bounded smooth hold – all subset of R^2. The body is subject to body forces $f(x) = (f_1(x), f_2(x))$, $x \in \Omega$. Moreover, surface tractions $p(x) = (p_1(x), p_2(x))$, $x \in \Gamma$, are applied to a portion Γ_1 of the boundary Γ. We assume, that the body is clamped along the portion Γ_0 of the boundary Γ, and that the contact conditions are prescribed on the portion Γ_2, where $\Gamma_i \cap \Gamma_j = \emptyset$, $i \neq j$, $i, j = 0, 1, 2$, $\Gamma = \bar{\Gamma}_0 \cup \bar{\Gamma}_1 \cup \bar{\Gamma}_2$.

We denote by $u = (u_1, u_2)$, $u = u(x)$, $x \in \Omega$, the displacement of the body and by $\sigma(x) = \{\sigma_{ij}(u(x))\}$, $i, j = 1, 2$, the stress field in the body. Consider elastic bodies obeying Hooke's law, i.e., for $x \in \Omega$ and $i, j, k, l = 1, 2$

$$\sigma_{ij}(u(x)) = a_{ijkl}(x) e_{kl}(u(x)). \qquad (1)$$

We use here and throughout the paper the summation convention over repeated indices (2). The strain $e_{kl}(u(x))$, $k, l = 1, 2$, is defined by:

$$e_{kl}(u(x)) = \frac{1}{2}(u_{k,l}(x) + u_{l,k}(x)), \qquad (2)$$

where $u_{k,l}(x) = \frac{\partial u_k(x)}{\partial x_l}$. The stress field σ satisfies the system of equations (2)

$$-\sigma_{ij}(x)_{,j} = f_i(x) \quad x \in \Omega, i, j = 1, 2, \qquad (3)$$

where $\sigma_{ij}(x)_{,j} = \frac{\partial \sigma_{ij}(x)}{\partial x_j}$, $i, j = 1, 2$. The following boundary conditions are imposed

$$u_i(x) = 0 \quad \text{on} \quad \Gamma_0, \quad i = 1, 2, \qquad (4)$$

$$\sigma_{ij}(x) n_j = p_i \quad \text{on} \quad \Gamma_1, \quad i, j = 1, 2, \qquad (5)$$

$$u_N \leq 0, \quad \sigma_N \leq 0, \quad u_N \sigma_N = 0 \quad \text{on } \Gamma_2, \qquad (6)$$

$$\mid \sigma_T \mid \leq 1, \quad u_T \sigma_T + \mid u_T \mid = 0 \quad \text{on } \Gamma_2, \qquad (7)$$

where $n = (n_1, n_2)$ is the unit outward versor to the boundary Γ. Here $u_N = u_i n_i$ and $\sigma_N = \sigma_{ij} n_i n_j$, $i, j = 1, 2$, represent the normal components of displacement u and stress σ, respectively. The tangential components of displacement u and stress σ are given by $(u_T)_i = u_i - u_N n_i$ and $(\sigma_T)_i = \sigma_{ij} n_j - \sigma_N n_i$, $i, j = 1, 2$, respectively. $\mid u_T \mid$ denotes the Euclidean norm in R^2 of the tangent vector u_T. The results concerning the existence of solutions to (1) - (7) can be found in (2).

Let us recall from (3) the cost functional approximating the normal contact stress on the contact boundary

$$J_\phi(u(\Omega)) = \int_{\Gamma_2} \sigma_N(u) \phi_N(x) ds, \qquad (8)$$

depending on the auxiliary given bounded function $\phi(x)$, $x \in \Omega$. Let us denote by U_{ad} the set of admissible domains. Consider the following

shape optimization problem: For a given function ϕ, find a domain $\Omega^\star \in U_{ad}$ such that

$$J_\phi(u(\Omega^\star)) = \min_{\Omega \in U_{ad}} J_\phi(u(\Omega)), \qquad (9)$$

where σ_N and ϕ_N are the normal components of the stress field σ corresponding to a solution u satisfying (1) - (7) and the function ϕ, respectively.

3. OPTIMALITY CONDITIONS

In the paper the optimality conditions for structural optimization problem (9) are formulated. Using material derivative method (1; 3) as well as asymptotic expansion method (1; 4) we calculate shape as well as topological derivatives of the cost functional (8). Finally the optimality condition for simultaneous shape and topology optimization problem is formulated.

4. LEVEL SET METHODS

In the paper the level set method (5) is employed to solve numerically problem (9). Consider the evolution of a domain Ω under a velocity field V. Let $t > 0$ denote the time variable. Under the mapping $T(t, V)$ we have

$$\Omega_t = T(t, V)(\Omega) = (I + tV)(\Omega), \quad t > 0.$$

By Ω_t^- we denote the interior of the domain Ω_t and by Ω_t^+ we denote the outside of the domain Ω_t. The domain Ω_t and its boundary $\partial\Omega_t$ are defined by a function $\Phi = \Phi(x, t) \;:\; R^2 \times [0, t_0) \to R$ satisfying

$$\begin{cases} \Phi(x,t) = 0, & \text{if } x \in \partial\Omega_t, \\ \Phi(x,t) < 0, & \text{if } x \in \Omega_t^-, \\ \Phi(x,t) > 0, & \text{if } x \in \Omega_t^+, \end{cases} \qquad (10)$$

i.e., the boundary $\partial\Omega_t$ is the level curve of the function Φ. Assume that velocity field V is known for every point x lying on the boundary $\partial\Omega_t$, i.e., with $\Phi(x, t) = 0$. Therefore the equation governing the evolution of the interface in $D \times [0, t_0]$ has the form (5)

$$\Phi_t(x, t) + V(x, t) \cdot \nabla_x \Phi(x, t) = 0, \qquad (11)$$

where Φ_t denotes a partial derivative of Φ with respect to the time variable t.

5. NUMERICAL METHODS

The structural optimization problem (9) is solved numerically as the shape and topology optimization problem. First the shape optimization problem is solved using the described level set method. In equation (11) velocity field V is set equal to the shape gradient of the cost functional (8). When the decrease in the cost functional value is less than the prescribed tolerance value the topology optimization problem is solved. The finite element method is used as the discretization method. Numerical results are provided. Obtained numerical results shows that the proposed algorithm allows for significant improvments from one iteration to the next.

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OPTIMAL GUIDANCE OF MOBILE SENSOR NETWORK NODES FOR FAULT DETECTION IN DISTRIBUTED PARAMETER SYSTEMS

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Keywords: distributed parameter systems, sensor location, fault detection, parameter estimation, algorithmic optimal control

1. INTRODUCTION

Although we witness an extremely fast development of methods of Fault Detection and Isolation (FDI) for dynamical systems in the last decade (1), (2), (3), (4), there is a grave lack of the corresponding effective techniques dedicated to distributed parameter systems (DPSs). Furthermore, within the framework of FDI systems, the optimization of data acquisition process which increases the reliability of the diagnosis is most often neglected and the contributions are very scarce. Within the framework of diagnostics, the crucial difficulty is the definition of a suitable criterion describing the relations between the quality of the system diagnosis and the observation strategy. One of the most prospective approaches in this context is to make use of techniques originating in parameter estimation, see the works (5) and (6) where the appropriate performance measure, the so-called D_s-optimality criterion, defined on the Fisher Information Matrix (FIM) associated with the unknown system parameters, was used as a measure of the 'goodness' of experimental conditions. Nevertheless, more efforts are needed in order to adapt this approach in the context of modern measurement systems encountered in applications.

In order to estimate the unknown parameters of DPS models in the form of partial differential equations (PDEs), the system's behaviour or response is observed with the aid of some suitable collection of sensors termed the measurement or observation system. For variables which can be measured on-line, it is usually possible to make the measurements continuously in time. However, it is generally impossible to measure process states over the entire spatial domain. What is more, the measurements are inexact by virtue of inherent errors of measurement associated with transducing elements and also because of the measurement environment.

The inability to take distributed measurements of process states leads to the question of where to locate sensors so that the information content of the resulting signals with respect to the distributed state and PDE model be as high as possible. This is an appealing problem since in most applications these locations are not prespecified and therefore provide design parameters. The importance of sensor planning has already been recognized in many application domains, e.g., air quality monitoring systems, groundwater-resources management, recovery of valuable minerals and hydrocarbon, model calibration in meteorology and oceanography, hazardous environments and emerging smart material systems.

The sensor location problem was attacked from various angles, but the results communicated by most authors are limited to the selection of stationary sensor positions (for reviews, see (7), (8), (9)). An appealing alternative to such an approach is to apply spatially-movable sensors, which leads to the so-called continuous scanning observations. This is somewhat intimidating because of the complexity of the resulting optimization problem, but in recompense for such efforts a number of benefits are derived. This is due to the fact that sensors are not assigned to fixed positions which are optimal only on the average, but are capable of tracking points which provide at a given time moment best information about

the parameters to be identified. Consequently, by actively reconfiguring a sensor system we can expect the minimal value of an adopted design criterion to be lower than the one for the stationary case. It is important to note that planning techniques developed for moving sensors can prove useful in many areas of automation. A possibility of using moving observations does arise in a variety of applications, e.g., air pollutants in the environment are often measured using data gathered by monitoring cars moving in an urban area and atmospheric variables are measured using instruments carried in an aircraft. What is more, technological advances in communication systems and the growing ease in making small, low power and inexpensive mobile systems now make it feasible to deploy a group of networked vehicles in a number of environments (10), (11). A cooperated and scalable network of vehicles, each of them equipped with a single sensor, has the potential to substantially improve the performance of the observation systems. Applications in various fields of research are being developed and interesting ongoing projects include extensive experimentation based on testbeds. The problem to be discussed in this paper cought our attention while working on one of such experimental platforms, namely the MAS-net lab testbed being a distributed system equipped with two-wheeled differentially driven mobile robots capable of sensing the states of DPSs described by diffusion and wave equations (12), (13).

In this work we outline an approach to determine D_s-optimal sensor nodes trajectories whose measurements are supposed to serve as a base for fault detection for a DPS defined in a two-dimensional spatial domain. As will be shown, this formulation allows for maintaining a low complexity regarding possible implementations of the resulting strategy in practice. Moreover, we also show how the proposed formulation can be transformed into an equivalent optimal control problem in Mayer form, which can be efficiently solved by the Matlab toolbox Riots, a high-performance tool for solving optimal control problems (15). The paper will be illustrated with numerical examples regarding determination of optimal sensor schedules for a parabolic DPS.

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FINITE ELEMENT MULTIOBJECTIVE DESIGN OF PERMANENT MAGNET GENERATOR BASED ON DIMENSIONALITY REDUCTION

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Keywords: heuristics, evolutionary multi-criteria optimization, electrical machines design, permanent magnet generator

1. INTRODUCTION

The paper describes metaheuristic optimisation of permanent magnet generator (PMG) design problem based on the novel finite element analysis model (Woźniak). This is nonlinear optimisation problem with many constraints with five objectives what is very challenging for most Pareto evolutionary multiobjective (EMO) algorithms. The majority of citations on EMO deal problems with lower dimensionality (Deb). Increasing criteria number causes difficulties in terms of reduced selection pressure for better solutions, runtime increase, as well as results visualisation to the decision maker problems. The dimensionality reduction is very appealing approach to ease this problems.

In this paper two procedures of dimensionality reduction are applied to the finite element PMG EMO design: principal component analysis (PCA) and partial dominance structure preservation (PDSP) based on δ-dominance approach (Brockhoff). Results are compared.

This paper has the following outline. Section 2 provides basic concepts on the dimensionality reduction problem. Section 3 contains the PMG design problem introducing the finite element model. Section 4 includes analysis of the PMG design problem objective space and EMO computational setup details. Results of the Pareto optimisation and dimensionality reduction are analysed in details.

2. PROBLEM FORMULATION

In this paper a minimisation problem is considered with n objective functions $f_i : X \to \mathbb{R}$ from set F, each mapping solution $x \in X$ from decision space X, to an objective vector $z \in Z$ from objective space Z, with partial order $rel \subseteq Z \times Z$ defined. The considered methods of dimensionality reduction seek the minimal set of objectives that can explain most of the design problem variance in the objective space.

3. DESIGN ISSUES

This section presents the full model and design constants of the PMG for the finite element analysis with the flat parameterisation. The two decision arguments {D, h}, are defined in Fig. 1.

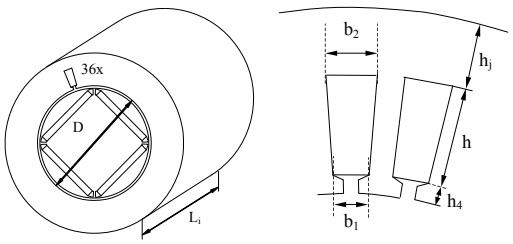

Fig 1. Machine dimensions and definition of optimisation problem arguments {D, h}.

The five objectives of the PMG MO problem are strongly nonlinear functions of the arguments.

4. OPTIMISATION OF THE PMG

In this Section the analysis all objectives are presented (as in Fig. 2) in the form of set of 3D views of surfaces generated for a set of solutions defining the mesh nodes X_{nodes} in the decision space. The Pareto set for the finite element PMG design cannot be considered as approximation of convex set.

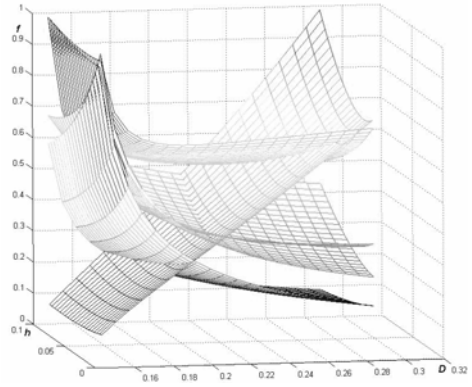

Fig. 2. Mesh 3D view of all scaled objectives of the PMG design problem

For the PMG EMO design the NSGA II was implemented within the MATLAB for Windows workspace. Dimensionality reduction by means of PCA NSGA II procedure (Deb) was performed. Sample results of the first step

$$\lambda^T = [3.2469 \quad 1.1795 \quad 0.4714 \quad 0.0745 \quad 0.0277]$$

$$V^T = \begin{bmatrix} 0.5416 & 0.5328 & -0.4503 & 0.1668 & 0.4384 \\ -0.0974 & -0.0610 & -0.0429 & -0.8682 & 0.4808 \\ 0.0564 & 0.2419 & 0.8458 & 0.1773 & 0.4376 \\ 0.5781 & -0.7744 & 0.0418 & 0.1131 & 0.2270 \\ -0.5998 & -0.2326 & -0.2798 & 0.4173 & 0.5776 \end{bmatrix}$$

i.e. elements of the eigenvector v_1 corresponding to the largest eigenvalue λ_1 (first principal component) shows that the first and second objectives are the least conflicting.

The same result is obtained in the first step of the PDSP-based procedure. It is presented in form of the parallel coordinates plot in Fig. 3.

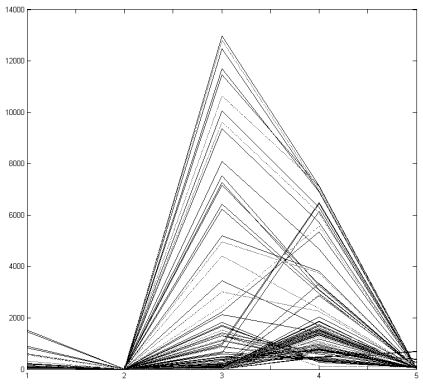

Fig. 3. Parallel coordinates plot.

The correlation assessments hold locally at the dominating solutions approximations, but not in set X_{nodes} evenly distributed (as mesh in Fig.2) in the two-dimensional decision space.

Consecutive steps of objectives reduction are described, results of the PCA NSGA II, and PDSP-based procedure are compared and discussed in final form of the paper.

This paper provides a basis for further research on design methods with a more detailed PMG models, including saturation of the magnetic circuit and 3D analysis. On the basis of this results author plans further research on shortening the Pareto front approximation to reflect decision maker's preferences.

5. CONCLUSIONS

In this paper results of application of two different methodologies, namely principal component analysis (PCA) and the one based on partial dominance structure preservation (PDSP) are presented and compared. The PDSP showed to be more restrictive, and let to reduce only two objectives (i.e. from five to three) what has been visualised on parallel coordinates plots.

This study is a continuation of author's research. The key contributions are:

- results for five-objective problems dimensionality reduction. To the author's best knowledge these are the first real-world show-case problem results for the PDSP δ-dominance approach (Brockhoff) presented,
- a comparison between dimensionality reduction results of EMO fine element design of the PMG, using the PCA NSGA II, and PDSP-based procedure.

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LAGRANGIAN RELAXATION FOR STOCHASTIC OPTIMIZATION WITH PROBABILISTIC CONSTRAINTS

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Nonlinear stochastic optimization problems with probabilistic constraints are examined. The concept of a p-efficient point of a probability distribution is used to derive equivalent problem formulations, and necessary and sufficient optimality conditions are derived. Lagrangian relaxation of the problem is analyzed, the dual functional and its subdifferential.

Two algorithms for solving the dual problem are developed. The algorithms are based on cutting plane techniques for approximation of the dual functional and the p-efficient frontier. The algorithms yield an optimal solution for problems involving r-concave probability distributions. For general probability distributions the algorithms provide an optimal solution of the convexified problem, and a suboptimal solution of the original problem, as well as upper and lower bounds for the optimal value of the original optimization problem.

The results are applied to solve a bond portfolio problem with probabilistic liquidity constraint. Numerical illustration is provided which demonstrates the numerical efficiency of the methods.

This is a joint work with Darinka Dentcheva, Stevens Institute of Technology, and Andrzej Ruszczynski, Rutgers University.

No degradation of efficiency in very high dimensional Monte Carlo computations

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Keywords: multidimensional normal distribution, Monte Carlo methods, probabilities of convex sets, efficiency of estimators, comparison of performances.

1 Introduction

Our aim is twofold in this paper: to show via computing numerical examples ranging from one-hundred to one-thousand dimensional integration problems, that normal probabilities of sets can be computed in thousand dimensions in a few minutes and second: the efficiency of some estimators does not decrease with increasing the number of dimensions. The examples concern the computation of the probabilities of convex sets (polyhedra and hyperellipsoids) in case of multidimensional normal probabilities. The FORTRAN subroutines used in testing can be found at `www.uni − corvinus.hu/ ∼ ideak1`.

2 Efficiency

Assume, that we have two Monte Carlo estimators Θ_1 and Θ_2 for computing a given integral I, where $E(\Theta_1) = E(\Theta_2) = I$, with variances $D^2(\Theta_1)$ and $D^2(\Theta_2)$, and the times necessary to evaluate the estimators are t_1 and t_2 respectively. Then the efficiency of the second estimator with respect to the first one is defined [3] as

$$\text{Efficiency} = \frac{t_1 D^2(\Theta_1)}{t_2 D^2(\Theta_2)}. \tag{1}$$

This measure of efficiency is used to compare different Monte Carlo estimators, and this is generally thought to be declining with increasing the number of dimensions.

3 Computing multidimensional normal probabilities

Consider the density function φ and the distribution function Φ of the n-dimensional normal distribution with mean $\mathbf{0}$ and correlation matrix R. In this case the probability of the n-dimensional set X is

$$I = Pr\{X\} = \int_X \varphi(\mathbf{z})d\mathbf{z} = \int_{R^n} f(\mathbf{z})d\Phi(\mathbf{z}). \tag{2}$$

The **crude estimator** suggested by the right hand side can be given as follows. Generate samples $\mathbf{x}_i, i = 1, \ldots, N$ of the normal random variable $\boldsymbol{\xi}$ with density function φ and compute an unbiased estimator of I as

$$\Theta_1 = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i). \tag{3}$$

The efficiency of all other estimators is given with respect to this basic estimator thorough this paper.

A normally distributed random vector $\boldsymbol{\xi}$ can be written as $\boldsymbol{\xi} = \chi_n T\boldsymbol{\eta}$, where χ_n is a χ-distributed scalar random variable, with n degrees of freedom, T is an upper triangular matrix, for which $TT' = R$, and the vector $\boldsymbol{\eta}$ is uniformly distributed on the surface of the unit sphere $S = \{\mathbf{x}|\sum_{i=1}^{n} x_i^2 = 1\}$. Note, that χ_n, and $\boldsymbol{\eta}$, are independent. Let us denote the distribution function of the χ-distributed random variable by $K(s), s \geq 0$ and the distribution function of $\boldsymbol{\eta}$ by $V(\mathbf{y}), \mathbf{y} \in S$. Then

$$I = \int_{R^n} f(sT\mathbf{y})dK(s)dV(\mathbf{y}) = \qquad (4)$$
$$\int_S \left(\int_0^\infty f(sT\mathbf{y})dK(s) \right) dV(\mathbf{y}).$$

Introducing a notation for the inner integral

$$g(\mathbf{y}) = \int_0^\infty f(sT\mathbf{y})dK(s),$$

clearly the function $g(\mathbf{y})$ gives the probability content of that portion of the ray $\lambda T\mathbf{y}, \lambda \geq 0$, which lies inside the set X. Since for convex bodies bounded by linear or quadratic constraints the intersection of a line with the boundaries can be evaluated, thus for these cases the function $g(\mathbf{y})$ can be evaluated (it is the difference of two χ distribution function values). Define the following function $e(\mathbf{y}) = \left(g(\mathbf{y}) + g(-\mathbf{y})\right)/2$ which is the result of applying the same idea to the vectors $\mathbf{y}$ and $-\mathbf{y}$ simultaneously.

Consider now a random orthonormalized system U of vectors on S, $U = \{\mathbf{u}^i, i = 1, \ldots, n | \mathbf{u}^i \in S, (\mathbf{u}^i)'(\mathbf{u}^j) = \delta_{ij}, i, j = 1, \ldots, n\}$. Then consider the normalized sum of any two vectors from U, that is let

$$\mathbf{v}^{i,j,\mathbf{s}} = \frac{1}{\sqrt{2}} \left(s_1 \mathbf{u}^i + s_2 \mathbf{u}^j \right),$$

where the pair of indices i, j and the sign vector $\mathbf{s}$ runs through all possible triplets from the set

$$J^* = \{(i, j, \mathbf{s}) | i = 1, \ldots, n, j = 1, \ldots, n, i < j, \\ s_1 = 1, s_2 = 1, \text{or } s_1 = 1, s_2 = -1\}. \quad (5)$$

The previous estimator is applied to the resulting $n(n-1)$ vectors $\mathbf{v}^{i,j,\mathbf{s}}$: this is called the **orthonormalized − 2**, or O_2 estimator.

So the complete estimator O_2 for $N = 1$ system U, when two vectors from U are added and subtracted in all possible ways, has the form

$$O_2 = \frac{1}{n(n-1)} \sum_{(i,j),\mathbf{s} \in J^*} e\left(T\mathbf{v}^{i,j,\mathbf{s}}\right) = \\ \frac{1}{n(n-1)} \sum_{(i,j),\mathbf{s} \in J^*} e\left(\frac{1}{\sqrt{2}} \left(s_1 T\mathbf{u}^i + s_2 T\mathbf{u}^j \right) \right).$$

This is called the orthonormalized-2, or O_2 estimator. Obviously, in actual computation we generate N diferent systems U and average the results.

4 Numerical results

To test the efficiencies of the orthonormalized estimators we computed the probabilities of a great number of randomly generated sets (polyhedra and hyperellipsoids). Computer experiences were carried out on a PC, with a 2.8 GHz processor, memory of 1 Gbyte, in dimensions up to $n = 1000$.

To summarize our experiences we can state, that about three accurate digits of probability can be obtained in 10–30 minutes even in $n = 1000$ dimensions. We obtained an average efficiency of 10–100 for examples from $n = 100$ to $n = 1000$ dimensions for polyhedra. For random hyperellipsoids our findings are about the same as for polyhedra: the efficiency remains between 10 and 1000 for n-dimensional sets. The efficiencies were somewhat greater for hyperellipsoids than for polyhedra.

We believe, that the reason, why efficiency does not deteriorate with increasing the number of dimensions is the following: an orthonormalized-2 estimator computes the function value at $O(n^2)$ points (as compared to the crude estimator, where the number of function evaluations can be kept constant – to preserve the same standard deviation of estimator Θ_1). This number of function evaluations is computationally feasible and sufficient to preserve the efficiency.

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COMPARISON OF THE EXACT AND APPROXIMATE ALGORITHMS IN THE RANDOM SHORTEST PATH PROBLEM

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Keywords: Multi-objective Shortest Path Problem

1. INTRODUCTION

The determination of the shortest path in a given graph i.e. the classical shortest path problem (CSPP) is one of the basic problems of computational geometry. It has been discussed and many algorithms were proposed in the literature. See, for instance (Ahuja et.al, 1993), (Cormen et.al, 1990). Usually the authors consider the deterministic models where distances between vertices are deterministic. In only a few papers this problem was stated in random case when the distances are defined by random variables and some algorithms were proposed (Murthy et.al, 1996), (Murthy et.al, 1997).

In this paper the static random shortest path problem with the second moment criterion is discussed and a comparison of proposed exact and approximate algorithm is given.

2. PROBLEM STATEMENT

Let $G = (V, E)$ be a directed graph with a finite set of vertices V and a set of edges $E \subseteq V \times V$. Further, let $s \in V$ be a source vertice and let $t \in V$ be a destination vertice.

In the Random Shortest Path Problem (RSPP) each edge $e \in E$ is associated with a random variable T_e taking positive values. The goal is to find the path, from the source vertice s to the destination vertice t, which minimize a function of moments of random variables related with edges of the path. We also assume that the random variables T_e, for $e \in E$, are independent. We propose to consider a criterion that is a minimal sum of the variance and a square of the expected value of the sum of random variables related with edges of the path, i.e. the second moment of the sum of random variables related with edges of the path, because of $(\mathbf{E}[X])^2 + \mathbf{V}[X] = \mathbf{E}[X^2]$. Similar criterion has been considered by I. Murthy and S. Sarkar in (Murthy et.al, 1996).

Now we formulate the RSPP with criterion of the second moment. Let

$$\mathcal{P} = \{\langle v_0, v_1, \ldots, v_{n-1}, v_n\rangle | v_0 = s \wedge v_n = t \wedge \wedge (v_0, v_1), \ldots, (v_{n-1}, v_n) \in E\}$$

be a set of all paths from the source vertice s to the destination vertice t. The goal in the RSPP is to find a path $\langle v_0, v_1, \ldots, v_{n-1}, v_n\rangle \in \mathcal{P}$ such that

$$\mathbf{E}\Big[\Big(\sum_{i=1}^{n} T_{(v_{i-1},v_i)}\Big)^2\Big] = = \min_{\langle u_0,u_1,\ldots,u_{m-1},u_m\rangle \in \mathcal{P}} \mathbf{E}\Big[\Big(\sum_{i=1}^{m} T_{(u_{i-1},u_i)}\Big)^2\Big].$$

To show that the problem can not be solved directly, for instance by Dijkstra algorithm it is presented an example of a random graph where the application of the Bellman Principle of optimality fails, i.e. where the subpath of the shortest path is not the shortest subpath.

3. MAIN RESULTS

In this section exact algorithms and approximate algorithms are introduced. It will be shown that the RSPP with the second moment criterion re-

duces to the Multi-objective Shortest Path Problem (MOSPP), thus the RSPP can be solved with a help of general methods for solving the MOSPP. First, two exact algorithms are presented, namely Extended Bellman-Ford algorithm (EBF) with a modified procedure of the relaxation of edge and a Generic Label Correcting algorithm (GLC) which is a kind of generalization of the classical Dijkstra algorithm. In this algorithm relaxations of edges are coming in a little bit more natural order than in the EBF algorithm. Unfortunately, the time complexity and also the space complexity of these general algorithms are exponential. Therefore a few approximate algorithms with the polynomial time complexity are proposed. One of them is a modification of EBF algorithm in which we have to assign with each vertice the list of all nondominated cost vectors related with all paths to this vertice. Unfortunately, for this reason EBF algorithm has an exponential complexity. The proposed approximate algorithm is a natural modification of EBF which assigns with the each vertice the list of a fixed number (the same for all vertices) of cost vectors. Another approximate algorithm is the Single Criterion Approximation algorithm (SCA). The idea of the algorithm is based on the fact that the RSPP with the second moment criterion reduces to the MOSPP. In this algorithm we permanently calculate the shortest path with respect to the one criterion and remove from the graph the edge with the greatest value of the second criterion.

The last proposed approximate algorithm is a variant of the algorithm presented in (Tsaggouris et.al, 2005) and (Tsaggouris et.al, 2006). The algorithm is a modification of classical Bellman-Ford algorithm to the MOSPP. In this algorithm we first estimate for each vertice v the minimal and the maximal distance from the source vertice s to the vertice v. Next, if some path from the source vertice s to the vertice v has the first criterion cost μ then we store the second criterion of the path at the position

$$\left\lceil k \cdot \frac{\mu - \mu_{min}(v)}{\mu_{max}(v) - \mu_{min}(v)} \right\rceil,$$

where μ_{min}, μ_{max} are the estimated minimal and maximal distances and k is the size of the array.

4. COMPUTATIONAL RESULTS

We performed our tests on quite large randomly generated graphs. Moreover, used graphs had from 10000 to 30000 vertices and each vertice had 10 outcoming edges. All the tests was made on Intel Celeron Mobile 1400MHz with 256MB RAM, working under control of Linux operating system with kernel version 2.6.11-6. Obtained results shows that the first proposed approximate algorithm works very well, i.e. its works very quickly and usually produce exact answer. The SCA algorithm is not so good and the last one works very longly, because the main loop of this algorithm usually can not be broken.

5. CONCLUSIONS

Computational results of the test of the presented exact and approximate algorithms, show that the approximate algorithms are much faster than the exact ones and could be very useful, for example, as a first approximation stage of some more difficult algorithm solving the RSPP. Moreover, carried out detailed analysis of different data representations can be used for solving the RSPP with criterion of higher moments.

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A STOCHASTIC ALGORITHM FOR ENGINEERING OPTIMIZATION PROBLEMS

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Key works: numerical optimization, stochastic, random, algorithm.

1. INTRODUCTION

There are many algorithms, traditional computation or evolutionary computation, for single-objective optimization problems. Almost all focus on the determination of positions neighbouring an optimal solution and handle constraints based on violated constraints. We can suppose that every decided variable of an optimization problem has digits that are listed from left to right; we have our remarks as follows:

- To evaluate objective function, the role of left digits is more important than the role of right digits of a decided variable; we calculate the changing probabilities of the appearance of a better solution than the current one on each iteration, and on the performance of SP algorithm, we create good conditions for its appearance.
- Based on the relation of decided variables in the formulas of constrains and objective function we select k variables ($1 \le k \le n$) to change their values instead of selecting all n variables on each iteration.
- Because we can not calculate exactly the number of iterations of a stochastic algorithm for searching an optimal solution the first time on each performance, we use unfixed number of iterations, which has more chance to find an optimal solution the first time with necessary number of iterations.

Based on these remarks we introduce a new stochastic algorithm, Search via Probability (SP) algorithm, the SP algorithm uses probabilities to control the process of searching for optimal solutions.

2. THE MODEL OF SINGLE-OBJECTIVE OPTIMIZATION PROBLEM

We consider a model of single-objective optimization problem as follows:

Minimize $f(x)$

subject to

$$g_j(x) \le 0 \quad (j = 1, \ldots, r)$$

where

$$x = (x_1, x_2, \ldots, x_n),$$
$$a_i \le x_i \le b_i,\ a_i, b_i \in R,\ i = 1, \ldots, n.$$

3. PROBABILITIES OF CHANGES AND SELECTING VALUES OF A DIGIT

We suppose that every decided variable x_i ($1 \le i \le n$) has m digits that are listed from left to right $x_{i1}, x_{i2}, \ldots, x_{im}$ (x_{ij} is an integer and $0 \le x_{ij} \le 9$, j=1, …,m). We calculate changing probabilities of digits which can find better values than the current ones on each iteration.

3.1. Probabilities of changes

Consider the j-th digit x_{ij} of variable x_i, let A_j be an event that digit x_{ij} can find a better value than the current one ($1 \le j \le m$). Event A_j is more important than event A_{j+1}, it means that the occurrence of event A_j has a decisive influence on the occurrence of event A_{j+1} and after event A_j occurs a certain number of times, it will

create good conditions for event A_{j+1} to occur. Let q_i (i=1,…, m) be probability of A_i, r_i be number of iterations of event A_i ($r_i \geq 1$, i=1,…, m). Because $A_1, A_2, \ldots, A_i$ are independent of one another, these probabilities are maximum if

$$q_i = r_i / \sum_{k=i}^{k=m} r_k \quad (i = 3, \ldots, m)$$

Because left events are more important than right events, it means that left events are more stable than right events, we have:

$$r_1 \leq r_2 \leq \ldots \leq r_m$$

Therefore:

$$q_1 \leq q_2 \leq \ldots \leq q_m \text{ and } q_i \leq 1/(m+1-i)$$

Ex: Let $r_1=r_2=\ldots=r_m=1$, we have:

$$q_1 = \frac{1}{m}, q_2 = \frac{1}{m-1}, \ldots, q_{m-1} = \frac{1}{2}, q_m = 1$$

We have average probabilities of changes:

$$p_j = \frac{1}{j}(1 + \frac{1}{2} + \ldots + \frac{1}{j}) \qquad (1 \leq j \leq m)$$

and m=7, we have:

p=(0.37, 0.41, 0.46, 0.52, 0.61, 0.75, 1)

The changing probabilities of digits of a variable increase from left to right. This means that left digits are more stable than right digits, and right digits change more than left digits. In other words, the role of left digit x_{ij} is more important than the role of right digit $x_{i,j+1}$ ($1 \leq j \leq m-1$) for evaluating objective function.

3.2. Probabilities for selecting values of a digit.

Consider j-th digit with changing probability q_j, let R_1 be the probability of choosing a random integer number between 0 and 9 for j-th digit, let R_2 be probabilities of j-th digit incremented by one or a certain value, let R_3 be probabilities of j-th digit decremented by one or a certain value. The average probabilities of R_1, R_2 and R_3 are:

$R_1=0.5$, $R_2=R_3=0.25$.

4. SELECTING K VARIABLES (1≤K≤N) TO CHANGE THEIR VALUES

On each iteration, if we select n variables to change their values, the ability of finding a better solution than the current one can be very small. Therefore we select k variables ($1 \leq k \leq n$) to change their values, and after a number of iterations the algorithm has more chance to find a better solution than the current one.

5. THE RANDOM SEARCH VIA PROBABILITY ALGORITHM

The main idea of SP algorithm is that variables of problem are separated into discrete digits, and then they are changed with the guide of probabilities and combined to a new solution. The SP algorithm has the following characteristics: The SP algorithm finds a better value than the current one of digits one by one from left digits to right digits of every variable with the guide of probabilities. Variable Loop that counts number of iterations will be set to 0 if SP algorithm finds a better solution than the current one; this means that SP algorithm can find an optimal solution the first time after a necessary number of iterations.

6. EXAMPLES

We chose 5 engineering optimization problems as follows:

1. Design of a Welded Beam.
   The version of Coello.
   The version of Ray and Liew.
2. Design of a Pressure Vessel.
3. Minimization of the Weight of a Tension/Compression String.
4. Minimization of the Weight of a Speed Reducer.

We tested this approach by implementing the SP algorithm on 6 test single-objective optimization problems, and we found very good and stable results.

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ON A CONSTRAINED CONTROL MAYER'S PROBLEM FOR SINGULARLY PERTURBED DELAYED SYSTEMS

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Keywords: time delay system, singular perturbation, optimal control

1. INTRODUCTION

Control problems for singularly perturbed systems are studied extensively for about four recent decades. Most of publications in the topic are devoted to analysis of undelayed dynamics control problems (see e.g. [1-3,10] and references therein). Control problems for singularly perturbed delayed systems are studied much less (see e.g [1,4-9,11] and references therein).

One of the important issues, arising in control theory, is the optimization of a controlled system with respect to a given performance index. The rich literature is devoted to studying this issue for singularly perturbed undelayed systems with unconstrained controls (see e.g. [10]) and constrained controls (see e.g. [2,3]). Optimal control problems for singularly perturbed systems with delays were studied only in several works. The problems with unconstrained controls were considered in [4-6,11] (the case of small delay) and in [8,9] (the case of nonsmall delay). For our best knowledge, optimal control problems with constrained controls for singularly perturbed delayed systems were not studied in the literature.

In this presentation we consider an optimal control problem with a prescribed duration for a singularly perturbed linear time-dependent system with a point-wise state delay. The initial condition for this system is given. The control is constrained by linear inequalities. The cost functional is a linear function of the terminal value of the slow state variable. The delay is small of order of the small parameter $\varepsilon > 0$ multiplying a part of the derivatives in the system. An asymptotic behavior (for $\varepsilon \to +0$) of the solution of the considered optimal control problem is studied.

It should be noted that singularly perturbed delayed systems with small delays of order of the small multiplier for a part of the derivatives have a significant importance in the theory (functional-differential equations, control theory) and various applications. A brief survey on this topic can be found in [7].

2. PROBLEM STATEMENT AND MAIN RESULTS

Consider the following system

$$dx(t)/dt = \sum_{i=0}^{1} \Big[A_{i1}(t)x(t-\varepsilon h_i) + A_{i2}(t)y(t-\varepsilon h_i)\Big] + B_1(t)u(t), \tag{1}$$

$$\varepsilon dy(t)/dt = \sum_{i=0}^{1} \Big[A_{i3}(t)x(t-\varepsilon h_i) + A_{i4}(t)y(t-\varepsilon h_i)\Big] + B_2(t)u(t), \tag{2}$$

where $t \in [0,T]$; $x(t) \in E^n$, $y(t) \in E^m$, $u(t) \in E^r$ (u is a control); $\varepsilon > 0$ is a small parameter; $h_0 = 0$; $h_1 > 0$ is a given constant independent of ε; $T > 0$ is a given time instant independent of ε; $A_{ij}(t)$ and $B_k(t)$, $(i = 0,1;\ j = 1,...,4;\ k = 1,2)$ are given matrices of corresponding dimensions.

For (1)-(2), the initial conditions are given

$$x(\tau) = \varphi_x(\tau), \quad y(\tau) = \varphi_y(\tau), \ \tau \in [-\varepsilon h_1, 0], \tag{3}$$

where $\varphi_x(\tau)$ and $\varphi_y(\tau)$ are given vectors.

The admissible controls are measurable functions for $t \in [0,T]$ satisfying the inequalities

$$\alpha_l \le u_l(t) \le \beta_l, \text{ for a.a. } t \in [0,T], \tag{4}$$

where α_l and β_l, $(\alpha_l < \beta_l)$, $(l = 1, ..., r)$ are given constants; $u_l(t)$, $(l = 1, ..., r)$ are components of the vector $u(t)$. The set of all admissible controls $u(t)$ is denoted by U.

The performance index, evaluating the control process, is

$$J(u(t)) \stackrel{\triangle}{=} c' x(T) \to \min_{u(t)\in U}, \qquad (5)$$

where $c \in E^n$ is a given vector; the prime denotes the transposition.

The problem (1)-(5) is called the Original Optimal Control Problem (OOCP).

In the sequel, we assume:

A1. All the eigenvalues of the matrix $\bar{A}_4(t) = A_{04}(t) + A_{14}(t)$ lie inside the left-hand half-plane for all $t \in [0, T]$.

Under this assumption, setting formally $\varepsilon = 0$ in (1)-(2) and eliminating y from the resulting system, we obtain the following system (in this system the state and control are redenoted by $\bar{x}$ and $\bar{u}$):

$$d\bar{x}(t)/dt = \Big(\bar{A}_1(t) - \bar{A}_2(t)\bar{A}_4^{-1}(t)\bar{A}_3(t)\Big)\bar{x}(t) + \Big(B_1(t) - \bar{A}_2(t)\bar{A}_4^{-1}(t)B_2(t)\Big)\bar{u}(t), t \in [0, T], \qquad (6)$$

where $\bar{A}_j(t) = A_{0j}(t) + A_{1j}(t)$, $(j = 1, 2, 3)$. For (6) the initial condition and the performance index are, respectively,

$$\bar{x}(0) = \varphi_x(0), \qquad (7)$$

$$\bar{J}(\bar{u}(t)) \stackrel{\triangle}{=} c' \bar{x}(T) \to \min_{\bar{u}(t)\in U}. \qquad (8)$$

The problem (6)-(8) is called the Reduced Optimal Control Problem (ROCP).

In the presentation, some connections between the solutions of the OOCP and the ROCP are established for all sufficiently small $\varepsilon > 0$, i.e. robustly with respect to the small parameter ε. One of these connections is presented in the following theorem.

Theorem 1. *Let the assumption A1 be satisfied. Let the matrix-functions $A_{ij}(t)$, $B_k(t)$, $(i = 0, 1;\ j = 1, ..., 4;\ k = 1, 2)$ be continuously differentiable for $t \in [0, T]$. Let the vector-function $\varphi_x(\tau)$ be continuously differentiable and the one $\varphi_y(\tau)$ be bounded for $\tau \in [-\varepsilon_0 h_1, 0]$ with some $\varepsilon_0 > 0$. Let the ROCP have a solution, and $\bar{J}^*$ be the optimal value of $\bar{J}(\bar{u}(t))$ in the ROCP. Then, for all sufficiently small $\varepsilon > 0$: $|J_\varepsilon^* - \bar{J}^*| \le a\varepsilon$, where $J_\varepsilon^* \stackrel{\triangle}{=} \inf_{u(t)\in U} J(u(t))$ in the OOCP; $a > 0$ is some constant independent of ε.*

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GENERATING SERIES FOR THE STUDY OF STABILITY OF BILINEAR SYSTEMS

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Keywords: bilinear systems, generating series, BIBO stability, rational expression

1. INTRODUCTION

The aim of this paper is to study the Bounded Input Bounded Output (BIBO) stability of bilinear systems. The stability of linear systems can be studied by computing their transfer function. In this paper, we use the generating series (generalization of the transfer function) as a tool for analysing the stability of bilinear systems. In fact, the generating series G of a bilinear system is a formal power rational series in noncommutative variables. It provides a formal expression of the output $y = \varepsilon(G)$ in iterated integrals form.
The stability/stabilization can be always studied from the generating series G: According to expression of G, three cases occur. In the first case, the output $y = \varepsilon(G)$ can be explicitly computed; in the second case, this output can be bounded (or unbounded) if the input $u(t)$ is bounded; in the third case, no conclusion about the BIBO stability can be easily deduced. Then, we look only for a stabilizing constant input $u(t) = \eta$, by studying the univariate series G_η

2. METHOD

A bilinear system (B) with inputs $(u_i(t))_{1\leq i\leq m}$ and drift $u_0(t) \equiv 1$ is given by its state equations

$$(B)\begin{cases} x^{(1)}(t) &= (M_0 + \sum_{i=1}^{m} u_i(t)M_i)x(t) \\ y(t) &= \lambda.x(t) \end{cases} \tag{1}$$

where $x(t) \in Q$, $R-$vector space, $M_0, M_1, \cdots, M_m, \lambda$ are $R-$linear.

• We compute the rational expression associated with the expansion of its generating series G built on the alphabet $Z = \{z_0, z_1, \cdots, z_m\}$

$$G = \lambda.x(0)+\sum_{\nu\geq 0}\sum_{j_0,\cdots,j_\nu=0}^{m} \lambda.M_{j_0}\cdots M_{j_\nu}x(0)z_{j_0}\cdots z_{j_\nu}$$

by generalizing the Schutzenberger's method (4) for computing the rational expression describing a rational series.

• From the rational expression of G, we obtain a formal expression of the output (1)

$$y(t) = \sum_{w\in Z^*} \langle G|w\rangle \int_0^t \delta(w) = \int_0^t \delta(G) = \varepsilon(G)$$

by computing directly the iterated integral $\int_0^t \delta(G)$ where G is a rational expression.

• According to the form of G, three cases occur

1. G **is a simple rational expression :**
   $G = z_0^p(c_0z_0)^*$, $z_0^p(c_1z_1)^*$, $z_i^p(c_0z_0)^*$, $z_i^p(c_iz_i)^*$, $(c_0z_0)^*z_i^p$, $(c_iz_i)^*z_0^p, \cdots \quad c_i \in R$
   Then we compute explicitly $y(t) = \varepsilon(G)$ and deduce the BIBO stability/instability.
   We obtain also an explicit computing of $y(t)$ when G is a shuffle product of such simple rational expressions since $\varepsilon(G_1 \sqcup G_2) = \varepsilon(G_1)\varepsilon(G_2)$.
2. G **is a concatenation product of some simple rational expressions:** $(c_0z_{j_0})^{*p_0}z_{i_1}(c_1z_{j_1})^{*p_1}\cdots z_{i_k}(c_kz_{j_k})^{*p_k}$
   We use the theorem of Hoang Minh (3) :
   Theorem 1:
   $\forall k$**, let us suppose that** G_k **is exchangeable and let us denote** $\varepsilon(G_k)$ **by** $g_k(\xi(t))$

   $$g_k(\xi(t)) = g_k(t, \xi_1(t), \cdots, \xi_m(t))$$

   where $\xi_j(t)$ **is the primitive of the input** $u_j(t)$ **cancelling for** $t = 0$**. Then,** $\forall k$**, the series**

   $$S_k = G_0z_{i_1}G_1\cdots z_{i_k}G_k$$

   where $z_{i_1}, \cdots, z_{i_k} \in Z$**, has the following evaluation:**

   $$\varepsilon(S_k) = y(t) =$$

$$\int_0^t \int_0^{\tau_k} \cdots \int_0^{\tau_2} g_0(\xi(\tau_1))g_1(\xi(\tau_2)-\xi(\tau_1))\cdots$$

$$g_k(\xi(t)-\xi(\tau_k))d\xi_{z_{i_1}}(\tau_1)\cdots d\xi_{z_{i_k}}(\tau_k)$$

So we can prove that $|y(t)|$ is bounded (or unbounded) if $|u(t)|$ is bounded and study the BIBO stability

3. **No conclusion seems available about the BIBO stability by using the generating series.**

For a single input system with drift (B) we prove the following proposition and corollaries.

Proposition 1
The output $(\varepsilon(G))_\eta$ of (B), the generating series of which is G, for the constant input $u(t) = \eta$, is equal to the output $\varepsilon(G_\eta)$ of some system, the generating series of which is G_η, obtained by substituting ηz_0 to z_1 in G.

Corollary 1
A necessary condition for the BIBO stability of (B), is that, for every $\eta \in R$, the real part of the poles of G_η is ≤ 0 and the imaginary poles of G_η are single.

Corollary 2
If there exists η such that every pole of G_η has a negative real part and if every imaginary pole is single, then $u(t) = \eta$ is a stabilizing input

So we look only for stabilizing constant inputs $u_i(t) = \eta_i$, by studying the univariate series G_{η_i}.

• Example : Bilinear approximants of the electric equation (2)

$$\dot{v}(t) = -k_1 v(t) - k_2 v^2(t) + u(t) \qquad (2)$$

1. **At order 2**
A bilinear system (B_2) approximating it at order 2 is

$$\begin{cases} x^{(1)}(t) &= \left(\begin{pmatrix} 0 & 0 \\ a^{(0)} & a^{(1)} \end{pmatrix} + u(t)\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right)x(t) \\ y(t) &= (x(0)\ \ 1)\ x(t) \end{cases}$$

The rational expression is:

$$G_2 = (a^{(0)}z_0 + z_1)(a^{(1)}z_0)^* + x(0)$$

By theorem 1, (B_2) is not BIBO for $a^{(1)} > 0$ and is BIBO for $a^{(1)} < 0$ (if $M_1 \leq u(t) \leq M_2$ then $\varepsilon(G_2)$ is bounded)
For instance, for $x(0) \geq 0,\ \ a^{(0)} > 0,\ \ a^{(1)} < 0,\ \ 0 \leq u(t) \leq M$, then
$y(t) \leq x(0) + \frac{M+a^{(0)}}{-a^{(1)}}$

2. **At order 3**
The generating series is,
for $a^{(1)} \neq 0,\ a^{(2)} \neq 0$:

$$G_3 = (z_1+a^{(0)}z_0)(a^{(1)}z_0+(z_1+a^{(0)}z_0)a^{(2)}z_0)^*+x(0)$$

$$G_{3,\eta} = x(0) + \frac{(a^{(0)}+\eta)z_0}{1-a^{(1)}z_0-(a^{(0)}+\eta)a^{(2)}z_0^2}$$

If $\eta = -a^{(0)}$ then $|y(t)|$ is bounded ($y_{3,\eta}(t) = x(0)$) else we decompose $G_{3,\eta}$ in partial fractions for studying the stabilizing inputs.

3. CONCLUSIONS

The BIBO stability of a bilinear system cannot be generally studied by considering its state equation. In this paper, we use the "evaluation" of its generating series G. If the rational expression of G is simple or obtained by concatenating some simple rational expressions, then the use of the generating series of the system provides an answer about the stability and a bound for the output. Otherwise, we can look for a stabilizant constant input $u(t) = \eta$ by using the univariate series G_η.

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Control of an Industrial Rolling Process Using The Theory of Switched Repetitive Processes

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1. INTRODUCTION

The unique characteristic of a repetitive process (also termed a multipass process in the early literature) can be illustrated by considering machining operations where the material or workpiece involved is processed by a series of sweeps, or passes, of the processing tool. Assuming the pass length $\alpha < +\infty$ to be constant, the output vector, or pass profile, $y_k(p)$, $p = 0, 1, \ldots, (\alpha - 1)$, ($p$ being the independent spatial or temporal variable), generated on pass k acts as a forcing function on, and hence contributes to, the dynamics of the new pass profile $y_{k+1}(p)$, $p = 0, 1, \ldots, (\alpha - 1)$, $k = 0, 1, \ldots$. This, in turn, leads to the unique control problem in that the output sequence of pass profiles generated can contain oscillations that increase in amplitude in the pass-to-pass direction, i.e. in the collection of pass profile vectors $\{y_k\}_k$.

Industrial examples include long-wall coal-cutting and metal rolling, see the original papers cited in, for example, (3) for further details. A number of so-called algorithmic examples also exist where adopting a repetitive process setting for analysis has clear advantages over alternative approaches to systems related analysis. These include iterative learning control schemes, e.g. (2) and iterative solution algorithms for dynamic nonlinear optimal control problems based on the maximum principle. In the case of iterative learning control for the linear dynamics case, the stability theory for differential (and discrete) linear repetitive processes is one method which can be used to undertake a stability/convergence analysis of a powerful class of such algorithms and thereby produce vital design information concerning the trade-offs required between convergence and transient performance.

In many practical applications, e.g. metal rolling, or processing operations using multiple operation robot arms, a number of passes may be completed under one regime and then the dynamics change to allow further processing to take place. One way of modeling such a case is by switching the dynamics from one state-space model to an alternative (or alternatives) and this paper continues the development of tools for the analysis of such models.

Note also that there is one other form of switching which can occur in repetitive process dynamics, i.e. along the pass. Here, however, we restrict attention to the pass-to-pass case since it has more obvious and immediate practical applications.

In this paper we consider a metal rolling process where the workpiece involved is passed through two successive rolling operations which are to be controlled to produce a desired final product. We show that this can be modeled as a discrete linear repetitive process which switched dynamics in the pass-to-pass direction. Then we develop new results on stability and control law design and give an illustrative numerical example.

2. PROCESS MODELING

In its simplest form a multi-roll roll system consists of two separate pairs of rolls which are con-

trolled by separate input signals, i.e. different rolling forces. The deformation of the workpiece takes place between these pairs of rolls with parallel axes revolving in opposite directions. The metal strip to be rolled to a pre-specified thickness (also termed the gauge or shape) through a series of rolls for successive reductions — here we consider the case when two sets of rolls are used since the case of more than two follows as a natural generalization.

In practice, a number of models of this process can be developed depending on the assumptions made about the underlying dynamics and the particular mode of operation under consideration. The particular task is to develop a simplified (but practically feasible) model relating the gauge on the passes through the rolls. The current pass is denoted by $y_{2k+2}(t)$, the previous passes – by $y_{2k+1}(t)$ and $y_{2k}(t)$.

As a starting point for analysis in this general area, we consider the following discrete model, which can be achieved by applying e.g. a backward Euler discretization procedure to the differential model

$$\begin{cases} x_{2k+1}(p+1) = A_1 x_{2k+1}(p) \\ \qquad +B_1 u_{2k+1}(p) + B_{01} y_{2k}(p), \\ y_{2k+1}(p) = C_1 x_{2k+1}(p) \\ \qquad +D_1 u_{2k+1}(p) + D_{01} y_{2k}(p), \\ \\ x_{2k+2}(p+1) = A_2 x_{2k+2}(p) \\ \qquad +B_2 u_{2k+2}(p) + B_{02} y_{2k+1}(p), \\ y_{2k+2}(p) = C_2 x_{2k+2}(p) \\ \qquad +D_2 u_{2k+2}(p) + D_{02} y_{2k+1}(p), \end{cases}$$

over $p = 0, 1, \ldots, (\alpha - 1)$, $k = 0, 1, \ldots$.

This last model structure is precisely that of a discrete linear repetitive process with dynamics which switch in the pass to pass direction after the completion of each pass. To complete this model description, it is necessary to specify the boundary conditions, i.e. the initial state vector on each pass and the initial pass profile. Without loss of generality we can assume that $x_{2k+1}(0) = d_{2k+1}$, $x_{2k+2}(0) = d_{2k+2}$, and $y_0(p) = f(p)$, where the vectors d_{2k+1} and d_{2k+2} have known constant entries and the vector $f(p)$ has entries which are known functions of p.

3. STABILITY AND CONTROL LAW DESIGN

The stability theory of repetitive processes consists of two separate concepts, termed asymptotic stability and stability along the pass (3). In effect, both of these are a form of bounded input bounded output stability of the pass profile sequence (recall the unique control problem for these processes) where asymptotic stability demands this property over the finite and constant pass length and as a consequence that the sequence of pass profiles converge to a steady or so-called limit profile as $k \to \infty$. The limit profile is described by a standard (or 1D) discrete linear systems state space model. The fact that the pass is finite, however, could mean that this limit profile is unstable, i.e. all eigenvalues of the state matrix do not lie in the open unit circle in the complex plane. (Over a finite duration even a unstable 1D linear system can only produce a bounded output.)

Stability along the pass prevents this undesirable situation by demanding the bounded input bounded output property uniformly, i.e. independent of the pass length.

The control aim here is to obtain the closed loop process stable along the pass but also to achieve the prescribed limit pass profile. For this reason we consider a switched control law of the form

$$u_{2k+1}(p) = K_1^1 x_{2k+1}(p) + K_2^1 y_{2k}(p),$$
$$u_{2k+2}(p) = K_1^2 x_{2k+2}(p) + K_2^2 y_{2k+1}(p),$$

To solve these problems we use a Lyapunov approach which can be computed using numerically efficient optimization methods, called Linear Matrix Inequalities (LMI), see (1).

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IDENTIFICATION PROBLEM AS A PROBLEM OF OPTIMAL CONTROL

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1. PROBLEM STATEMENT

Let us consider a linear dynamic system with scalar control $u(t)$

$$\dot{X}(t) = F\,X(t) + B u(t), \qquad (1)$$

where $X(t) = (x_1(t), x_2(t), \ldots, x_n(t))^T$ – vector of state variables; F, B – matrices with constant elements $\{f_{ik}\}_{i=1,k=1}^{i=n,k=n}$, $\{b_{ii}\}_{i=1}^{i=n}$.

Denote

$p_1 = (f_{11}, f_{12}, \ldots, f_{nn})^T$, $p_1 \in R^{n_1}$, $n_1 = n\,n$;

$p_2 = (b_{11}, b_{22}, \ldots, b_{nn})^T$, $p_2 \in R^n$;

$p = p_1 + p_2 \in R^m$, $m = n_1 + n$; $(.)^T$ is the sign of transposition.

It is assumed that the function $\tilde{x}_1(t)$ is obtained as a record of measurement ($t \in [0, T]$).

Let us now consider the following problem: to find the control $u_0(t)$ after action of which the solution $x_1(t)$ of system (1) satisfies the conditions:

$$\left\| \tilde{x}_1(t) - x_1(t) \right\|_X \le \delta, \qquad (2)$$

$$x_1(0) = x_1^0, x_2(0) = x_2^0, \ldots, x_n(0) = x_n^0 \qquad (3)$$

$$\inf_{u \in U} \Omega[u] = \Omega[u_0], \qquad (4)$$

where $\Omega[u]$ is the functional of control quality; U is the functional space of controls; X is the functional space of vector functions of state variables; δ is a given value; $\|.\|$ is the norm in the respective space.

In this paper we assume that the initial values $x_2(0), x_3(0), \ldots, x_n(0)$ of state variables are unknown.

For example, the identification of external loads leads to problems of the type (2),(3),(4) [1,2,3]. There are also other practical problems which can be similarly formulated. Let us call this problem *the problem of control under conditions of uncertainties*.

Problems of this type were formulated and investigated in works of N.N.Krasovsky [4], A.B.Kurzhansky [5] and others [6].

2. METHOD OF SOLUTION

It was shown that the uncertainties in the initial conditions $x_2(0), x_3(0), \ldots, x_n(0)$ lead to occurrence of additional terms as delta-functions and their derivatives in the solution which concentrate at the point $t = 0$. A special filtration of the function $\tilde{x}_1(t)$ was suggested for eliminating the influence of uncertainty in initial conditions. Thus, the initial problem (2),(3),(4) with unknown values $x_2(0), x_3(0), \ldots, x_n(0)$ can be reduced to a problem with zero conditions (3).

If the functional of control quality is stabilizing, then the solution of problem (2),(3),(4) is stable to small changes of initial data [7].

It is assumed that the relationship between the functions $x_1(t)$ and $u(t)$ has the form:

$$C_p u = x_1, \qquad (5)$$

where C_p is a compact operator ($C_p : U \to X$) which depends on the parameter vector p of the mathematical model.

The solution of problem (2),(3),(4) can be reduced to the following extremal problem [7]:

$$\Omega[u_0] = \inf_{u \in Q_{\delta,p}} \Omega[u], \qquad (6)$$

$$x_1(0) = 0, x_2(0) = 0, \dots, x_n(0) = 0, \quad (7)$$

where $Q_{\delta,p} = \{u : u \in U, \left\| C_p u - \tilde{x}_1(t) \right\|_X \le \delta\}$.

If the coefficients of matrices F, B are defined with some errors ($p_1 \in D_1$, $p_2 \in D_2$, $D_1 \subset R^{nn}$, $D_2 \subset R^n$, $p = p_1 + p_2 \in D = D_1 \oplus D_2 \subset R^m$), then the set of possible solutions in the extremal problem (6) has to expand to the set $Q_{\delta,h}$:

$$Q_{\delta,h} = \{u : u \in U, \left\| C_p u - \tilde{x}_1(t) \right\|_X \le \delta + h \left\| u \right\|_U\},$$

where $h = \sup_{p \in D} \left\| C_p - C_T \right\|_{U \to X}$, C_T is the exact operator.

The set $Q_{\delta,h}$ can be changed in some cases to a more narrow set $Q^* = \bigcup_{p \in D} Q_{\delta,p}$ and the extremal problem (6) can be changed to the extremal problem:

$$\Omega[\tilde{u}_0] = \inf_{p \in D} \inf_{u \in Q_{\delta,p}} \Omega[u]. \qquad (8)$$

It was shown that the solution of problem (8) exists, is unique and stable to small changes of initial data if $\Omega[u]$ is a stabilizing functional [7].

3. CONCLUSIONS

An attempt has been made to consider a typical problem of identification as a problem of optimum control of dynamic system under conditions of uncertainty. An algorithm for its solution with the use of regularization method is offered.

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ADAPTIVE PARAMETER ESTIMATION FOR INFINITE-DIMENSIONAL FACTOR MODEL BY USING PARTICLE FILTER

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Keywords: Stochastic Parabolic systems, Particle filter, Factor model, Parameter estimation

1. INTRODUCTION

In this paper, we select the parabolic type stochastic partial differential equation with stochastic boundary inputs for the term structure dynamics. The stochastic boundary inputs are generated by the linear stochastic equations with mean-reverting property. Noting that the instantaneous forward process is unobservable, we need to construct an observation mechanism from market instruments. Choosing the yield curve data as the observation process, we set the finite dimensional discrete- time observation mechanism. For fixed parameters included in the parabolic systems, the optimal filter is the Kalman filter which can be computed exactly. However once we construct the augmented state including the systems' parameters, the linearity is lost and the Kalman filter can not be applied. For circumventing these difficulties, we propose a new algorithm which is a combination of the Kalman filter for the state and the particle filter for the included parameters. For checking the feasibility of the proposed algorithm, several digital simulation studies are performed.

2. MATHEMATICAL MODEL

Musiela [1] derives the Heath, Jarrow and Morton arbitrage-free interest rate dynamics under the time-to-maturity parameterization as follows:

$$df(t,x) = \frac{\partial f(t,x)}{\partial x}dt + \nu(x)dt + dw(t,x), \quad (1)$$

where $f(t,x)$ denotes the instantaneous forward rate curve ,$\nu(x)$ is identified by using the argument of absence of arbitrage and $w(t,x)$ is a Brownian motion process which depends on x(time-to maturity). In order to support the smoothness property of the forward process $f(t,x)$ with respect to x, the parabolic type systems are proposed:

$$\begin{aligned} df(t,x) &= \frac{k}{2}\frac{\partial^2 f(t,x)}{\partial x^2}dt + \frac{\partial f(t,x)}{\partial x}dt \\ &+\nu(x)dt + dw(t,x), \ f(0,x) = f_o(x), \end{aligned} \quad (2)$$

where $x \in G =]0, \hat{T}[$ and for simplicity we set

$$\begin{aligned} \frac{1}{2}\frac{\partial f(t,0)}{\partial x} &= \mu_{00}f(t,0) + \mu_{01}f(t,\hat{T}) \\ &+g_0(t) + \sigma_{01}g_1(t) \end{aligned} \quad (3)$$

$$\begin{aligned} -\frac{1}{2}\frac{\partial f(t,\hat{T})}{\partial x} &= \mu_{10}f(t,0) + \mu_{11}f(t,\hat{T}) \\ &+g_1(t) + \sigma_{10}g_0(t) \end{aligned} \quad (4)$$

where for $i = 0, 1$

$$dg_i(t) = (a_i g_i(t) + b_i)dt + \sigma_i dw_i(t), \text{for .} \quad (5)$$

3. OBSERVATION MECHANISM

It is well known that the instantaneous forward rate is unobservable and Libor,FRA's (forward rate agreements) etc are market instruments. Hence the yield curve process is constructed from these instruments. Noting that the relation between the yield curve and the forward rate process is theoretically given by

$$\begin{aligned} \tilde{Y}(t,T) &= \log(1 + Y(t,T)) \\ &= \frac{1}{T-t}\int_0^{T-t} f(t,x)dx, \end{aligned} \quad (6)$$

our observation can be set as the following discrete-time type;

$$\tilde{Y}(t_i, T_k) = \frac{1}{T_k - t_i} \int_0^{T_k - t_i} f(t_i, x)dx + \epsilon_{ik} \quad \text{for } i = 1, 2.3, \cdots \text{and } k = 1, 2, 3, \cdots, p \quad (7)$$

where ϵ denotes the white Gaussian noise with $E\{\epsilon_{ik}\} = 0$, and $E\{\epsilon_{ik}\epsilon_{\ell k}\} = \sigma\delta_{ik\ell m}$.

4. FILTERING PROBLEM

In this section, we assume that all parameters included in system and observation are known. Hence it is possible to construct the optimal filter for the continuous-discrete systems (2) and (7). For the finite-dimensional systems, Jazwinski [2] has proposed such an optimal filter. Th extension to the infinite-dimensional system is straightforward.

Now the minimum variance estimates of $f(t, x), g_0(t)$ and $g_1(t)$ for $t_i \leq t < t_{i+1}$ are given by

$$\hat{f}(t, x) = E\{f(t, x)|\mathcal{Y}_{t_i}\} \quad (8)$$

and

$$\hat{\vec{g}}(t) = [E\{g_0(t)|\mathcal{Y}_{t_i}\} \;\; E\{g_1(t)|\mathcal{Y}_{t_i}\}]' \quad (9)$$

for $\mathcal{Y}_{t_i} = \{\vec{Y}_1, \vec{Y}_2, \cdots, \vec{Y}_i\}$.

5. PARAMETER ESTIMATION

We denote the optimal estimates for the fixed θ by $\hat{f}(t; \theta)$ and $\hat{\vec{g}}(t; \theta)$, which are obtained from the previous section. Hence with the aid of Bayesian rule, we have for $t_i \leq t < t_{i+1}$

$$\begin{aligned} E\{f(t, x)|\mathcal{Y}_i\} &= \int_\Theta \hat{f}(t, x; \theta)dP(\theta|\mathcal{Y}_i), \\ E\{\vec{g}(t)|\mathcal{Y}_i\} &= \int_\Theta \hat{\vec{g}}(t; \theta)dP(\theta|\mathcal{Y}_i) \\ E\{\theta|\mathcal{Y}_i\} &= \int_\Theta \theta dP(\theta|\mathcal{Y}_i). \end{aligned}$$

To realize above equations , we need to compute the conditional distribution $P(\theta|\mathcal{Y}_i)$ which is given by

$$dP(\theta|\mathcal{Y}_i) = \frac{p(\vec{Y}_i|\theta)p(\theta|\mathcal{Y}_{i-1})d\theta}{\int_\theta p(\vec{Y}_i|\theta)p(\theta|\mathcal{Y}_{i-1})d\theta}. \quad (10)$$

By using an idea of particle filter algorithm, we can realize (5):

- At $t = 0$ the M independent particles $\{\theta_j^{(0)}\}_{j=1,2,\cdots,M}$ are generated with the initial law $P(\theta)$.
- For $0 \leq t < t_1$ obtain $\hat{f}(t_1^-, \cdot; \theta_j^{(0)})$, $\hat{\vec{g}}(t_1^-; \theta_j^{(0)})$, and $P_{g_i g_i}(t_1^-; \theta_j^{(0)})$.
- At $t = t_1$, we obtain $\hat{f}(t_1^+, \cdot; \theta_j^{(0)})$, $\hat{\vec{g}}(t_1^+; \theta_j^{(0)})$, and compute

$$p(\vec{Y}_1|\theta_j^{(0)}) = \frac{1}{\sqrt{2\pi\sigma}} \exp\{-\frac{1}{2\sigma}|\vec{Y}_1 - H_1\hat{f}(t_1^+, x : \theta_j^{(0)})|^2\}. \quad (11)$$

- From (11), we get

$$P(\theta_j^{(0)}|\mathcal{Y}_1) = \frac{p(\vec{Y}_1|\theta_j^{(0)})P(\theta_j^{(0)})}{\Sigma_i^M p(\vec{Y}_1|\theta_i^{(0)})P(\theta_i^{(0)})} \quad (12)$$

  where the distribution $P(\theta_j^{(0)}$ is approximated by the empirical distribution determined by the set of particles,i.e., $P(\theta = \theta_j^{(0)}) = \frac{1}{M}$.
- Hence at the time t_1, we got the optimal state and parameter estimates $E\{f(t_1, x)|\mathcal{Y}_1\}$, $E\{\vec{g}(t)|\mathcal{Y}_1\}$ and $E\{\theta|\mathcal{Y}_i\}$ from (??) with their optimal covariances, respectively.
- At $t = t_1$, we generate the M independent particles $\{\theta_j^{(1)}\}_{j=1,2,\cdots,M}$ with the law $P(\theta|\mathcal{Y}_1)$ where the measure $P(\theta|\mathcal{Y}_1)$ is reconstructed by using the resampling algorithm.
- Get $\hat{f}$ and $\hat{\vec{g}}$ for $t_1 \leq t < t_2$ with the initial condition $\hat{f}(t_1, x : \theta_j^{(1)}) = E\{f(t_1, x)|\mathcal{Y}_1\}$ and $\hat{\vec{g}}(t_1 : \theta_j^{(1)}) = E\{\vec{g}(t_1)|\mathcal{Y}_1\}$ for all j.
- Repeat the above steps.

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A CONSERVATIVE CONTROL SYSTEM DESCRIBED BY THE SCHRÖDINGER EQUATION

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Keywords: Schrödinger equation, well-posed linear systems, conservative systems

1. Introduction

A conservative system is a system for which a certain energy balance equation is satisfied both by its trajectories and by those of its dual system. In [1] -[3], Tucsnak and Weiss identified a large class of conservative linear systems described by a second order differential equation in a Hilbert space and an output equation and they may have unbounded control and observation operators.

In this paper, we construct an example of conservative systems described by a linear Schrödinger equation with boundary control and boundary observation. This example does not fit into the framework of [1] -[3].

2. The Schrödinger equation with Dirichlet type boundary feedback

Let Ω be an open domain in R^n with C^2-boundary $\Gamma = \overline{\Gamma_0 \cup \Gamma_1}$ where Γ_0 and Γ_1 are disjoint parts of Γ with $\Gamma_1 \neq$.

Let $A : H^{-1}(\Omega) \to H_0^1(\Omega)$ be the operator defined by:

$Af = \varphi$ if and only if $\varphi \in H_0^1(\Omega)$ and $-\Delta\varphi = f$

We consider the system described by the equations

$$y_t = \mathbf{i}\Delta y \text{ in } \Omega \times (0,+\infty) \quad (1)$$

$$y(x,0)=y_0(x) \quad \text{in } \Omega \quad (2)$$

$$y=0 \text{ on } \Gamma_0 \times (0,+\infty) \quad (3)$$

$$y + \tfrac{\mathbf{i}}{2}\tfrac{\partial}{\partial\nu}(Ay) = u \text{ on } \Gamma_1 \times (0,+\infty) \quad (4)$$

The input of this system is the function u in (4). The output associated with this system is

$$z=-y+ \tfrac{\mathbf{i}}{2}\tfrac{\partial}{\partial\nu}(Ay) \quad (5)$$

The precise statement of the conservativity of the system described by (1)-(5) is given in the following theorem

Theorem 1 *The equations* (1)-(5) *determine a conservative linear system* (Σ) *with input and ouput space* $U = L^2(\Gamma_1)$ *and state space* $X = H^{-1}(\Omega)$.
If
$y_0 \in Z_D = \{f \in L^2(\Omega) : \Delta f \in H^{-1}(\Omega),$
$f|_\Gamma \in L^2(\Gamma)$ *and* $f = 0$ *on* $\Gamma_0\}$,
$u \in H^1(0,+\infty;U)$
and the compatibility condition
$y_0(x) + \frac{\mathbf{i}}{2}\frac{\partial}{\partial\nu}(Ay_0)(x) = u(0,x)$ *for* $x \in \Gamma_1$
holds, then (1)-(5) *have a unique solution* y, z *satisfying*
$y \in BC(0,+\infty;Z_D) \cap BC^1(0,+\infty;H^{-1}(\Omega))$,
$z \in H^1(0,+\infty;U)$

3. Schrödinger equation with Neumann type boundary feedback

In this section, we suppose that the boundary Γ is of class C^2 and satisfies:

$\Gamma = \Gamma_0 \cup \Gamma_1$ with $\overline{\Gamma_0} \cap \overline{\Gamma_1} =$ where both Γ_0 and Γ_1 are nonempty.

Let $a(.)$ be an element of $L^\infty(\Gamma_1)$ such that $a(x) \neq 0$ for almost every $x \in \Gamma_1$.

We are interested in the linear system described by:

$$y_t = \mathbf{i}\Delta y \text{ in } \Omega \times (0,+\infty) \quad (6)$$

$$y(x,0)=y_0(x) \text{ in } \Omega \quad (7)$$

$$y=0 \text{ on } \Gamma_0 \times (0,+\infty) \quad (8)$$

$$\tfrac{\partial y}{\partial\nu} + \mathbf{i}\,|a(x)|^2\, y = \sqrt{2}a(x)u \text{ on } \Gamma_1 \times (0,+\infty) \quad (9)$$

$$\tfrac{\partial y}{\partial\nu} - \mathbf{i}\,|a(x)|^2\, y = \sqrt{2}a(x)z \text{ on } \Gamma_1 \times (0,+\infty) \quad (10)$$

Theorem 2 *The equations* (6)-(10) *determine a conservative linear system* (Σ) *with input and output space* $U = L^2(\Gamma_1)$ *and state space* $X = L^2(\Omega)$. *If*

$y_0 \in Z_N = \{f \in H^1_{\Gamma_0}(\Omega) : \Delta f \in L^2(\Omega), \frac{\partial f}{\partial \nu} \in aL^2(\Gamma_1)\}$,
$u \in H^1(0, +\infty; U)$,
and the compatibility condition
$\frac{\partial y_0}{\partial \nu} + |a(x)|^2 y_0 = \sqrt{2}a(x)u(0, x)$
holds then (6)-(10) *have a unique solution* y, z *satisfying*
$y \in BC(0, +\infty; Z_N) \cap BC^1(0, +\infty; L^2(\Omega))$,
$z \in H^1(0, +\infty; U)$

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Modelling a gas network through a parabolic DAE system

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Keywords: DAE systems, Gas network modelling, Gas Network Optimisation, Linear Quadratic Games, Nash Games, Parabolic Differential Equations, Riccati Differential Equations.

Abstract. *As natural gas is becoming increasingly important in modern life, its transmission and distribution through ever expanding pipeline networks is dependent on efficient control and management. However, the problem characteristics, namely its large dimension, nonlinearity, geographical dispersion, and transient properties of the gas behaviour, make the design of efficient algorithms for optimisation of gas networks crucial.*

Therefore, we see the optimisation of the gas dynamics in the pipelines as a LQ Nash game, where the different, and many times conflicting, objectives to be taken into account in the optimisation of the network can be modelled as players of the LQ game. The dynamics in the network, as well as the coupling conditions, are modelled through a parabolic DAE system, which is formed by the two Kirchhoff's Laws and a space discretised parabolic model which describes the gas transients in the pipelines. Thence, complex networks, i.e., complex with loops and noncontrollable elements, can be considered.

It is important to observe that the main time-variation in the problem comes through the constraints which represent offtakes' demand. Therefore, offtakes are viewed in this work as disturbances to the system from a nominal usual value. Other parts of the network, such as the value of Linepack (i.e., the gas stored in the pipelines) also change with time. Hence, we distinguish two different parts in the network: the active part which is formed by the controllable units, and the passive part composed by the controllable units' connections, i.e., the pipelines.

This framework can also set up a holistic interactive approach that brings together different network features—e.g. compressor stations, sources, regulators, pipelines and valves—whose optimisation objectives are different. A single optimisation procedure becomes, thus, possible without having to feed results from different software packages into others. In addition, this mathematical model, where independent entities take action, also offers the ideal modularity and subsequent problem decomposition. A modular approach is also well-suited to the high, and ever changing, dimension of the gas networks.

Besides the pipelines, the network also comprises offtakes, valves, reservoirs, compressor stations, supplying sources, and regulators. With the last three being controllable units, which means that we will set some of its variables in order to run the system in a desirable, or suitable, manner.

The network is first decomposed into controllable elements and pipelegs, with the latter being aggregated into subsystems which express vicinity properties. Thus, in the game framework, the players communicate trough network connectivity constraints.

The network overall objective, i.e., to ensure the delivery of the service at the customer offtakes, is represented as disturbances. We do this since the customers demand is usually variable, which highly contributes for the unsteady nature of flow in the pipelines. The pressure of the gas delivered to the customers should be up to a contracted minimum. This can be provided by variable gas supply realised by compressor stations

or the development of the network in order to increase its flow capacity. The large extent of the network makes that even small improvements in the system might involve significant profits.

Conditions for the existence and uniqueness of a solution for the game are related to the solution of certain Riccati differential equations and a bounary value problem. The approach used is the construction of a value function which leads to existence assertions in terms of solvability of certain Riccati differential equations and a boundary value problem. Furthermore, this approach directly provides a calculation procedure for the equilibrium controls.

A simple network, where the players are two controllable elements relevant to the network dynamics, is used to illustrate the calculation procedure.

MODELLING REAL TIME AUTHENTICATION PROTOCOLS USING ALGEBRAIC SPECIFICATION TECHNIQUES – THE CASE OF TESLA PROTOCOL

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Keywords: Algebraic Specification and Verification, CafeOBJ, Authentication, TESLA protocol

1. INTRODUCTION

We present how to model real time authentication protocols with CafeOBJ algebraic specification language [1]. The protocols are specified as Timed Observational Transition Systems or TOTSs [2]. Based on this specification, we can verify desirable properties of the protocols through induction and/or case analysis, thanks to the CafeOBJ system and its support to the interactive theorem proving. The method we apply is a combination of [2] and [3]. As a case study we model TESLA protocol [4], which is used for the source authentication in multicast communication settings, and verify a safety property. The paper is organized as follows. Section 2 describes informally the TESLA protocol while section 3 presents how to model it with CafeOBJ. Section 4 concludes the paper.

2. THE TESLA PROTOCOL

The Timed Efficient Stream Loss-tolerant Authentication (TESLA) broadcast authentication protocol is distinguished from other types of cryptographic protocols in both its key management scheme and its use of timing. Basic TESLA that is the simplest version of the protocol informally works as follows. An initial authentication is achieved using a public key signature. The subsequent messages are authenticated using Message Authentication Codes (MACs) linked back to the initial signature. In message *n-1*, the sender *S* generates a key k_n , and transmits $f(k_n)$, where *f* is a suitable cryptographic hash function, to the receivers *R*, as a commitment to that key. In message *n*, *S* sends a data packet m_n, authenticated using a MAC with key k_n. The key itself is revealed in message *n+1*. Each receiver checks that the received k_n corresponds to the commitment received in message *n-1*, verifies the MAC in message *n*, and then accepts the data packet m_n as authentic. Message *n* also contains a commitment to the next key k_{n+1}, authenticated by the MAC, thus allowing a chain of authentications [5]. The messages exchanged are as follows:

Init Message: $R \rightarrow S$: n_R
Reply Message $S \rightarrow R$: $\{f(k_1), n_R\}_{SK(S)}$
Msg_1: $S \rightarrow R$: $d_1, f(k_2)$, MAC($k_1, d_1, f(k_2)$)
Msg_n: $S \rightarrow R$: $d_n, f(k_{n+1}), k_{n-1}$, MAC($k_n, d_n, f(k_{n+1}), k_{n-1}$)

where n_R is a nonce generated by the receiver to ensure freshness and d_1, d_n the data transmitted. The protocol requires an important time synchronization assumption, the *security condition*: the receiver will not accept message *n* if it arrives after the sender might have sent message *n+1*, otherwise an intruder can capture message *n+1*, and use the key k_n from within it to fake a message *n*. Thus the agents' clocks need to be loosely synchronized.

3. MODELLING TESLA USING CAFEOBJ

We have modeled TESLA as a Timed Observational Transition System in CafeOBJ. The specification consists of sorts (or types), operators on the sorts, and equations that define operators. The specification is executable. The visible sorts corresponding to the basic data types and the related operators are as follows:

- sort **Agent** denotes agents; constant **enemy** denotes the enemy,
- sort **SKey** denote the secret key used for the encryption of the initial packet,
- sort **Key** denotes the key used for MACs,
- sort **Prf** denotes the pseudorandom function *f*; given a key *k*, *f(k)* returns the commitment for the key, while operator *k* returns the argument of *f(k)*.
- sort **Nonce** denotes nonces. Given agents p1, p2 and random number r, n(p1,p2,r) denotes a nonce generated by agent p1 to authenticate agent p2, where r makes the nonce globally unique and unguessable.
- sort **Cipher** denotes the ciphertexts encrypted with sender's private key.
- sorts **Mac1**, **Mac2** denote the message authentication codes of messages *m1* and *mn* correspondingly.

The four operators to denote the four kinds of messages are **im**, **rm**, **m1** and **mn** which are declared as:

op im : Agent Agent Agent Nonce → Msg
op rm : Agent Agent Agent Cipher → Msg
op m1 : Agent Agent Agent Prf Mac1 → Msg
op mn : Agent Agent Agent Prf Key Mac2 Nat → Msg

where **Msg** denotes messages. We mention the indexing of each message **mn**. The network is modeled as a multiset of messages, which is used as the storage that the intruder can use. The enemy tries to glean seven kinds of values from the network, which are *Nonces*, *Ciphertexts*, *Pseudorandom function values*, *Message Authentication Codes* of two kinds and *Keys*.

The state space of the protocol is declared as the hidden sort **Tesla**. The specification consists of seven observations and twelve parameterized transitions. The four transitions formalize sending messages exactly following the protocol and the remaining the enemy's faking messages. In addition there is a time advancing transition rule *tick* that advances the master clock. Each transition is executed between a lower and an upper bound. We assume that the sender sends messages at discrete time units, while an enemy can send messages whenever he wants.

Based on the specification we have proved the following invariant property

At any reachable state, if a key can be obtained by the enemy, then either the key belongs to the enemy or it has been revealed as part of a message.

The above property is denoted by operator inv1.

inv1(T, K) =
K \in keys(nw(T)) implies
(p(K) = enemy) or (s s i(K)) * d1 <= now(T) .

where **T** denotes any reachable state of the protocol, **K** the key, **i(K)** is the index of the key, $\mathbf{d_1}$ is the time delay of sending action, **s** denotes the successor index, **\in** is the membership operator and **now(T)** denotes the current time.

The proof is done by induction on the number of transitions applied. The methodology [2] includes case analysis and appropriate lemma discovery.

We have used two additional lemmas to prove the above property.

4. CONCLUSIONS

We have formally specified and verified TESLA protocol using the TOTS/CafeOBJ method, to show its application to the modeling of real time authentication protocols. The protocol has also been modeled and verified in [5], [6], and [7]. CafeOBJ provides a flexible human computer interaction mechanism in good balance such that humans make proof plans and machines conduct tedious and detailed computations, and proof scores have flexible structure.

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P-FACTOR METHOD FOR NONREGULAR INEQUALITY-CONSTRAINED OPTIMIZATION PROBLEMS.

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Keywords: p-regularity, singularity, factor-operator.

1. INTRODUCTION

Let us consider the nonregular optimization problem

$$\min_{x\in R^n} \varphi(x)$$

subject to (1)

$$g_i(x) \le 0, \quad i = \overline{1,m}$$

where gradients $\nabla g_i(x^*)$ are linearly dependent at the solution point x^*. Classical methods for solving such a type of optimization problems became non effective or are not applicable since the Lagrange multiplier λ_0 in the following equation

$$\lambda_0\varphi'(x^*) + \lambda_1 g_1'(x^*) + \ldots + \lambda_m g_m'(x^*) = 0,$$

may be equal zero at the solution point x^*.

2. THE P-REGULARITY THEORY AND NUMERICAL METHOD

We propose to reduce inequality-constrained optimization problem to equality-constrained optimization problem of the following form:

$$\min_{x\in R^n} \varphi(x)$$

subject to (2)

$$g_i(x) + y_i^{2q} = 0, \quad i = \overline{1,m}$$

where $q = \left[\frac{p}{2}\right] + 1$, and $p \ge 2$.

Obviously if x^* is a local minimum for the problem (1) then (x^*, y^*) is local minimizer for (2) (see e.g.[2]). We would like to show how to apply so called the p-regularity theory for solving the problem (2). This theory introduced earlier in [3,4] is applied in different branches of mathematics.

Main idea of the our method is to replace the necessary optimality conditions by new onces obtained earlier for p-regular problems. Combining these with some nondegenerate modification of constraints $F(x)$, we obtain a regular system of equations. This new system reduces to the system of classical necessary optimality conditions in regular case, but it is a basis for constrained optimization algorithms in degenerate case, it means for constructing new method (p-factor Lagrang`e method).

Iterative sequences constructed for solving the system converge to the solution of the original nonlinear optimization problem with quadratic rate.

3. CONCLUSIONS

We present methods for solving degenerate nonlinear optimization problems with inequality constraints. The results are based on the constructions of p-regularity theory and on reformulating the inequality constraints as equalities. Namely, by introducing the slack variables we get the equality constrained

problem, where gradients are linearly dependent. The Jacobian matrix of the constraints is assumed to be singular at the solution point.

In considered method we construct non singular matrix. If matrix is nondegenerate at the solution point (x^*, y^*) we can use the p-factor Lagrange method to solve the problem (1). We prove that the constructed iterative process converges to the solution of the original nonlinear optimization problem with quadratic rate of convergence.

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REMARKS ON 0-1 OPTIMIZATION PROBLEMS WITH SUPERINCREASING AND SUPERDECREASING OBJECTIVE FUNCTIONS

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Keywords:0-1 optimization problem, upper-bound, lower-bound, superincreasing sequence.

1.INTRODUCTION

The most met formulation of 0-1 problem is

$$\max \sum_{j=1}^{n} c_j x_j \qquad (1)$$

subject to

$$\sum_{j \in N_i} a_{ij} x_j \le d_i \quad i = \overline{1,m} \qquad (2)$$

$$x_j \in \{0,1\},\ j \in N = \{1,2,...,n\},\ N_i \subset N \qquad (3)$$

For $m = 1$ and positive a_{ij}, d_i, c_j the problem becomes the knapsack one which is effectively applied in knapsack-type public key cryptosystem (Koblitz (1994)).

For $m = 2$ and positive c_j, a_{ij}, d_i we obtain two-constraint 0-1 knapsack problem. An exact method for solving this problem is given in (Martello and Toth(2003)).

In general 0-1 optimization problem belongs to $NP-hard$ class but there are many particular cases solvable in polynomial time.

Such cases are discussed for example in (Jenner B. (1995)), (Alfonsin R. (1998)).

We want to refer to these cases. It turns out that we can extend the set of 0-1 optimization problems solvable in polynomial time. It is possible when the coefficients of the objective function belongs to the set of superincreasing or superdecreasing type of sequence.

2. SUPERINCREASING SEQUENCE AND 0-1 OPTIMIZATION PROBLEM

Definition 1.

A sequence (c_j) is called superincreasing

when $\sum_{i=1}^{j-1} c_i < c_j \quad for\ j = 2,3...$ (4)

We will consider sequences containing only n elements and assume that for $n = 1$ a sequence is superincreasing.

Proposition 1.

If the problem (1)-(3-) satisfies the following assumptions:

- a sequence (c_j) is the superincreasing and non negative one,
- elements $a_{ij} \ge 0$

the optimal solution of the problem (1)-(3) is given by the procedure

$$x_j^* = \begin{cases} 1 & when\ a_j \le d - \sum_{k \in N_j^+} a_k \\ & j = n, n-1, ..., 1 \\ 0 & otherwise \end{cases} \qquad (5)$$

where

a_j -the j-th column of the constraint matrix (2)

$d = (d_1, d_2, ..., d_m)^T$, $N_n^+ = \Phi$

$N_j^+ = \left\{k : x_k^* = 1,\ k \in \{n, n-1, ..., j = 1+1\}\right\}$

The complexity of the procedure (5) is polynomial - $O(n^3)$.

3. UPPER-BOUND AND LOWER-BOUND OF OPTIMAL OBJECTIVE FUNCTION VALUE

Denote by

H^n – the set of possible, integer and superincreasing sequences $(h_i), i = \overline{1,n}$

A^n – the set of superincreasing sequences with integer elements not smaller than suitable elements of sequence (c_j),

$A^n = \left\{h \in H^n : h_j \ge c_j \quad j = \overline{1,n}\right\}$

Let (c_j) be not decreasing.

Definition 2.

A superincreasing sequence (h_j^*) is called the nearest up to the sequence (c_j) when

$$h^* \in A^n$$
$$\left\|c - h^*\right\| = \min_{h \in A^n} \|c - h\| = \tag{6}$$
$$= \min_{h \in A^n} \sum_{j=1}^{n} \left|c_j - h_j\right|$$

The complexity of setting the sequence (h_j^*) is polynomial - $O(n^2)$.

Upper-bound of optimal objective function value is given by

$$\sum_{j=1}^{n} h_j^* x_j \geq \sum_{j=1}^{n} c_j x_j^* \tag{7}$$

for $a_{ij} \geq 0, \quad c_j \geq 0$

and $x_j = 1$ only then if it follows from the procedure (5) and when we replace the sequence (c_j) by sequence (h_j^*).

Similarly we can define a superincreasing sequence (h_j^o), which is called the nearest down to the sequence (c_j). Using (h_j^o), the lower-bound of optimal objective function value is given by formula $\sum_{j=1}^{n} h_j^o x_j$ when

$$x \in S = \left\{x \in E^n : constr. \quad (2),(3)\, hold\right\}.$$

4. MINIMALIZATION PROBLEM

We consider the following 0-1 problem:

$$\min \sum_{j=1}^{n} c_j x_j \tag{8}$$

subject to

$$\sum_{j \in N_i} a_{ij} x_j \geq d_i \quad i = \overline{1,m} \tag{9}$$

$$x_j \in \{0,1\}, \quad j \in N = \overline{1,n},\ N_i \subset N \tag{10}$$

This problem needs another approach.

Definition 3.

A sequence (c_j) is called superdecreasing one when

$$c_j > \sum_{i=j+1}^{n} c_i \quad j = 1,...,n-1 \tag{11}$$

Proposition 2.

If the problem (8)-(10) satisfies: (c_j) superdecreasing sequence, $c_j \geq 0, a_{ij} \geq 0$, there exists j such that $a_{ij} \geq d_i, i = \overline{1,m}$ then optimal solution of problem (8)-(10) can be expressed in following way

$$x_{j*}^* = 1 \; and \; x_j^* = 0 \quad for \; j \neq j*$$

when

there exists i such that

$$\sum_{j=j_*+1}^{n} a_{ij} < d_i, i \in \{1,2...,m\} \text{ and } j* < n$$

where $j* = \max\left\{j : a_{ij} \geq d_i, i = \overline{1,m}\right\}$

or $j* = n$.

The complexity of computing optimal solution according to procedure given bellow is polynomial- $O(n^2)$.

We have also considered several other cases (Chudy M.(2005)).

5. CONCLUSIONS

Superincreasing and superdecreasig sequences can be widely used to find effectively an upper- or lower- bound of optimal objective function value.

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A GENETIC LOCAL SEARCH ALGORITHM FOR WEIGHTED MAXIMUM LEAF SPANNING TREE PROBLEM

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Keywords: discrete optimization, genetic algorithm, WMLSTP.

1. INTRODUCTION

The importance of the NP-hard weighted maximum leaf spanning tree problem (WMLSTP) derives form its direct applications in the design of computer and communication networks, VLSI circuit, as well as from its appearance in theoretical investigations connected with some graph properties [2].

Given an undirected and connected graph $G = (V, E(G))$ where $V = \{1, 2, \ldots, n\}$ is a non-empty set of vertices, E is a set of edges and a non-negative function w: $V \rightarrow \Re^+$. For $i \in V$, let $\delta_G(i)$ denote a set of edges adjacent to i in graph G. For a spanning tree $T = (V, E(T))$, $E(T) \subset E(G)$, in G, the vertex $i \in V$ with $|\delta_T(i)| = 1$ is called a leaf and the set of all tree T leafs is denoted $L(T) = \{ i \in V : |\delta_T(i)| = 1\}$, where $\delta_T(i)$ is a set of edges adjacent to i in tree T, $\delta_T(i) \subseteq \delta_G(i)$. The WMLSTP is to find a spanning tree T in G, which maximizes the sum of leafs weight $\sum_{i \in L(T)} w_i$. This problem is a generalization of the maximum leaf spanning tree problem (MLSTP) where the problem is to find a spanning tree T in G, which maximizes the number of the leafs $|L(T)| \rightarrow \max$. The difference between problem WMLSTP and MLSTP is displayed in figure 1, where tree c) in weighted graph a) has the weight 8 whereas tree b) has greater number of leafs and the weight equals 0.

2. GTS ALGORITHM

For WMLSTP problem solution we propose a modified genetic local search algorithm called GTS where each spanning tree, individual of the population, generated by crossover procedure is improved by designed for WMLSTP randomized tabu search (RTS) instead of hill climbing algorithm. The population of GTS consists only of feasible solutions that is of spanning trees thus crossover and RTS algorithms have to generate only feasible descendents. Figure 2 presents the process of feasible descendent T_3 generation on the base of two parents T_1 and T_2 crossover where $T_1 \cup T_2$ stands for the joint genetic material (set-theoretic sum of tree edges) of parents.

3. COMPUTATIONAL RESULTS

For the purpose of GTS algorithm quality verification we make some series of computer experiment for problem WMLSTP instances where number of graph G vertices are n = 25, 50, 75, …, 250. For each n 50 test graphs (20 grid, 10 cubic, 20 with random connections in graphs) were generated randomly; for each test 10 optimizations were performed. Fig. 3 displays mean values of all series of computer experiments where one series consist of 10*50*10 = 5000 optimization processes. The first column of the Fig. 3 diagrams present the percentage improvement of the objective function realized by investigated SA (simulated annealing algorithm [1] taken for the comparison) and GTS algorithms in proportion to best spanning tree in the randomly generated initial population and the second column in proportion to the best spanning tree determined by 90 constructive heuristics. Besides, the third column presents the improvement index of the SA and GTS algorithms.

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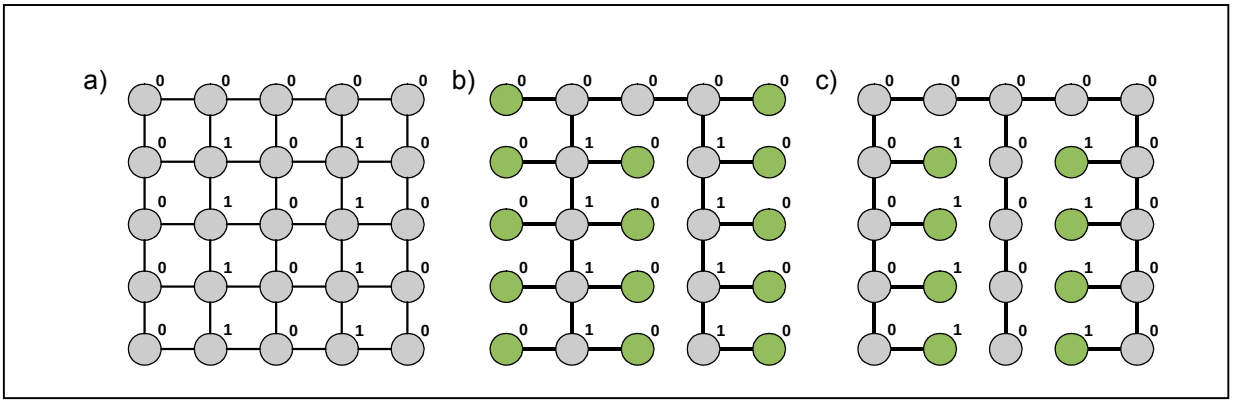

Fig. 1. Differences among WMLSTP and MLSTP problems.

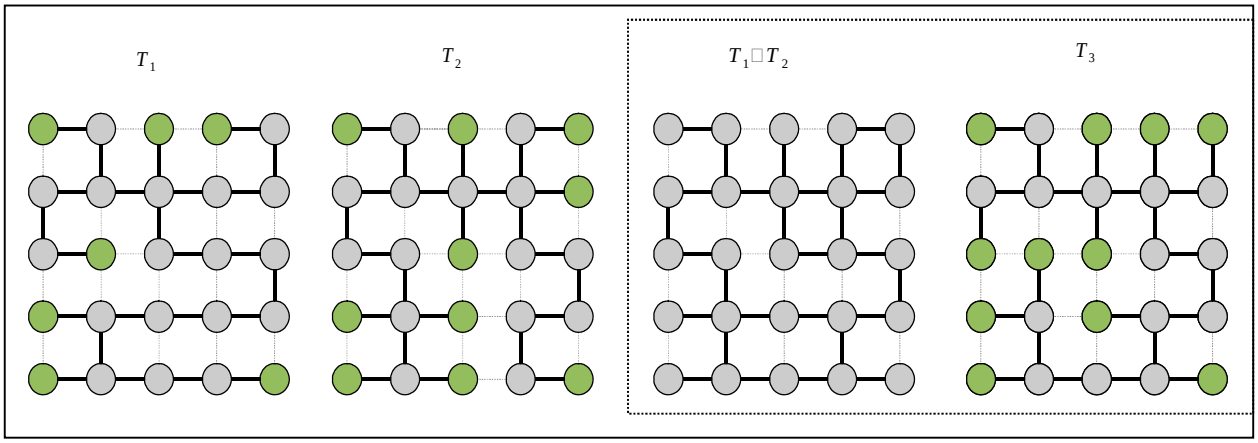

Fig. 2. Example of the crossover process.

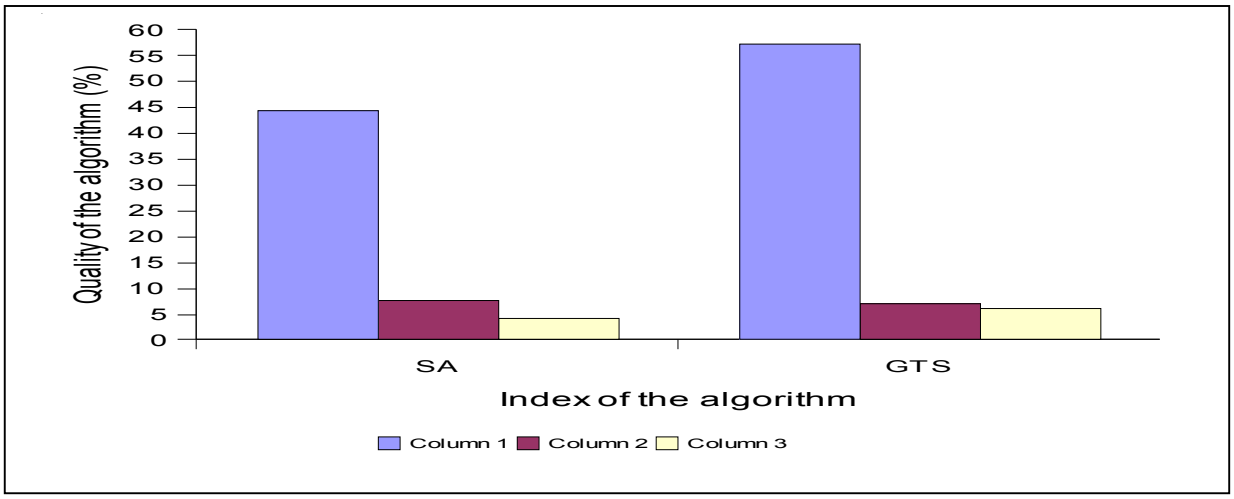

Fig. 3. Computational results.

PARALLEL NONMONOTONE DERIVATIVE FREE ALGORITHM FOR BOUND CONSTRAINED OPTIMIZATION

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Keywords: non monotone, derivative free, bound constrained

1. PRELIMINARIES

This paper presents a parallel iterative algorithm for solving the bound constrained optimization problem **(BCOP)**

$$\min_{x\in\mathcal{F}} f(x),\ \mathcal{F}=\{x\in I\!R^n : s\le x\le t\},$$

where the vector inequalities $s\le x\le t$ hold component wise, i.e., $s^k\le x^k\le t^k, k=1,\ldots,n$ and $f(\cdot):\mathcal{F}\to I\!R$ is a real valued function of n variables with inaccurate or absent derivative information. Starting with $x_0\in\mathcal{F}$, the algorithm generates a sequence $\{x_i\}_1^\infty\subseteq\mathcal{F}$ that, under suitable assumptions, possesses a subsequence $\{x_i\}_{i\in I}$ converging to a point $x_*\in\mathcal{F}$ satisfying a necessary condition for optimality linked to the differentiability properties of $f(\cdot)$. A salient feature of our *parallel* algorithm is that it exhibits a *fault tolerance* fixed by the user, say π; i.e., the algorithm still works even if π processors are idle or faulty at the same time.

The parallel algorithm is a natural outgrowth of previous sequential algorithms for unconstrained optimization problems, which assume that a numerical approximation of derivatives is unreliable. The forerunner derivative free algorithm was introduced by García and Rodríguez (1). Later García et al (2) suggested the non monotone version to deal with global optimization. A key concept needed for the convergence analysis of these algorithms is the generation of a set of r unit directions $D_i=\{d_{ik}\in I\!R^n, k=1,\ldots,r\}$ that positively spans $I\!R^n$; that is, any $x\in I\!R^n$ can be represented as a non negative linear combination of elements in D_i. For solving (BCOP) the set $D_i=\{\pm e_1,\ldots,\pm e_n\}$ of unit vectors along the axis positively spans $I\!R^n$ and has been suggested in previous works (1; 2; 3). Numerical experiments with unconstrained problems reveal that this choice in general deteriorates the algorithm's performance. Therefore, this paper suggests a new scheme to form D_i that takes into account the geometry of the constrained region, which seems to be necessary to prove convergence (4).

2. ALGORITHM

Due to space limitations this section describes a simplified implementation of the algorithm (table 1) and outlines the convergence proof. Complete details will be given in the full length version of this paper. There are, say p processors, with a common memory accessible by them all, where the best estimate $z, f(z)$ is saved. The j-th processor fetches this information around every Γ^j seconds. Besides, the j-th processor has the following handy information at the i-th iteration:

$K_i=\{k : s^k+\delta\le x_i^k\le t^k-\delta\}, \delta>0$
$P_j\subseteq\{1,\ldots,n\}$ variables pertaining to j
$\tau_{ij}>0$, radius of search
$\gamma_{ij}\ge 1$, expansion factor
$\mu_{ij}<1$, contraction factor
$x_{ij}\in\mathcal{F}$, solution estimate
$\varphi_{ij}\ge f(x_{ij})$, upper bound of $f(x)$

P_j is an index set of those components of x that can be modified by processor j. In fact, starting at any x_{ij} the j-th processor *attempts to* solve the BCOP on the subspace generated by the unit vectors $e_k, k\in P_j$; i.e. it tries to solve

$$\min_{x\in\mathcal{C}} f(x),\ \mathcal{C}=\{x\in\mathcal{F} : x^k=x_{ij}^k, k\notin P_j\}.$$

The algorithm ensures convergence to $x_*\in\mathcal{F}$ if $\bigcup_{j=1}^{p} P_j=\{1,\ldots,n\}$. When $P_j=\{1,\ldots,n\}$ for $j=1,\ldots,p$, the algorithm simply uses each

D_{ij} spans positively the subspace spanned by $e_k, k \in (P_j \cap K_i)$.
$D_{ij} = D_{ij} \cup \{\pm e_k : k \in (P_j \cap \neg K_i)\}$.
success = false
for $d \in D_{ij}$
  $y = \text{median}(s, x_{ij} + \tau_{ij} d, t)$
  if $f(y) \leq \varphi_{ij} - 0.01(\tau_{ij})^2$
    $x_{i+1,j} = y;\ \tau_{i+1,j} = \min(\tau, \gamma\tau_{ij})$
    success= true; break
if success= false
  $x_{i+1,j} = x_{ij};\ \tau_{i+1,j} = \mu\tau_{ij}$
Update $\varphi_{i+1,j}$
if time Γ^j to retrieve z is surpassed
  if $f(x_{i+1,j}) < f(z)$
    $z = x_{i+1,j}$
  elseif $f(z) \leq \varphi_{i+1,j} - 0.01(\tau_{i+1,j})^2$
    $x_{i+1,j} = z$
    $\tau_{i+1,j} = \min(\tau, \gamma\tau_{ij});\ \varphi_{i+1,j} = f(z)$

Table 1. i-th iteration, j-th processor

processor for solving BCOP. Although highly inefficient, let us point out that we have a fault tolerance $\pi = p - 1$. We could distribute the components $1, \ldots, n$ in such a way that any q processors randomly taken may modify all components; in which case $\pi = p - q$.

We say that x_{ij} is blocked by τ_{ij} if

$$[d \in D_{ij}] \Rightarrow f(y) > \varphi_{ij} - 0.01(\tau_{ij})^2,$$

where $y = \text{median}(s, x_{ij} + \tau_{ij} d, t)$. We observe that the upper bound φ_{ij} influences the performance of the algorithm significantly. Large values allow to succeed (success= true in table 1) more often and ease the *hill climbing* ability of the algorithm; on the other hand, the closer the value of φ_{ij} is to $f(x_{ij})$ the more similar the behaviour of the algorithm is to its monotone version and it might converge to the closest local minimum.

Convergence theorem. We need the following assumptions:

A1: $f(\cdot)$ is bounded below on $\mathcal{F}$, and $\{x_i\}_1^\infty$ remains in a compact set.

A2: $f(x_{ij}) \leq \varphi_{ij}; \varphi_{i+1,j} \leq \varphi_{ij}$.

Let $I \subseteq \{1, \ldots, \}$ and let i, k be two subsequent elements in I; then $\varphi_{kj} \leq \varphi_{ij} - 0.01\tau_{kj}^2$.

A3: $D_i \to D$, and D spans positively $I\!R^n$.

Let x_* be a limit point of blocked points and let $B(x_*, \rho)$ be a ball around it. If $f(\cdot)$ is convex in B with smooth directional derivatives $f'(x, d)$, then $f'(x_*, d) \geq 0$ for all feasible directions $d \in D$. Moreover, if $f(\cdot)$ is strictly differentiable at x_*, then $\nabla f(x_*)^T d \geq 0$ for all feasible directions $d \in D$.

Remark. If $K_* = \{k : s^k + \delta \leq x_*^k \leq t^k - \delta\} = \{1, \ldots, n\}$, the algorithm solves an unconstrained optimization problem and the theory developed in (1; 2) is valid. The proof of convergence is based on this fact, but it is rather lengthy and technical. It is omitted in this extended abstract.

3. CONCLUSIONS

We have sketched an algorithm for solving the Box Constraint Optimization Problem, which shares many important properties of its counterparts in unconstrained optimization; mainly *i:* It can deal with noisy functions, *ii:* Convergence for smooth convex functions, and for strictly differentiable functions is ensured under rather weak conditions, *iii:* It is non monotone, and may scape from local minima; and finally, *iv:* practical versions can be easily implemented in a multiprogramming environment with a fault tolerance fixed by the user.

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A Scheduling Method for R&D Projects with the Minimum Risk

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Keywords: Keywords : Risk, Scheduling, R&D Projects, Optimization.

A scheduling method has been developed for multi-task R&D projects in which technical and market risk factors are critical issues. The R&D risk is controlled by stage-wise investment decisions and the use of real options of stage-wise development type.

The project scheduling method employs the expected sum of total investment as a risk index, and minimizes the index through task ordering and task scheduling steps subjective to constraints.

Expected loss of a project with 3 tasks is evaluated for schedule A and B in Fig.1. Schedule B with shorter project term has increased expected loss, because test3 starts even if test 2 fails. Expected loss is linearly correlated to expected investment, which is the risk index, in multi-task projects.

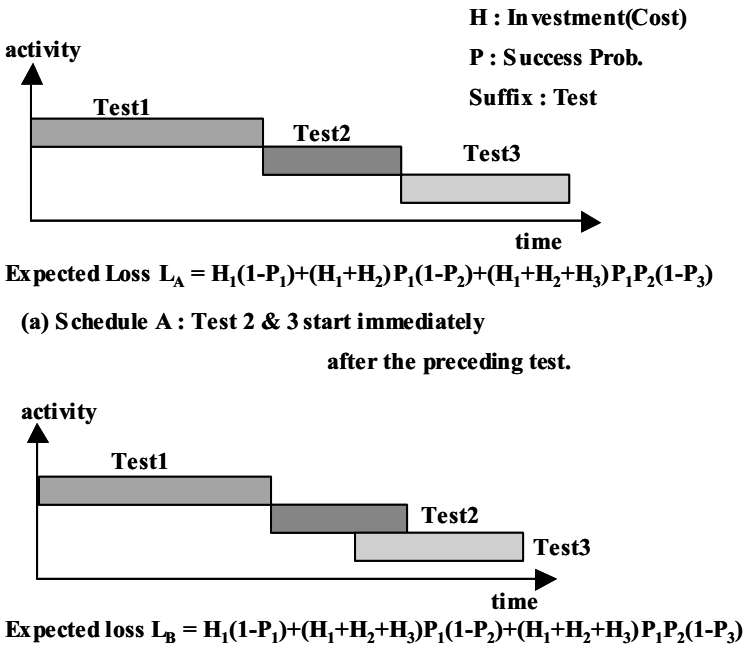

Fig. 1 Project schedule and expected loss

A risk directed ordering measure (task investment/ task failure probability) is analytically derived from the minimum expected loss criteria, and extended to satisfy task order constraints for Step 1. The total expected investment V for a project with n serial tasks is given as:

$$V=H_1+P_1H_2+\text{---}+P_1P_2\text{---}P_{n-1}H_n$$

,where H_k and P_k are investment (cost) and success probability of k-th task, respectively. The optimal ordering condition assures that no task pair exchange reduces the expected investment, and is described as follows:

$$H_{k+1}/(1-P_{k+1}) > H_k/(1-P_k)$$

The ordered tasks are scheduled by the dynamic programming for resource allocation at Step 2 as illustrated in Fig.2.

The project scheduling method has been successfully applied to a sample pharmaceutical R&D project with 28 tasks as in Fig.3, and the applicability of the method has been confirmed with numerical results from the two scheduling steps.

Numerical results reveal some characteristics of the minimum risk schedule of the multi-task project:

- Flattened resource is obtained throughout the project term in the expected resource profile, though remarkable peak is found at later stage of the project in the success-based resource profile.

- Delayed start of tasks at earlier stage of the project contribute to improve the risk index, because those tasks tend to have critical impact on the expected investment.

(a) The possible schedules are defined for each task ordered at Step 1 on the basis of the decision tree describing the binary choice of task initiation month.

(b) The optimal path with the minimum expected loss is searched in the decision tree subjective to constraints on resource and time.

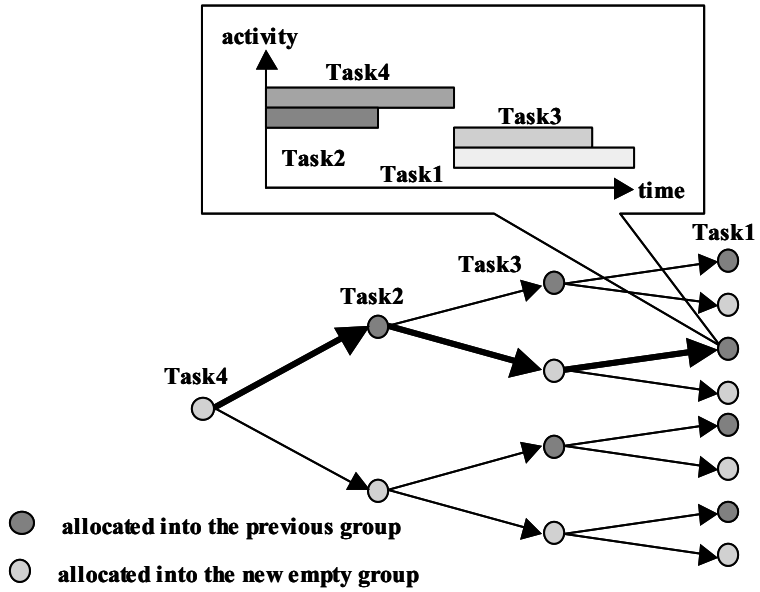

Fig.2 Schedule optimization scheme for Step 2

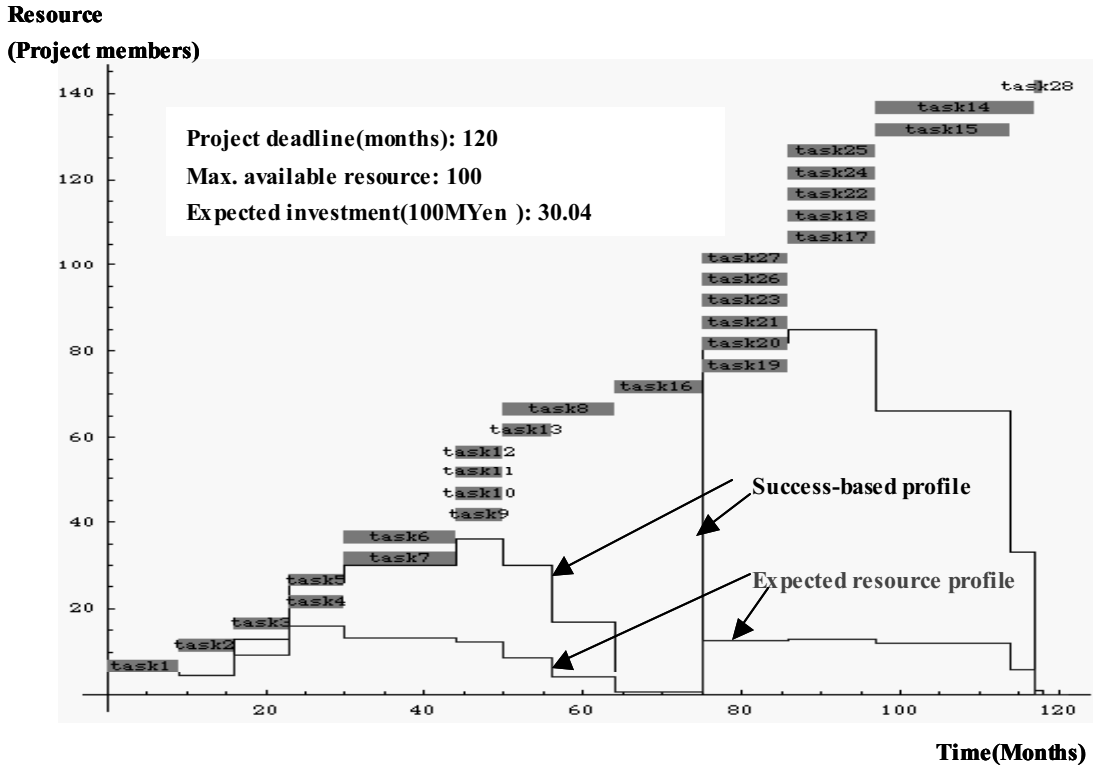

Fig3. Project schedule with the minimum risk

SCHEDULING PROBLEMS FOR SYNCHRONIZATION OF MULTI-OBJECTS MOVEMENT

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Keywords: movement scheduling and synchronization, shortest paths, disjoint paths, multicriteria shortest paths problems.

1. INTRODUCTION

In the paper a problem of determining movement schedule of many objects is considered. The problem is used in many domains such as: routing in computer networks, movement planning of mobile robots, tasks processing in parallel or distributed computing systems, arms control of independent robots, planning and synchronization of many objects movement in computer simulation games, e.g. in Computer Generated Forces (CGF) systems (Petty, 1995). A special type of movement is such one that objects must be moved simultaneously. And a special type of system with this requirement is system for movement planning and simulation of military objects (units) in combat simulators. Movement scheduling has an influence on accuracy, adequateness, effectiveness and other characteristics of these systems. Then, the problem is to model and optimize such movement of detachments to achieve intended goals of commands (such as: achievement of destinations on restricted time, avoiding of losses during redeployment etc.). Regardless of kind of military actions military objects are moved according to some group pattern. For example, each object being moved in group (e.g. during attack, during redeployment) must keep distances between each other inside group.
Therefore, the paper presents some problems of movement scheduling for many objects to synchronize their movement.

2. DEFINITIONS AND NOTATIONS

We assume that we have Berge's graph G defining structure of the terrain (divided on the squares, hexagons, etc.) $G=\langle V_G, A_G\rangle$, $V=|V_G|$, V_G – set of graph's nodes (as centre of terrain squares), A_G – set of graph arcs, $A_G \subset V_G \times V_G$, $A=|A_G|$. We assume that on each arc we have defined value $d_{n,n'}$ of function d which describes terrain distance between the graph nodes n and n'. We have K objects (columns, trucks, tasks) for movement from the vector $s=(s_1, s_2, ..., s_K)$ of source nodes to the vector $t=(t_1, t_2, ..., t_K)$ of destination nodes of G. For further discussion we accept following notations:

$$I_k(s_k,t_k)=I_k=\left(i^0(k)=s_k,...,\ i^r(k),...,i^{R_k}(k)=t_k\right)$$

$$T_k(I_k)=T_k=\left(\tau^0(k),\tau^1(k),...,\tau^r(k),...,\tau^{R_k}(k)=\tau(I_k)\right)$$

$$V_k(I_k)=V_k=\left(v_{i^0(k),i^1(k)}, v_{i^1(k),i^2(k)},\ \ldots,\ v_{i^{R_k-1}(k),i^{R_k}(k)}\right)$$

where I_k - vector of nodes describing path for the k-th object, $\forall_{m\in\{1,...,R_k\}}\left(i^{m-1}(k),i^m(k)\right)\in A_G$; $i^r(k)$ - the r-th node on the path for the k-th object; s_k, t_k – source and destination nodes for the k-th object; T_k - vector of time instances of achieving the nodes belonging to the path for the k-th object; $\tau^r(k)$ - time instance of achieving node $i^r(k)$ by the head of the k-th object, $\forall_{k=\overline{1,K}}\ \forall_{r=\overline{0,R_k-1}}\ \tau^{r+1}(k)\geq\tau^r(k)\geq 0$ and $\forall_{k=\overline{1,K}}\ \tau^0(k)=0$; $\tau(I_k)$ - time of achieving destination node by the k-th object; V_k - vector of velocities $v_{i^r(k),i^{r+1}(k)}$ of the k-th object on the arc $\left(i^r(k),i^{r+1}(k)\right)$ of its path; R_k - number of arcs belonging to the path of the k-th object.

Let $IP_k=\left\{i_1(k),\ i_2(k),...,\ i_p(k),...,\ i_{P_k}(k)\right\}$ denotes set of nodes at which we must align the head of the k-th object in relation to the heads of other objects, where $i_p(k)$ - the p-th element of IP_k satisfying: $\forall_{p=\overline{1,P_k}}\ \exists_{r\in\{1,...,R_k\}}\ i_p(k)=i^r(k)$ and $r_p(k)=r\in\{1,...,R_k\}\Leftrightarrow i_p(k)=i^r(k)$. The form of IP_k

and $r_p(k)$ say that path for the *k*-th object must cross by nodes belonging to IP_k. Let, by analogy $TP_k = \{\tau_1(k),\ \tau_2(k),...,\ \tau_p(k),...,\ \tau_{P_k}(k)\}$ denotes set of time instances of achievement particular alignment nodes from the set IP_k by the *k*-th object head, $\tau_p(k)$ denotes moment of achieving the *p*-th alignment node by the *k*-th object,

$$\tau_p(k) = \tau^0(k) + \sum_{\substack{r\in\{0,...,R_k-1\} \\ r \le r_p(k)}} \frac{d_{i^r(k),i^{r+1}(k)}}{v_{i^r(k),i^{r+1}(k)}}$$

We make additionally assumption that $P_1=P_2=...=P_K=N$, i.e. for all objects the same number of alignment points (nodes) exist. Moreover, we define for each p=1,..,N following characteristic: $\tau_p^{\max} = \max_{k\in\{1,...,K\}} \tau_p(k)$.

3. FORMULATION OF THE PROBLEM

We define the problem of synchronous movement of K objects as follows: for each $k \in \{1,...,K\}$ to determine the path I_k crossing by points from IP_k and for each arc $\left(i^r(k), i^{r+1}(k)\right)$, $r \in \{0,...,R_k-1\}$ belonging to the path I_k to determine such a velocity $0 < v_{i^r(k),i^{r+1}(k)} \le v^{\max}(k)$, that some goals (one or more) are satisfied, where $v^{\max}(k)$ describes maximal velocity of the *k*-th object resulting from its technical properties.

The most important goals for movement synchronization can be divided into two categories. The first category is time of movement of K objects. We can define two basic measures of this category:

$$\tau^{\max} = \max_{k\in\{1,...,K\}} \tau^{R_k}(k) \quad , \qquad \sum_{k=1}^{K} \tau^{R_k}(k)$$

The second category is "distance" between times of achieving alignment points by all of K objects. We can define two main measures of this category: $\sum_{p=1}^{N}\sum_{k=1}^{K} \tau_p^{\max} - \tau_p(k)$,

$\min_{p\in\{1,...,N\}} \max_{k\in\{1,...,K\}} \left(\tau_p^{\max} - \tau_p(k)\right)$.

One of the formulations of optimization problem for movement synchronization of K objects using defined two categories of measures can be presented as follows: for fixed paths I_k of each *k*-th object to determine such $v_{i^r(k),i^{r+1}(k)}$, $r = \overline{0, R_k-1}$, $k = \overline{1,K}$ that

$$\sum_{p=1}^{N}\sum_{k=1}^{K} \tau_p^{\max} - \tau_p(k) \to \min$$

with the constraints :

$$v_{i^r(k),i^{r+1}(k)} \le v^{\max}(k), \qquad r = \overline{0, R_k-1},\ k = \overline{1,K}$$

$$v_{i^r(k),i^{r+1}(k)} > 0, \qquad r = \overline{0, R_k-1},\ k = \overline{1,K}$$

Paths for K objects may be disjoint or not and they must cross by fixed alignment points or we dynamically determine these points.

4. CONCLUSIONS

In the final version of the paper a nonlinear movement scheduling problem in order to minimize sum of delays of all (K) objects in checkpoints with some additional constraints will be defined. Two equivalent formulation of two-criteria mathematical programming problems taking into account two categories of the goals will be also presented. It will be proved that constraint coefficient matrices for both problems are totally unimodular and we can use effective algorithms for solving linear programming problems to find lexicographic solution of two-criteria problems. Two algorithms for synchronous movement scheduling will be proposed and their properties will be shown. Similarities and differences between defined problems and classical tasks scheduling problem before critical lines on parallel processors will be discussed. Some extensions of movement scheduling problem will be presented, too.

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TARIFF OPTIMIZATION PROBLEM - FORMULATION AND ALGORITHMS

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1. INTRODUCTION

The problem we consider concerns the optimal tariff offered to a customer of a mobile telecommunication company. The company proposes the best possible combination of services within several contracts to an individual customer, or a corporation. The considered services are such as: domestic and foreign calls, local and long distance calls, SMS and MMS messages, etc. In general the number of these services can be quite significant especially when corporate client is considered. Some of these services can be packed into packages which we call contracts which require fixed monthly payments if the specified number of services included in them are not exceeded. If a customer uses more services than those specified in the contract he is charged for each exceeding service.

The tariff optimization problem is then defined as a problem of finding the best possible choice of contracts such that the monthly payment of a client is the lowest provided that the customer's profile is known. By the customer's profile we mean his average use of services during some pre–specified period of time. Once the mobile telecommunication company decides to propose to its customers optimal tariffs it must take into account an avalanche of questions from its customers concerning its new proposition. It translates into a bulk of optimization problems which have to be solved in short time in order not to discourage the customers from this proposition.

2. THE PROBLEM FORMULATION

Let us denote by y_i the number of contracts of ith type and by x_{ij} the number of jth services within the ith type of contract. Then the tariff optimization problem–$\mathbf{P}$–is as follows (more general formulations with the option for substitute services are possible)

$$\min_{x,y} \sum_{i=1}^{m} \left[c_i y_i + \sum_{j=1}^{n} c_{ij} \max\left[0, x_{ij} - y_i b_{ij}\right] \right]$$

$$\text{s. t.} \sum_{i=1}^{m} x_{ij} = x_j^h, \quad j = 1, \ldots, n \tag{1}$$

$$0 \le y_i \le M_i, \ i = 1, \ldots, m \tag{2}$$

$$0 \le x_{ij}, \ i = 1, \ldots, m, \ j = 1, \ldots, n. \tag{3}$$

Here, $x = \{x_{ij}\}_{i=1,\ldots,m, j=1,\ldots,n}$, $y = \{y_i\}_{i=1,\ldots,m}$, c_i is the monthly cost of the ith contract, c_{ij} is the unit cost of the jth service in the ith contract and b_{ij} is the limit of the jth service in the ith contract which is included in the contract as free of charge. Furthermore, x_j^h denotes the average number of units of the jth service measured in the pre–specified period of time. In order to complete the description of the problem we have to indicate that variables y are integer variables, furthermore we assume that x are real numbers. Problem $\mathbf{P}$ can be stated as a standard linear MIP problem by introducing auxiliary variables z_{ij} which transform the problem to the problem with a differentiable cost function ((3)):

$$\min_{x,y} \sum_{i=1}^{m} \left[c_i y_i + \sum_{j=1}^{n} c_{ij} z_{ij} \right] \tag{4}$$

$$\text{s. t. } x_{ij} - y_i b_{ij} - z_{ij} \leq 0 \quad (5)$$

$$0 \leq z_{ij},\ i = 1, \ldots, m,\ j = 1, \ldots, n \quad (6)$$

and constraints (1)–(3).

3. DECOMPOSITION METHOD FOR MIP PROBLEM

Problem (4)–(6), (1)–(3) can be solved by various algorithms (some exemplary results are presented in the next section), however for problems with large m and n the performance of these methods couldn't allow to use them in on–line computations (an offer for a corporate client can refer to as many 20 different contracts which can have 200 different services). In order to circumvent the dimensionality problem we advocate to use the relaxation methods based on the Lagrangian of the problem. Since only constraints (1) unable us to solve the problem in the decomposed way–each subproblem corresponds to each contract i–we introduce the Lagrange function with respect to these constraints:

$$\mathcal{L}(x, y, \lambda) = \sum_{i=1}^{m} \left[c_i y_i + \sum_{j=1}^{n} c_{ij} z_{ij} \right] + \sum_{j=1}^{n} \lambda_j \left[\sum_{i=1}^{m} x_{ij} - x_j^h \right], \quad (7)$$

where λ_j are the Lagrange multipliers corresponding to (1).

The problem can then be solved by using two–stage algorithm where at the lower level subproblems $\mathcal{P}_i$, $i = 1, \ldots, m$ are solved:

$$\min_{y_i, x_{ij}, z_{ij}, j=1,\ldots,n} \left[y_i c_i + \sum_{j=1}^{n} c_{ij} z_{ij} + \sum_{j=1}^{n} \lambda_j x_{ij} \right]$$

$$\text{s. t. } 0 \leq y_i \leq M_i$$

$$0 \leq x_{ij},\ j = 1, \ldots, n.$$

$$x_{ij} - y_i b_{ij} - z_{ij} \leq 0$$

$$0 \leq z_{ij},\ j = 1, \ldots, n$$

assuming that λ_j, $j = 1, \ldots, n$ from the upper level of the algorithm are given.

At the upper level of the algorithm variables λ_j, $j = 1, \ldots, n$ are updated in order to maximize the function

$$\bar{\mathcal{L}}(\lambda) = \mathcal{L}(x(\lambda), y(\lambda), \lambda), \quad (8)$$

Problem	B & B	B & C (G)	B & C (P)	B & C (G + P)
small	0.08 s. 2 nodes	0.047 s. 1 node	0.062 s. 1 node	0.084 s. 1 node
medium	1.74 s. 84 nodes	0.87 s. 28 nodes	0.61 s. 32 nodes	0.84 s. 8 nodes

Table 1. Numerical results

where $x(\lambda)$ and $y(\lambda)$ are solutions to the problems $\mathcal{P}_i$.

Since the upper level of the optimization algorithm is nondifferentiable problem subgradient methods such as those described in (2) should be used to solve it.

4. CONCLUSIONS

The paper presents a practical problem of determining an optimal tariff for a customer of a mobile telecommunications company. The formulated problem can be solved on–line as results presented below show.

Suppose that the number of possible contracts and services are equal to $m = 6$ and $n = 14$ respectively–then we have small tariff problem. In the second problem we have $m = 13$ and $n = 80$–we call it a medium size problem. In order to solve these problems we applied CBC (COIN-OR Branch and Cut) framework for solving MIP problems (see (1) and (4)). Some numerical results are given in Tab. 1–(G) means Gomory, (P) means Probing and (G+P) Gomory and Probing. The table reports CPU time obtained on Intel PC with 1.86MHZ processor with 1GB of main memory.

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MULTICRITERIA COORDINATED CONTROL OF WATER RESERVOIR SYSTEMS IN CASE OF FLOOD EMERGENCY

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Keywords: multicriteria optimal control, multicriteria decision support reference sets, preference structures, environmental protection, water reservoir systems, flood control.

1. PRELIMINARIES

In this paper we will present an approach to solving the problem of choice of an optimal reservoir control strategy in the situation of flood emergency. The potential and often adopted actions include spontaneous releases of water from the reservoir based on the emergency precipitation forecasts. As side effects, the water level sinks below the minimum necessary to sustain the ecosystems in reservoir lakes, while the fluvial ecosystems below the reservoir are often destroyed. We show that these effects may be minimised by a suitable coordination: the problem to be solved is a multicriteria coordination one, with the environmental, financial and human-life-protection-related criteria.

We assume that in the region, which is endangered by the flood, there exist n water reservoirs, which can be used for the flood-control. The reservoirs are divided into N subsystems , each of them having a separate direction, economical goals, individual instructions on how to act in case of flood emergency, and a specified region, which should be protected in the first order of importance. The latter information can be regarded as components of the *i-th* subsystem preference structure, for $i=1,\ldots,N$. Motivated by the situation in the Upper Vistula Basin, which served as a playground for an implementation and experiments, we consider the case where all reservoirs are located on the feeders, while the flood wave on the recipient between and beneath the mouths of the feeders is controlled by the coordinated release of water from reservoirs belonging to different subsystems. Such situation may occur when larger cities and industrialised areas are situated in the main river valley.

This paper bases on an earlier research on modelling and control of water flows in river systems and reservoirs. Based on the above we will formulate a new problem concerning

- modelling the preferences of single reservoir management responsible for local flood-control activities; and
- coordination of their activities by constructing a common preference structure to be applied by a supervisory control centre.

In the model here presented the water reservoirs and river beds are modelled by the system of controlled ordinary differential equations:

$$x' = f(x,u,t,\eta),\ x\in\mathbb{R}^n,\ t\in[t_0,T],\ u\in\mathbb{R}^k,\ \eta\in\mathbb{R}^n \quad (1)$$

The above eqs. (1) results from a discretisation of the system of Saint-Venant equations. The latter describe the water flows more accurately, but require the real-time data on the flows and other hardly accessible information, such as exact description of river bed profiles, which change usually in the high water flow circumstances, therefore are not suitable for real-time control. The state variables x_j in the discretised models may be identified with the volumes of real, or hypothetical reservoirs (i.e. those resulting from a partitioning of river beds when discretising the Saint-Venant eqs.), while the controls u_i are interpreted as the velocity of

the water issue from the controlled reservoirs. The precipitation forecasts η may be input into the model as expected values or as deterministic scenarios, and should be updated at each step of the control strategy choice procedure. Other weather forecasts can be included into the problem analysis at the water inflow modelling stage. The described model makes possible efficient computation and proved useful in real-time control systems, when the dimension of the system (1) was between 37 and 140.

2. OPTIMISATION PROBLEM STATEMENT

Management staff of reservoirs is responsible for the flood protection in the recipient' s valley as well as in their own protection regions. For measuring the overall performance of each subsystem we have introduced the aggregated trajectory objectives $J_i(u,t)$ quantifying the value of the flood losses in the whole *i-th* subsystem protection region from the beginning of the observation period t_0 to t. We assume that they may be expressed in the form:

$$J_i(u,t) := \int_{[t_o,t]} g_i\left(x_{k(i)}, x_{k(i)+1}, \ldots x_{k(i)+1(i)}, t\right)dt, \quad (2)$$

for $i=1,\ldots N$, $t_o \le t \le T$, where t_o and T denote the moments of foreseen beginning and termination of the flood emergency situation, respectively, $x_{k(i)},\ldots x_{k(i)+1(i)}$ are the state-space coordinates of the *i-th* subsystem, and g_i, $i=1,..n$, are piecewise differentiable functions describing the dependence of the flood losses on the state of reservoirs. The criteria J_i describe the losses in ecological, financial, and human life emergency terms and cannot be easily aggregated. Obviously, they are to be the minimised simultaneously.

First, let us assume that the functions J_i conform to the local preference structures in each subsystem. Thus the goal of the supervisory control centre is to coordinate the subsystems' actions in order to assure the sustainability of ecosystems, and - when the flood danger becomes salient – to protect highly populated areas in the recipient's valley. Let us observe that the above criteria J_i are conflicting, i.e. the strategy minimizing the losses in the *i-th* region may not be optimal for the *j-th* subsystem, for $j \neq I$ and the ecological, economical and emergency criteria for each single reservoir are conflicting as well. The experiments point out that the coordinating centre is both capable and willing to keep the losses – in unavoidable – combined with the costs of anti-flood operations in certain limits, uniformly bounded for all reservoirs. At the same time the function J_{N+1}, which describes the losses in the recipients valley is to be minimised as an additional criterion. The role of the coordinating superior decision centre will thus consist in ensuring that the values of the criteria are nondominated and belong to the specified reference set *Q(t)*, i.e.

$$\left(J_1(u,t),\ldots,J_N(u,t)\right) \in Q(t) \quad (3)$$

The values of the multifunction *Q(t)* may be regarded as the sets of safe, or desired values of the criteria. Since the moment of termination of the flood danger is uncertain, and the indirect values of the losses play also an important role, we assume that the relation (3) shall be fulfilled on certain subinterval $[t_1,T]$ of the control period $(t_1>t_0)$, whereas t_1 may be meant as the beginning of anti-flood activities according to emergency rules. The optimisation task thus posed is a multicriteria optimal control problem with output trajectory objectives. We provide methods of finding a nondominated trajectory of the system fulfilling the additional demands (3). For the case, where the values of Q cannot be achieved for all $t \in [t_1,T]$, we propose a collection of methods to regularise the problem based on the distance scalarisation techniques.

There are diverse environmental, social, economical, and benefits of applying the coordination of control actions in case of a flood, or preceding an expected flood. The most important, yet not quantifiable indicator, is the number of human lives that can be saved if the flood wave is kept within safe limits or at least it grows in an observable and predictable manner. The environment can be kept intact by preventing non-justified and unnecessary water releases. The economic criteria, i.e. the value of potential losses, that could be avoided is another widely used objective. All that should be considered in the dynamical context and over a multi-year period.

Finally, we describe the numerical methods, which have been applied to solve the problem. A potential application is generating a flood-control strategy in the real-time control of eight water reservoirs in the Upper Vistula basin (the ninth reservoir is under construction) will also be presented. We will point out other areas in Europe and worldwide, which are endangered by floods in a similar manner and could be protected using the results here presented.

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FORMULATION OF OPTIMIZATION PROBLEM OF THE HORIZONTAL AXIS WIND TURBINE BLADE

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Keywords: Horizontal Axis Wind Turbine, Multidisciplinary Optimization, Genetic Algorithm

1. FORMULATION OF OPTIMIZATION PROBLEM

The optimal design of the wind turbine blade requires a number of optimization criteria to be taken into account, as: minimization of generated blade vibrations; maximization of output generated; minimization of blade material cost; stability of the blade structure; fulfillment of appropriate strength requirements by the blade structure.

The amplitude of generated vibrations of the wind turbine blade depends on its stiffness, which is a function of material density and thickness of its components. Therefore, when the vibration minimization criterion be taken into account, the wind turbine blade should be provided with the highest possible stiffness.

Such a formulation of optimization problem also satisfies the criterion of generated output maximization, as the output of a wind turbine depends also on the optimum shape of blades, i.e. on their optimum geometrical features.

The mass and fabrication cost of a blade depend on the same parameters as the amplitude of blade vibrations. If the cost minimization criterion were considered, then the optimization task would have to be formulated as a weight minimization task. However, in order to ensure stability of the structure, the weight should be maximized.

The side effect of such approach is possibility that eigenfrequencies of designed blade's will be the same as resonance frequencies.

In order to fulfill strength conditions it is necessary to optimize blade's maximal displacement, having strain constraints.

It is important that optimizations process gives proper dynamic characteristics. Such a characteristics are eigenfrequencies and spectral function. When excluding dumping, dynamic properties of mechanical system are taken from inertial matrix and stiffness matrix, which should be modified in optimizations process using proper objective function. The stiffness matrix can modify using dependence on blade's static deflection. Then the optimization task should be formulated as the minimization of the tip blade displacement task. Next step in optimizations process is mass reduction. The best way it would be to take mass reduction and minimizing the tip blade's displacement into account simultaneously, having effect all criteria fulfilled.

The problem of multidisciplinary discrete-continuous optimization of the wind turbine blade was formulated as a single criterion optimization task using the ε - limitations method:

A) formulating objective function as a weighted sum of most important criteria (mass reduction and minimizing of the tip blade's displacement);
B) choosing spectacular criteria as objective function, and formulating other criteria as limitations:
   - Minimization of the blade mass;
   - Minimization of the tip blade displacement.

Decision design variables in optimizations process are: shell thickness, web thickness, number of stiffening ribs and their arrangement along blade span.

The other criteria:
- fulfillment of appropriate strength requirements by the blade structure,
- ensure local and global stability of the blade structure,
- the natural frequency of the blade must be separated from the harmonic vibration associated with rotor rotation,
- the natural frequency of the blade must be separated from the frequency of the Karman's vortex,
- ensure minimal material cost of the blade,

were expressed in the form of inequality limitations.

4. CONCLUSIONS

Numerical calculations for all three variants of optimization processes and results of numerical simulations of displacement vibration signals determined for chosen nodes of the blade, makes conclusions:
- Mass reduction criteria reduces slightly blade vibrations (26% mass reduction);
- The tip blade displacement criteria reduces significantly the blade vibrations (about 30 %) making system more stable but increases significantly the blade mass (about 32%);
- Using the weighted objective function allows slightly reduce the tip blade displacement, increasing slightly it's mass;
- Such paretooptimal solution is good compromise between reducing the blade's mass and keeping good stiffnesses parameters.

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Joint solution to the long-term power generation planning and maintenance scheduling

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Keywords: Long-term power planning, maintenance schedule, warmstarting in interior point methods, global optimization, DC representation

1. LTGMP problem

Long-term electric power planning is a stochastic optimization problem. It has to be solved for new plant planning, fuel acquisition, and long- and short-term operation. Another decision that can be optimized is where to set the maintenance periods of the thermal units.

The Bloom and Gallant formulation (1) with the maximization of the profit (for a liberalized market) is a quadratic programming model that optimizes the expected generation of each unit of the pool in the intervals in which the long term period is split. The maintenance scheduling model is a linear binary problem (4). The union of both models results in a quadratic mixed binary problem (QMBP):

$$\begin{aligned}
&\text{minimize } h'x + \frac{1}{2}x'Hx && \text{(1a)}\\
&\text{subject to: } Ax \geq b && \text{(1b)}\\
&\qquad Cy = d && \text{(1c)}\\
&\qquad 0 \leq x_j^i \leq \overline{x}_j^i y_j^i \quad \forall\, i,\, j && \text{(1d)}\\
&\qquad y_j^i \in \{0,1\} \quad \forall\, i,\, j && \text{(1e)}
\end{aligned}$$

where constraints (1b) are part of the generation planning model (with continuous variables) and constraints (1c) models the maintenance schedule (with binary variables). The constraints on the upper bound (1d) links the two models. The subindex j indicates the unit and the supraindex i indicates the interval.

2. LTGMP solution approach

We solve problem (1) using some global optimization methods together with a specialized interior point technique.

Therefore, problem (1) is transformed into the continuous equivalent programming problem

$$\begin{aligned}
&\text{minimize } h'x + \frac{1}{2}x'Hx - \lambda y(y-1) && \text{(2a)}\\
&\text{subject to: } Ax \geq b && \text{(2b)}\\
&\qquad Cy = d && \text{(2c)}\\
&\qquad 0 \leq x_j^i \leq \overline{x}_j^i y_j^i \quad \forall\, i,\, j && \text{(2d)}\\
&\qquad 0 \leq y_j^i \leq 1 \quad \forall\, i,\, j && \text{(2e)}
\end{aligned}$$

by using the non-convex constraint

$$y_j^i(1 - y_j^i) = 0 \quad \forall\, i,\, j,$$

with $\lambda \geq 0$.

For a suitable given values of $\lambda := \lambda^*$ the global optimal solution of both problems, (1) and (2), are the same.

The objective function (2a) is a difference of two convex functions. By using global optimization techniques (2; 3) we can transform problem (2) into an equivalent convex minimization problem with a reverse convex constraint:

$$\begin{aligned}
&\text{minimize } h'x + \frac{1}{2}x'Hx - t && \text{(3a)}\\
&\text{subject to: } Ax \geq b && \text{(3b)}\\
&\qquad Cy = d && \text{(3c)}\\
&\qquad t - \lambda y(y-1) \geq 0 && \text{(3d)}\\
&\qquad 0 \leq x_j^i \leq \overline{x}_j^i y_j^i \quad \forall\, i,\, j && \text{(3e)}\\
&\qquad 0 \leq y_j^i \leq 1 \quad \forall\, i,\, j && \text{(3f)}
\end{aligned}$$

The new problem introduces a new variable, t, and one quadratic reverse convex constraint (3d). Notice that problem (2) and (3) are equivalents for any nonnegative value of λ, but the problems

(1), (2) and (3) are equivalent only for a suitable $\lambda := \lambda^*$.

By using problem (3) a sequence of programming problems are generated in order to obtain a good approximation to λ^*, and therefore, to the optimal solution of the original problem (1). Each new problem updates the λ value and adds linear constraints that limit the feasible domain.

Each generated problem is initialized with warm-start techniques and solved with interior point methods.

In the presentation the main parts of the model and the relevant details of the implementation will be further developed. Application to the solution of realistic cases of the Spanish electricity system will be presented.

References

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