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Numerical Techniques for Optimization Problems with PDE Constraints

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Abstract. The development, analysis and implementation of efficient and robust numerical techniques for optimization problems associated with partial differential equations (PDEs) is of utmost importance for the optimal control of processes and the optimal design of structures and systems in modern technology. The successful realization of such techniques invokes a wide variety of challenging mathematical tasks and thus requires the application of adequate methodologies from various mathematical disciplines. During recent years, significant progress has been made in PDE constrained optimization both concerning optimization in function space according to the paradigm 'Optimize first, then discretize' and with regard to the fast and reliable solution of the large-scale problems that typically arise from discretizations of the optimality conditions.

The contributions at this Oberwolfach workshop impressively reflected the progress made in the field. In particular, new insights have been gained in the analysis of optimal control problems for PDEs that have led to vastly improved numerical solution methods. Likewise, breakthroughs have been made in the optimal design of structures and systems, for instance, by the so-called 'all-at-once' approach featuring simultaneous optimization and solution of the underlying PDEs. Finally, new methodologies have been developed for the design of innovative materials and the identification of parameters in multi-scale physical and physiological processes.

Mathematics Subject Classification (2000): 35Rxx, 49-xx, 65Kxx, 90Cxx, 93Cxx.

Introduction by the Organisers

The workshop *Numerical Techniques for Optimization Problems with PDE Constraints*, organised by Matthias Heinkenschloss (Houston), R.H.W Hoppe (Augsburg/Houston), and Volker Schulz (Trier), held January 25th–January 31st, 2009, was the third in series, following two Oberwolfach workshops on the same subject in 2003 and 2006. One of the main objectives of the first two meetings was to bring together leading experts from the fields of optimal control/optimization on one hand and the efficient and reliable numerical solution of PDEs on the other hand in order to encourage and foster new approaches by the exchange of state-of-the-art methods and fresh ideas. The achievement of this goal was well reflected by the 2009 workshop which was attended by almost fifty active researchers from nine countries including a few students and postdoctoral fellows. A total of thirty-one presentations was given at the workshop covering a wide spectrum of issues ranging from the analysis of specific theoretical problems to more algorithmic aspects of computational schemes and various applications in aerodynamics and fluid mechanics as well as life and material sciences.

A particular area of active research, where the adaptation of new insights from optimization and numerical PDEs was extremely beneficial, is the

Numerical solution of control and/or state
constrained optimal control problems for PDEs.

This topic was one of the central themes of the workshop addressed in several talks including the a priori and a posteriori error analysis of numerical schemes (Hinze, Vexler, Weiser), a convergence analysis for the approximate solution of controlled conservation laws (St. Ulbrich), numerically verified bang-bang controls (Tröltzsch), as well as recent progress in mathematical programs with equilibrium constraints (Hintermüller), optimal control of state constrained dynamical systems with ODEs and PDEs (Pesch), robust solution methods via the virtual control approach (Ridzal), and interior-point methods for state constrained problems (Schiela). The important class of semi-smooth Newton methods was studied focusing on independence results (M. Ulbrich) as well as on its application to time-optimal control problems (Kunisch) and to systems of Allen-Cahn variational inequalities (Blank). Further contributions dealt with the efficient solution of PDE control problems with random coefficients (Borzi), the combination of the Hamilton-Jacobi-Bellman approach and Pontryagin's minimum principle (Cristiani), and control problems for elliptic and parabolic PDEs promoting directional sparsity (Griesse).

Another central theme of the workshop was

Optimal Design/Shape and Topology Optimization.

Researchers in these areas reported on the use of game theoretic concepts in multi-objective optimization (Desideri), the state-of-the-art in the analysis and numerics of topology optimization (Leugering), the optimal design of metamaterials (Sigmund), and recent analytical results for shape optimization of the compressible Navier-Stokes equations (Sokolowski). Applications included a PDE approach to optimization/optimal control of high performance buildings (Burns), efficient and

fast numerical methods in aerodynamic shape design (Gauger, Schmidt), acoustic optimization of plates and shells (Hardesty), and robust shape optimization in computational fluid dynamics (Schillings). The aspect of shape optimization based on reduced order modeling was covered by a contribution dealing with a combination of domain decomposition and balanced truncation techniques (Antil).

The important topic of

Parameter Identification/Inverse Problems

was the subject of four talks concerned with PDE-based statistical inverse problems in geology (Ghattas), adaptive concepts for parameter identification (Kaltenbacher), reduced order modeling by proper orthogonal decomposition for hydrological inverse problems (Kelley), and parameter estimation for diffusion processes in hippocampal neuron nuclei (Wittum).

The efficient solution of large-scale optimization problems was addressed by a survey on methods based on iterative linear solvers (Gill) and on a priori bounds for the ratio between the cost of an optimization run and a single system simulation (Griewank).

Workshop: Numerical Techniques for Optimization Problems with PDE Constraints

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Abstracts

Shape Optimization Governed by the Heat and the Stokes Equations Using Domain Decomposition and Model Reduction

Harbir Antil

(joint work with M. Heinkenschloss, R.H.W. Hoppe)

This work is concerned with the numerical solution of shape optimization problems governed by time dependent partial differential equations (PDEs) using derivative based methods. In particular, we are interested in problems where only a small part of the spatial domain on which the governing PDE is posed can be modified. This is, e.g., the case in the applications discussed in [1] and [3].

Our goal is to reduce the cost of the numerical solution of such problems using domain decomposition [6] and model reduction [2]. We use domain decomposition techniques to decouple the problem into a subproblem that involves only the subdomain that can be varied and a subdomain that corresponds to the fixed subdomain. These two subdomains could be subdivided further, but this is not considered here. Introducing the additional problem structure introduced by domain decomposition into the shape optimization is already beneficial for computation of shape sensitivities and other parts of the optimization algorithms. We use the decomposition further to apply model reduction to the subproblem corresponding to the fixed subdomain. The goal is to derive a reduced order model of much smaller size than the original one, but with the property that the solution of the shape optimization problem corresponding to the reduced order model approximates that of the full order model. To describe the ideas in more detail, we consider a shape optimization problem governed by the heat equation.

The domain $\Omega \subset \mathbb{R}^2$ is decomposed into $\bar{\Omega} = \bar{\Omega}_1 \cup \bar{\Omega}_2$, $\Omega_1 \cap \Omega_2 = \emptyset$ such that only subdomain Ω_2 is allowed to be modified by shape optimization. We use the method of mapping, i.e., we assume that Ω_2 can be mapped onto a reference domain Ω_{ref} by a bijective map Φ which is parametrized by $\alpha \in \mathcal{A}_{ad} \subset \mathbb{R}^k$. We assume that the set of admissible parameters $\mathcal{A}_{ad}$ is closed and convex. In our applications, parts of the boundary of Ω_2 are described by Bézier polynomials. We write $\Omega(\alpha), \Omega_2(\alpha)$ to emphasize the dependence on the shape parameters. We assume that the subdomain $\Omega_2(\alpha)$ is much smaller than the fixed subdomain Ω_1.

We consider the model problem

$$\min \int_0^T \int_D |y(x,t) - d(x,t)| dx + \int_{\Omega_2(\alpha)} \ell(y,t,\alpha) dx \; dt$$

subject to heat equations

$$\begin{aligned} \partial_t y(x,t) - \nabla(k(x)\nabla y(x,t)) &= f(x,t) && (x,t) \in \Omega(\alpha) \times [0,T] \,, \\ y(x,t) &= g(x,t) && (x,t) \in \partial\Omega(\alpha) \times [0,T] \,, \\ y(x,0) &= y_0(x) && x \in \Omega(\alpha) \end{aligned}$$

and to the parameter constraints $\alpha \in \mathcal{A}_{ad}$. Here $D \subset \Omega_1$. After a finite element discretization in space we obtain the semi-discretized shape optimization problem

$$\min \int_0^T l(\mathbf{y}(t), t, \alpha)\ dt \tag{1a}$$

subject to semi-discretized heat equations

$$\mathbf{M}(\alpha)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\alpha)\mathbf{y}(t) = \mathbf{B}(\alpha)\mathbf{u}(t)\,, \quad t \in [0, T]\,, \tag{1b}$$

$$\mathbf{M}(\alpha)\mathbf{y}(0) = \mathbf{M}(\alpha)\mathbf{y}_0\,, \quad \alpha \in \mathcal{A}_{ad}\,. \tag{1c}$$

The term $\mathbf{B}(\alpha)\mathbf{u}(t)$ captures the inhomogeneous right hand side f and boundary data g.

We use domain decomposition [6] in a standard way to arrive at

$$\min \frac{1}{2}\int_0^T \|\mathbf{C}_1^I\mathbf{y}_1^I - \mathbf{d}_1^I(t)\|_2^2 + \widetilde{l}(\mathbf{y}^\Gamma(t), \mathbf{y}_2^I(t), t, \alpha)dt$$

subject to

$$\begin{aligned}
\mathbf{M}_1^{II}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_1^{II}\mathbf{y}_1^I(t) + \mathbf{A}_1^{I\Gamma}\mathbf{y}^\Gamma(t) &= \mathbf{B}_1^I\mathbf{u}_1^I(t)\\
\mathbf{M}_2^{II}(\alpha)\frac{d}{dt}\mathbf{y}_2^I(t) + \mathbf{M}_2^{I\Gamma}(\alpha)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{II}(\alpha)\mathbf{y}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\alpha)\mathbf{y}^\Gamma(t) &= \mathbf{B}_2^I(\alpha)\mathbf{u}_2^I(t)\\
\mathbf{M}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}^{\Gamma\Gamma}(\alpha)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{M}_2^{\Gamma I}(\alpha)\frac{d}{dt}\mathbf{y}_2^I(t)&\\
+\mathbf{A}_1^{\Gamma I}\mathbf{y}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\alpha)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\alpha)\mathbf{y}_2^I(t) &= \mathbf{B}^\Gamma(\alpha)\mathbf{u}^\Gamma(t)\\
\mathbf{y}_1^I(0) = \mathbf{y}_{1,0}^I\,,\ \mathbf{y}_2^I(0) = \mathbf{y}_{2,0}^I\,,\ \mathbf{y}^\Gamma(0) = \mathbf{y}_0^\Gamma\,,\ \alpha \in \mathcal{A}_{ad}\,.&
\end{aligned}$$

To apply model reduction, we derive the first order necessary optimality conditions. Due to the domain decomposition of the problem, the first order necessary optimality conditions is a system of coupled differential equations, which is decomposed into two subdomain optimality systems, which are coupled by interface conditions. Since the heat equation is linear and since we assumed that the objective function corresponding to subdomain Ω_1 is quadratic, the subdomain optimality system corresponding to the fixed subdomain Ω_1 and its interface conditions with the second subdomain optimality system is exactly of a form that is needed for balanced truncation model reduction [2]. We apply balanced truncation model reduction to the subdomain optimality system corresponding to the fixed subdomain Ω_1 and interface the reduced subdomain optimality system with the (original) subdomain optimality system for $\Omega_2(\alpha)$. The existing error bounds for balanced truncation model reduction indicate that if we apply balanced truncation model reduction to the subdomain optimality system corresponding to the fixed subdomain Ω_1, then the coupled optimality system closely approximates the original optimality system. This conjecture is supported numerically.

From the model reduction of the first order necessary optimality conditions we also construct a reduced order shape optimization problem which is given by

$$\min \frac{1}{2}\int_0^T \|\widehat{\mathbf{C}}_1^I\widehat{\mathbf{y}}_1^I - \mathbf{d}_1^I(t)\|_2^2 + \widetilde{l}(\mathbf{y}^\Gamma(t), \mathbf{y}_2^I(t), t, \alpha)dt$$

subject to

$$\widehat{\mathbf{M}}_1^{II}\frac{d}{dt}\widehat{\mathbf{y}}_1^I(t) + \widehat{\mathbf{M}}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \widehat{\mathbf{A}}_1^{II}\widehat{\mathbf{y}}_1^I(t) + \widehat{\mathbf{A}}_1^{I\Gamma}\mathbf{y}^\Gamma(t) = \widehat{\mathbf{B}}_1^I\mathbf{u}_1^I(t)$$

$$\mathbf{M}_2^{II}(\alpha)\frac{d}{dt}\mathbf{y}_2^I(t) + \mathbf{M}_2^{I\Gamma}(\alpha)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{II}(\alpha)\mathbf{y}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\alpha)\mathbf{y}^\Gamma(t) = \mathbf{B}_2^I(\alpha)\mathbf{u}_2^I(t)$$

$$\widehat{\mathbf{M}}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}^{\Gamma\Gamma}(\alpha)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{M}_2^{\Gamma I}(\alpha)\frac{d}{dt}\mathbf{y}_2^I(t)$$
$$+\widehat{\mathbf{A}}_1^{\Gamma I}\mathbf{y}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\alpha)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\alpha)\mathbf{y}_2^I(t) = \mathbf{B}^\Gamma(\alpha)\mathbf{u}^\Gamma(t)$$

$$\widehat{\mathbf{y}}_1^I(0) = \widehat{\mathbf{y}}_{1,0}^I\,,\ \mathbf{y}_2^I(0) = \mathbf{y}_{2,0}^I\,,\ \mathbf{y}^\Gamma(0) = \mathbf{y}_0^\Gamma\,,\ \alpha \in \mathcal{A}_{ad}\,.$$

Here the state variables $\widehat{\mathbf{y}}_1^I$ are of much smaller size than the state variables $\mathbf{y}_1^I$ in (1). The $\widehat{\cdot}$-matrices are generated by balanced truncation model reduction.

The number of state variables in the reduced order shape optimization problem is much smaller than the number of state variables in the original shape optimization problem (1). Moreover, one can show that the first order necessary optimality conditions for the reduced order shape optimization problem is identical to the reduced first order necessary optimality conditions. This is important, since we solve the reduced order shape optimization problem, but can only expect error bounds for the reduced order optimality system.

We have also successfully applied domain decomposition and model reduction to a shape optimality system governed by the Stokes equations. Because of the incompressibility conditions, domain decomposition and model reduction becomes more involved. See [4, 5]. In particular, it is not so obvious that in this case there exists a reduced order shape optimization problem such that its first order optimality conditions are the reduced first order necessary optimality conditions. We are able to derive a reduced order shape optimization problem with this property. The results mirror those obtained for the heat equation.

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Systems of Allen-Cahn Variational Inequalities

Luise Blank

(joint work with Harald Garcke, Lavinia Sarbu, Vanessa Styles)

Interface evolution in time can be studied using a phase field model. The Cahn-Hilliard, the Allen-Cahn equation and other phase field type equations are based on the Ginzburg Landau energy using e.g. a double well potential or an obstacle potential. Considering two possible phases they correspond to the values ± 1. In interfacial regions solutions rapidly change from values close to 1 to values close to -1 and the thickness of this interfacial region is proportional to a parameter ε. The *Cahn-Hilliard approach* modells the evolution with mass conservation and results in a variational inequality of fourth order. Discretizing in time the corresponding gradient flow equation results into a control problem with box constraints and with a cost functional including the H^1-semi-norm as well as the norm of the dual space H^{-1}. Hence, we face problems similar to control problems with state constraints.

Our approach for solving the Cahn-Hilliard variational problems efficiently is based on a *primal-dual active set strategy* which can also be formulated as a *semi-smooth Newton method*. In each iteration step one has to solve a subproblem given by a coupled system of PDEs where one is given on the whole domain while the other is to be solved on the interface only. Hence the size of the problem is drastically reduced. In the discrete setting we have shown local superlinear convergence where we first had to show the existence of the solutions of all subproblems. Global convergence is not of large interest here, as we study a discrete time evolution and hence we always have good starting values from the previous time step. However, the appropriate scaling of the arising Lagrange multiplier μ by $\frac{1}{\varepsilon}$, or respectively the choice of the parameter c in the PDAS method is essential to avoid oscillatory behaviour due to bilateral constraints.

Computations have been performed in two and three space dimensions using adaptive meshes. The number of primal dual active set iterations are typically between one and four, when the active set is initialized using the solution at the previous time step. As far as we can compare the results with other methods the PDAS-method outperformed previous approaches. Up to now one of the bottle necks for a speed-up is the linear algebra solver. Currently a multigrid solver is under consideration. However, this freedom of choosing a linear algebra solver is one of the advantages of using the primal-dual method instead of other simulation approaches. A further advantage is the enourmos reduction of the dimension due to small inactive sets.

As in the case of Cahn-Hilliard variational inequalities we studied successfully also the PDAS approach for the L^2-gradient flow of Ginzburg-Landau energy, namely the *Allen-Cahn variational inequality*. Then mass conservation is not of interest.

In many applications more than two phases or materials appear. In case that several materials appear one can introduce a concentration vector. In this formulation one component is the concentration of the "void" and the other components are the concentrations of the materials. Examples where such an approach can be used appear in in structural topology optimization, materials science (different grains or phases) or fluid mechanics. The simplest phase field method in this context is the *vector valued Allen-Cahn system* for which we studied primal-dual active set methods for systems of Allen-Cahn variational inequalities. Apart from the consideration of systems we face additional constraints due to the fact that the components have to lie in the Gibbs simplex.

We first established H^2-regularity in space for the vector valued parabolic variational inequality. This made it possible to reformulate the problem using complementarity conditions or in other words employing Lagrange multipliers. For the fully discretized setting we proved local superlinear convergence of the PDAS-algorithm for the corresponding optimization problem in a situation where in addition to unilateral bounds the unknown is vector-valued and has to fulfill an equality constraint.

Also the computations for Allen-Cahn systems have been performed with adaptive meshes using ALBERTA as mesh generator. We performed computations for a system of 30 phase field variables (a situation which frequently arises in materials science) as well as in 3D for a double bubble as initial data. In the test cases our ansatz outperforms previous solution techniques in CPU-time. Additional gain is expected with a problem adapted linear algebra solver. Moreover, it is important to note that the PDAS-method allows for the more accurate fully implicit time discretization and also for much larger time steps than other approaches in the literature.

One of our goals is to solve *multimaterial structural topology optimization problems* with a phase field approach. In this context also additional mass constraints have to be taken into account when using the Allen-Cahn modell. Incorporating these constraints into the primal-dual active set method leads to additional difficulties as Lagrange multipliers for the non-local constraints have to be considered. To our knowledge such a situation has not been studied yet before within the context PDAS-methods.

In case of this *vector-valued and nonlocal mass-conserving Allen-Cahn system* we can also show H^2-regularity. In spite of nonlocal mass constraints it is possible to use a semi-smooth Newton method to solve the discretized system. Being able to solve such a system will be a key ingredient for the application of a phase field approach to structural topology optimization problems.

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Multigrid and Sparse-Grid Techniques for PDE Control Problems with Random Coefficients

Alfio Borzì
(joint work with Greg von Winckel)

An established tool for the construction of control strategies for real systems is provided by optimal control theory [4] where an optimal control problem is formulated as the minimization of an objective, that models the purpose of the control and describes the cost of its action, under the constraint given by the modeling equations. We focus on the control of nonlinear elliptic and parabolic PDEs with random coefficients where the nonlinearity is nonmonotonic. Therefore the resulting optimal control problem may be singular in the sense that without control the model equation may not admit solutions.

With this benchmark, we discuss elliptic and parabolic optimal control problems with random coefficients that describe the reaction nonlinearity and the linear diffusion. The present work is based on previous work on deterministic models [2] and on recent research [8] on modeling and optimization problems where the coefficients of the problem are described by random fields. We present efficient multigrid [6] schemes and sparse-grids methodology to solve these problems. Our setting is based on the work in [1, 5, 7] on elliptic problems with random inputs. We assume that the reaction coefficient is modeled by random fields that can be approximated by a truncated Karhunen–Loève expansion on the probability space. With this representation, we can use the Smolyak sparse-grid algorithm [3] to model a high-dimensional stochastic coefficient space.

We use a stochastic collocation method, where the solution of the stochastic optimal control problem is obtained solving, in the physical space, a deterministic optimality system for each point of the sparse-grids coefficient space. For the solution of the deterministic optimality system, we use a collective-smoothing multigrid (CSMG) scheme [2] that provides optimal computational performance independently of the values of the optimization parameters and of the problem's coefficient. The combination of sparse-grids and multigrid techniques results in a solution process with optimal computational complexity with respect to the sizes of the physical and probability grids.

We discuss the modeling of random fields and their representation by the Karhunen–Loève expansion and define the concept of solution of a stochastic PDE problem. We formulate representative nonlinear elliptic and parabolic optimal control problems with a random coefficient and consider a deterministic objective. Then, we discuss the discretization of the stochastic parameter space using sparse-grids collocation and describe the Smolyak scheme. A collective-smoothing

multigrid scheme for nonlinear PDE optimal control problems is discussed. Numerical experiments for validating the numerical performance of the CSMG multigrid scheme combined with sparse-grids collocation techniques are illustrated. Typical multigrid convergence rates and robustness with respect to a large choice of optimization parameters is obtained. Results of computation of stochastic optimal control solutions are reported with a focus on the moments of the tracking ability of the optimization scheme. We discuss the construction of a robust control obtained as the mean of the controls resulting from different realizations of reaction fields and demonstrate that this control represents an improvement compared with the control obtained considering a mean field reaction coefficient.

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A PDE Approach to Optimization and Control of High Performance Buildings

J. A. Burns

(joint work with J. Borggaard, E. M. Cliff, L. Zietsman)

Commercial buildings are responsible for a significant fraction of the energy consumption and greenhouse gas emissions in the U.S. and worldwide. Consequently, the design, optimization and control of energy efficient buildings can have a tremendous impact on energy cost and greenhouse gas emission. Mathematically, building models are complex, multi-scale, multi-physics, highly uncertain dynamical systems with wide varieties of disturbances. By itself, building simulation is a significant computational challenge. However, when addressing the additional requirements that center on design, optimization (for energy and CO_2) and control (both local and supervisory) of whole buildings, it becomes an immense challenge to develop practical computational tools that are scalable and widely applicable to current and future building stock. The development of mathematical and computational methods to deal with such complex systems will be an enabling science

because at some point in the design and control process, numerical methods must be employed. In this paper we use a model problem to illustrate that distributed parameter control based on PDEs, combined with high performance computing can be used to provide practical insight into important issues such as optimal sensor/actuator placement and optimal supervisory building control. In order to illustrate some of the ideas, we consider the problem illustrated by a single room shown in Figure 1.

Here, the goal is to design the room (locate vents, place sensors, etc.) in order to control the room temperature near the workspace and minimize energy. The problems of design and control should be considered simultaneously because the type and effectiveness of the controller depends on the type and quality of the sensed information and conversely. For simplicity, we assume flow $\mathbf{v}(t,\mathbf{x})$ is given, the thermal control input is given by $u(t)$ and the noise is $v(t)$. The fully coupled flow-energy case where the control is applied at the boundary is slightly more complex and requires a different technical framework. However, for the discussion here it is sufficient to focus on the thermal equation

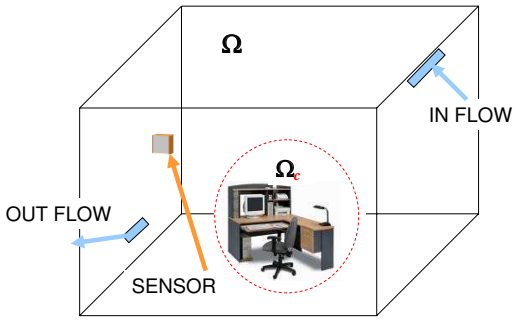

FIGURE 1. Room Control Problem

$$\frac{\partial T(t,\mathbf{x})}{\partial t} + \mathbf{v}(t,\mathbf{x}) \cdot \nabla T(t,\mathbf{x}) = \frac{1}{\mathrm{RePr}} \Delta T(t,\mathbf{x}) + b(\mathbf{x})u(t) + g(\mathbf{x})v(t) \,, \tag{1}$$

and to think of $b(\mathbf{x})$ as a function with support near the wall vent defined on the domain $\Omega \subset \mathbb{R}^3$ and $T(t,\mathbf{x})$ is the temperature. The control term is given by $b(\mathbf{x})u(t)$ and we assume there is a noise term $g(\mathbf{x})v(t)$ where $b(\mathbf{x})$ and $g(\mathbf{x})$ are given functions in $L_2(\Omega)$. The controlled output, $\xi(t)$, of the system will be defined by a weighted average over the sub-domain in the room occupied by the workspace. In particular, let

$$\xi(t) = \int_{\Omega_c} d(\mathbf{x})T(t,\mathbf{x})d\mathbf{x} + w(t) \,, \tag{2}$$

where $\Omega_c \subset \Omega$ is specified to be a region around the workspace and $w(t)$ represents sensor noise. Consider the problem of finding the control that minimizes

$$J(u) = \int_0^\infty \left\{ [\xi(t) - r(t)]^2 + R[u(t)]^2 \right\} dt \,, \tag{3}$$

where $R > 0$ and $r(t)$ is a desired average temperature to be tracked. For the discussion here, we set $r(t) = 0$ and note that this is a "zonal control problem" in that we care only about controlling the average temperature in the zone Ω_c.

Under suitable assumptions and applying the appropriate boundary conditions, we formulate (1) as a differential equation on the Hilbert space $Z = L_2(\Omega)$, of the

form

$$\dot{z}(t) = \mathcal{A}z(t) + \mathcal{B}u(t) + \mathcal{G}v(t)\,, \quad t > 0\,,\ z(0) = z_0 \in Z\,, \tag{4}$$

where $\mathcal{A} : D(\mathcal{A}) \subseteq Z \to Z$ generates a C_0-semigroup $S(t)$ on Z, $\mathcal{B} : \mathbb{R} \to Z$ and $\mathcal{G} : \mathbb{R} \to Z$ are linear input operators defined in the natural way

$$[\mathcal{B}u](\mathbf{x}) = b(\mathbf{x})u \ \text{ and } \ [\mathcal{G}v](\mathbf{x}) = g(\mathbf{x})v\,,$$

respectively. If the operator $\mathcal{D} : Z \to \mathbb{R}$ is defined by (2) and $\mathcal{Q} = \mathcal{D}^*\mathcal{D}$, then the linear quadratic regulator (LQR) control problem is defined by minimizing the cost (3) subject to the linear dynamics (4). In this simple case one can show that under reasonable conditions (see [4]) the LQR problem has an optimal control, in feedback form,

$$u^{opt}(t) = -\mathcal{K}z(t)\,, \tag{5}$$

where $\mathcal{K} : Z \to \mathbb{R}$ is the bounded linear gain operator. Moreover, $\mathcal{K} = R^{-1}\mathcal{B}^*\Pi$ where $\Pi : Z \to Z$ is a bounded linear operator, $\Pi = \Pi^*$ and Π satisfies the Riccati equation

$$\mathcal{A}^*\Pi + \Pi\mathcal{A} - \Pi\mathcal{B}R^{-1}\mathcal{B}^*\Pi + \mathcal{Q} = 0\,. \tag{6}$$

The operator Π is nuclear and there exist a function $k_T(\mathbf{x})$ such that

$$\mathcal{K}z(t) = \int_\Omega k_T(\mathbf{x})T(t,\mathbf{x})d\mathbf{x}\,, \tag{7}$$

where the kernel $k_T(\mathbf{x})$ is called the functional feedback gain. The functional gain defines the optimal LQR controller and can be used to place sensors and design low order controllers (see [4]). We have developed practical methods for computing 3D functional gains $k_T(\mathbf{x})$ (see [3]), and we can use this gain to guide the choice and placement of the sensors. As we show below, the functional gains often have localized (or nearly localized) support and one can use this fact to determine what regions in space are most important to the controller. For example, if

$$k_T(\mathbf{x}) = \begin{cases} k_T(\mathbf{x}) \gg 0, & \mathbf{x} \in \omega_k \subset \Omega \\ k_T(\mathbf{x}) \approxeq 0, & \mathbf{x} \notin \omega_k \subset \Omega \end{cases}\,,$$

then it is important (when possible) to place sensors in the region ω_k where $k_T(\mathbf{x}) \gg 0$. In particular, in this case

$$\mathcal{K}z(t) = \int_\Omega k_T(\mathbf{x})T(t,\mathbf{x})d\mathbf{x} \approxeq \int_{\omega_k} k_T(\mathbf{x})T(t,\mathbf{x})d\mathbf{x}\,, \tag{8}$$

and one would optimally place sensors so that the integral in (8) is best approximated by a quadrature evaluated at the sensor locations.

If one can not place sensors in ω_k, then one needs to estimate the state only inside the zone ω_k. This is a zonal estimation problem (see [1], [2]). For example, assume that there is one sensor with support in the region $\Omega(\mathbf{q})$ located near a wall given by

$$y(t) = \int_{\Omega(\mathbf{q})} c(\mathbf{x})T(t,\mathbf{x})d\mathbf{x} + w(t) = \mathcal{C}(\mathbf{q})z(t) + w(t)\,, \tag{9}$$

where $\Omega(\mathbf{q}) = \left\{\mathbf{x} \in \bar{\mathbf{\Omega}} : \|\mathbf{x} - \mathbf{q}\| < \epsilon\right\} \subset \bar{\Omega}$ contains the support of the function $c(\mathbf{x}) \in L_2(\Omega)$. Standard linear state estimators (observers) have the form

$$\dot{z}_e(t) = \mathcal{A}_e z_e(t) + \mathcal{F} y(t) \ , \tag{10}$$

where $\mathcal{F} : \mathbb{R} \to Z$ has the representation $[\mathcal{F}y](\mathbf{x}) = f_T(\mathbf{x})y$ and $z_e(t)$ is an estimate of the restricted state $T(t, \mathbf{x})|_{\omega_k}$.

In Figure 2 we show the functional feedback gain for the room problem above. Note that the "support" ω_k of $k_T(\mathbf{x})$ is largest near the workspace as expected. The optimal zonal estimation problem will be addressed in the full talk.

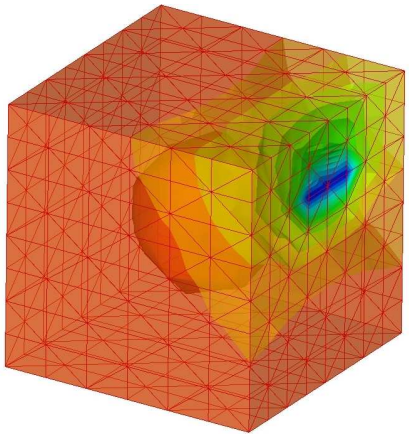

FIGURE 2. Feedback Functional gain

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Coupling the Hamilton-Jacobi-Bellman and the Pontryagin's Minimum Principle Approach to Solve Optimal Control Problems

EMILIANO CRISTIANI

(joint work with Pierre Martinon, Hasnaa Zidani)

We investigate the possibility of coupling the Hamilton-Jacobi-Bellman (HJB) approach and the Pontryagin's Minimum Principle (PMP) approach to solve a class of control problems. We show that a rough approximation of the value function computed by the HJB equation can be used as optimal initial guess for a shooting method based on the PMP.

We deal with the following controlled dynamics

$$\begin{cases} \dot{y}(t) = f(y, u) \, , & t > 0 \, , \\ y(0) = x \, , & x \in \mathbb{R}^d \, , \end{cases} \tag{1}$$

where $u = u(t)$ is the control and can be chosen in a set of admissible controls $\mathcal{U} = \{u : [0, +\infty) \to U\}$, and U is a compact set of $\mathbb{R}^m$. We denote by $y_x(t; u)$ the solution of the system (1) starting from the point x with control u. Let $\mathcal{T} \subset \mathbb{R}^d$ be

a given closed *target*. We denote by $t_f(x,u)$ the first time the trajectory $y_x(t;u)$ hits $\mathcal{T}$ (we set $t_f(x,u) = +\infty$ if the trajectory never hits the target). We also define a *functional cost* J

$$J(x,u) := \int_0^{t_f(x,u)} \varphi(y_x(t;u),u)dt \tag{2}$$

for some cost function $\varphi : \mathbb{R}^d \times U \to \mathbb{R}$. The final goal is to find

$$u^* \in \mathcal{U} \text{ such that } J(x,u^*) = \min_{u\in\mathcal{U}} J(x,u) \, .$$

We also define the *value function* T as $T(x) := J(x,u^*)$ for every $x \in \mathbb{R}^d$. Choosing $\varphi \equiv 1$ in (2) we obtain the classical *minimum time* problem.

The Hamilton-Jacobi-Bellman (HJB) approach is based on the resolution of the following first-order nonlinear hyperbolic PDE

$$\begin{cases} v(x) + \sup_{u\in U}\{-f(x,u)\cdot\nabla v(x) - \varphi(x,u) + (\varphi(x,u)-1)v(x)\} = 0\,, & x \in \mathbb{R}^d\backslash\mathcal{T}\,, \\ v(x) = 0\,, & x \in \mathcal{T}\,, \end{cases} \tag{3}$$

where $v = 1 - e^{-T}$ [1]. Once solved (3) and computed T, we easily obtain the optimal control u^* and the corresponding optimal trajectory [1]. The main advantages of this approach are: 1) the optimal control u^* realizes the *global* minimum of J, 2) u^* is obtained in feedback form, 3) once T is computed, the initial point x can be changed at will, the computation of the optimal trajectory is done in real time. The main drawbacks are: 1) it is needed to fix a box Ω where T is approximate, this results in not desired state constraints, 2) to obtain a good precision a very fine discretization of Ω is required, 3) this approach suffers from the "curse of dimensionality", so in general it is restricted to problems in low dimension ($d \leq 3$). Otherwise, parallel computation is needed.

The shooting method (SM) consists in finding trajectories that satisfy the necessary conditions stated by the PMP. This is done in practice by searching a zero of a certain shooting function, typically with a (quasi-)Newton method [4]. In order to evaluate the shooting function, a system of ODEs for y and the costate p must be solved in the time interval $[0, t_f^*]$, starting from the initial condition $y(0)$ and $p(0)$. Note that the exact values of t_f^* and $p(0)$ are not known. The main advantages of this approach are: 1) it is fast, 2) u^* is computed very accurately. The main drawbacks are: 1) finding a suitable initial guess for t_f^* and $p(0)$ for the convergence of the shooting method can be extremely difficult in practice, 2) u^* is in general only a local minimum of J, 3) u^* is open-loop.

The proposed algorithm consists in solving the HJB equation on a very coarse grid computing a rough approximation of T and t_f^*. Then we exploit the fact that if T is differentiable at x, then $p(0) = \nabla T(x)$ [3]. With these information we can initialize the shooting method and obtain in most cases an immediate convergence to the optimal solution.

Equation (3) is solved in a bounded domain Ω by the semi-Lagrangian scheme described in [6]. We denote the approximate value function by T_k^h, where k and h are the two discretization steps needed by the numerical method. Then, the

approximate gradient $\widetilde{\nabla} T_k^h$ is computed by first order centered finite differences (with step z). We have the following

Theorem 1. Let $\varphi \equiv 1$ and let $\hat{\eta}(x)$ be the exterior unit normal vector of $\partial\mathcal{T}$ at x. Assume $f(x,u)\cdot\hat{\eta}(x) < 0$ for $x \in \partial\mathcal{T}$. Assume $T \in C^1(\Omega)$ and $T < +\infty$. Finally assume that $k = Ch$ for some constant C. Then it exists $\Omega' \subset \Omega$ (explicitly computable) such that

$$\|\widetilde{\nabla} T_k^h - \nabla T\|_{L^\infty(\Omega')} \leq O\left(\frac{\sqrt{h}}{z}\right) + O(z^2)\ .$$

Here we show the results of our algorithm for the Goddard problem (see f.e. [5]):

$$\begin{cases} \dot{r} = v \\ \dot{v} = -\frac{D(r,v)}{m} - \frac{1}{r^2} + T_{max}\frac{u}{m} \\ \dot{m} = -T_{max}\ b\ u \end{cases}$$

where $D(r,v) = 310v^2 e^{-500(r-1)}$, $T_{max} = 3.5$, $b = 2$, $\phi(x,u) = u$, $U = [0,1]$, $(r(0), v(0), m(0)) = (1, 0, 1)$, $\mathcal{T} = \{r \geq 1.01\}$ and $\Omega = [0.998, 1.012]\times[-0.02, 0.18]\times[0.1, 1.8]$.

The three state variables are the altitude, velocity and mass of a rocket which climbs in the vertical direction. Here the goal is to find the optimal control to steer the rocket at a given altitude minimizing the fuel consumption. The HJB equation needs a huge number of iterations to converge, and the approximate value of $p(0)$ is sensible to the choice of Ω. For the SM, the problem is hard because it involves singular arcs. Solving the HJB equation on a 20^3 grid with 21 discrete controls we find in 211 seconds $p(0) = (-7.79,\ -0.31,\ 0.04)$ and $t_f^* = 0.17$. It is also possible to locate the singular arc, $t_{entry} = 0.02$ and $t_{exit} = 0.06$. On the other hand, the HJB approach is not able to compute a good approximation of the optimal control as we can in the last plot of Fig. 1. The application of the PMP to this problem and the resulting shooting formulation are described in [2]. With the initialization provided by the HJB solution, the shooting method converges in 1 sec to the solution $t_f^* = 0.1741$, $p(0) = (-7.2753, -0.2773, 4.382e-2)$, $t_{entry} = 0.02350$ and $t_{exit} = 0.06684$. The corresponding trajectory and optimal control are shown in Fig. 2, with the expected singular arc clearly visible on the control.

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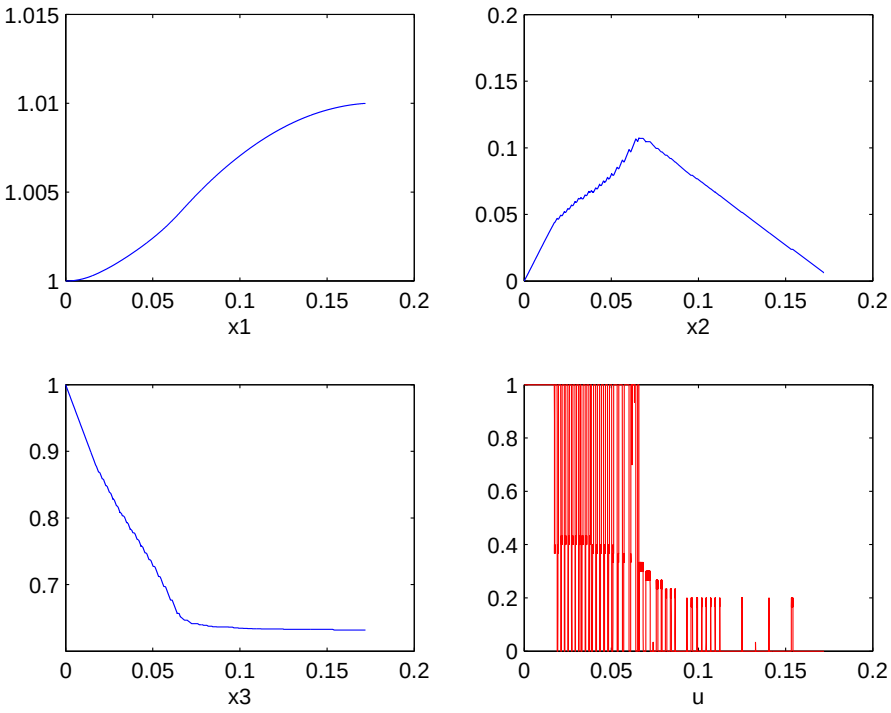

FIGURE 1. Results by HJB

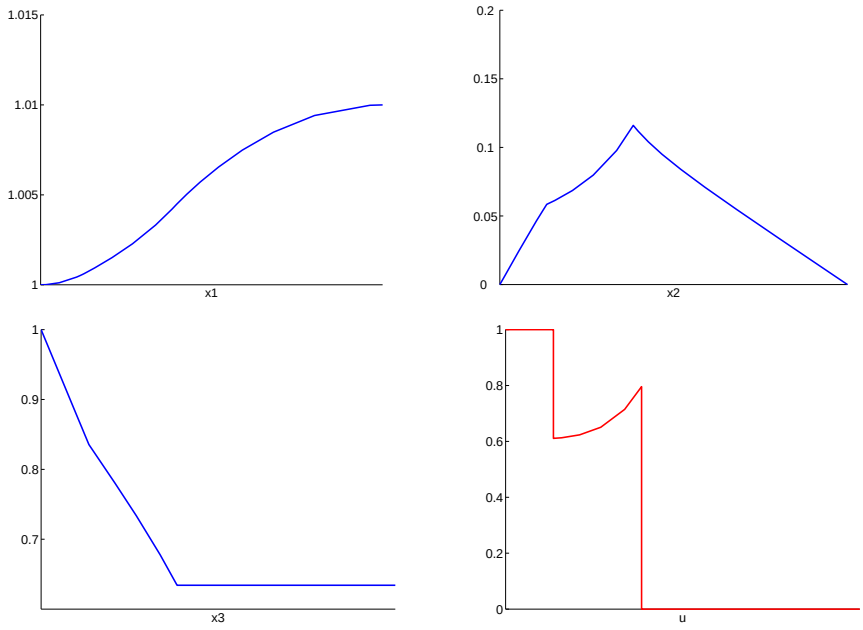

FIGURE 2. Results by SM

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Two-Discipline Optimization: Split of Territory for Optimum-Shape Design in Aerodynamics with Coupling to Another Discipline

Jean-Antoine Désidéri

A difficult issue in applied optimization and related numerical analysis, is the treatment of multi-objective problems when the criteria originate from different physical phenomena, each one being governed by a non-trivial set of PDEs. For such problems, the most general method consists in identifying the front of Pareto-optimal solutions. However, this identification is logically complicated in cases where more than two criteria are considered. Additionally, to realize this identification computationally, the *Non-dominated Sorting Genetic Algorithm (NSGA)* by Srinivas and Deb [7] is a well-known and effective algorithm, but it is very costly in distributed problems where the criteria are functionals of fields that are computed by finite-volume or finite-element-type simulations. Thus a challenging area of research in computational optimization is the definition and analysis of more economical algorithms to handle several physics concurrently in design.

We first focus on Nash games associated with a special split of variables to handle multi-objective shape optimization problems in which one criterion is either fragile or preponderant. A treatment of multi–criterion problems that removes the question of adjusting penalty constants, and that is computationally more economical than identifying the Pareto equilibrium front, is to seek a pseudo-optimal solution as the equilibrium point of a simulated dynamic game in which the set of design parameters is split into subsets, each subset being considered as the strategy (or territory) of a given functional. Nash or Stackelberg games [6], [2] are usually considered. Of course, the adopted definition of the splitting also introduces a bias, but one demonstrated to be weaker. Examples of successful concurrent optimizations realized numerically by such dynamic games have been provided from [8], [9] where the necessity to define a proper split of design variables in adequacy with the physics of the problem has also been strongly pointed out.

A sensitivity-analysis-based theoretical splitting strategy has been introduced in [5] for the treatment of cases in which a hierarchy between a primary and a secondary criteria to be minimized is introduced. An algorithm has been proposed in which the absolute optimum of the primary criterion is first identified, presumably numerically. Then, a secondary criterion is improved in a virtual Nash game, in which the design variables have been split, according to the diagonalization of a *reduced Hessian*, and assigned to the two virtual players, in a way that is devised to cause the least possible degradation to the primary criterion from its absolute optimum. Additionally, the approach puts in evidence the existence of a *continuum of Nash equilibrium points* originating from the initial absolute optimum of the primary criterion considered alone. Certain properties of *robust design* have also been established for the proposed formulation. Successful implementations and algorithmic generalizations can be found in [1].

These elements have been extended recently to cases where the initial point is arbitrary instead of resulting from the optimization of a single discipline alone.

We have proposed to define a notion of "Pareto-stationarity", according to which a design-point Y^0 is said to be Pareto-stationary w.r.t. a set of criteria iff a convex combination of these criteria is stationary at Y^0. Evidently, for smooth criteria, Pareto-optimal points are Pareto-stationary. Thus, inversely, if Y^0 is not such a Pareto-stationary point, a simple formula provides the definition of a direction along which all the criteria diminish from Y^0. For example, for two criteria, the descent direction can be $-w$, where

$$w = \frac{\|v\|\, u + \|u\|\, v}{\|u\| + \|v\|} \ ,$$

in which u and v are the local values of the gradients of the two criteria. Thus, a "cooperative phase of optimization" is conducted by successive steps along such common descent directions and until a Pareto-stationary point is achieved (in a finite or infinite number of steps). Then, the confrontation of the criteria can be organized in a "competitive phase of optimization", according to a Nash game in which information on local gradients and Hessians is used to guide the definition of a special split of variables, in a way similar to the first analyzed situation where the Nash game was initiated from a stationary point of the single primary criterion.

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Efficient One-Shot Methods for Aerodynamic Shape Design

Nicolas R. Gauger

Two different one-shot optimization techniques for aerodynamic shape design problems will be presented. These methods enable aerodynamic shape designs for the computational effort of a small, constant multiple of the effort of an aerodynamic simulation.

The first methodology is applicable to all areas of scientific computing, where large scale governing equations involving discretized PDEs are treated by custom made fixed point solvers. To exploit the domain specific experience and expertise invested in these simulation tools, it is proposed to extend them in a semi-automated fashion by the use of automatic differentiation (AD) tools. First they are augmented with adjoint solvers to obtain (reduced) derivatives and then this sensitivity information is immediately used to determine optimization corrections. In other words, rather than applying an outer optimization loop we prefer the 'one-shot' strategy of pursuing optimality simultaneously with the goals of primal and adjoint feasibility.

The second methodology presented follows the 'first optimize then discretize' philosophy. Integral parts of this approach are gradient preconditioning and shape derivatives in order to ensure efficiency.

The aerodynamic shape design examples, solved by the two presented one-shot methodologies, are drag reduction without and with constraints on lift under transonic flight conditions (with compressible Euler as governing equations) and the control of a viscous channel flow around a cylinder (here the governing equations are the incompressible Navier-Stokes equations with pressure correction).

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A Stochastic Newton Method for Bayesian Inverse Problems

Omar Ghattas
(joint work with James Martin, Lucas Wilcox, and Carsten Burstedde)

The problem of estimating uncertain parameter inputs to a mathematical model from output observations is fundamentally an inverse problem. The *forward problem* seeks to predict the outputs given the inputs by solving the governing equations. The forward problem is usually well-posed (the solution exists, is unique, and is stable to perturbations in inputs), causal (later-time solutions depend only on earlier time solutions), and local (the forward operator includes derivatives that couple nearby solutions in space and time). The *inverse problem*, on the other hand, reverses this relationship by seeking to estimate uncertain parameters from observations. The great challenge of solving inverse problems lies in the fact that they are usually ill-posed, non-causal, and non-local: many different sets of parameter values may be consistent with the data, and the inverse operator couples solution values across space and time.

Non-uniqueness stems from sparsity of the observations and uncertainty in both the measurements and the model itself. The popular approach to obtaining a unique "solution" to the inverse problem is to formulate it as an optimization problem: minimize the misfit between observed and predicted outputs in an appropriate norm while also minimizing a *regularization* term that penalizes unwanted features of the inputs. This has been called *Occam's approach*: find the "simplest" set of inputs that are consistent with the measured data. The inverse problem thus leads to a nonlinear optimization problem that is constrained by the forward problem. When the forward model is governed by PDEs, the result is an optimization problem that is large-scale in the (discretized) state variables, even when the number of inversion parameters is small. More generally, when the uncertain parameters represent fields (as in the case of medium or source functions), the inverse problem is of large scale in the (discretized) model parameters as well.

Solution of this optimization problem using this regularization approach to inverse problems will yield an estimate of the "best" values of input parameters that simultaneously fit the data and minimize the regularization penalty term. However, we are interested in not just point estimates of the best-fit inputs, but a *complete statistical description* of the input parameters that are consistent with the data. The *Bayesian* approach does this by reformulating the inverse problem as a problem in *statistical inference*, incorporating uncertainties in the measurements, the forward model, and prior information on the inputs [3, 5]. The solution of this inverse problem is the joint "posterior" probability density of the inputs, which reflects the degree of confidence in their values. Thus we are able to quantify the resulting uncertainty in the inputs, taking into account uncertainties in the data, model, and prior information.

The Bayesian solution of the inverse problem proceeds as follows. Suppose the relationship between output observables y and uncertain input parameters p is denoted by $y = f(p, e)$, where e represents noise due to measurement and/or

modeling errors. In other words, given the inputs p, the function $f(p)$ invokes the solution of the forward problem to yield y, the predictions of the observables. Suppose also that we have the prior probability density $\pi_{\text{pr}}(p)$, which encodes the confidence we have in prior information on the unknown inputs (i.e. independent of information from the present observations), and the likelihood function $\pi(y_{\text{obs}}|p)$, which describes the conditional probability that the inputs p gave rise to the actual measurements y_{obs}. Then Bayes' theorem of inverse problems expresses the posterior probability density of the inputs, π_{post}, given the data y_{obs}, as the conditional probability

$$\pi_{\text{post}}(p) \stackrel{\text{def}}{=} \pi(p|y_{\text{obs}}) = k\,\pi_{\text{pr}}(p)\,\pi(y_{\text{obs}}|p)\ , \tag{1}$$

where k is a normalizing constant. The expression (1) provides the statistical solution of the inverse problem as a probability density for the model inputs p.

While it is easy to write down expressions for the posterior probability density such as (1), making use of these expressions poses a challenge, because the posterior probability density is a surface in high dimensions (equal to the number of inputs), and because the solution of the forward model is required at each point on this surface. Straightforward grid-based sampling is out of the question for anything other than a few inputs or cheap forward simulations. Special sampling techniques, such as Markov chain Monte Carlo (MCMC) methods, have been developed to generate sample ensembles that typically require many fewer points than grid-based sampling [2, 3]. Even so, MCMC methods become prohibitive as the complexity of the forward simulations and the dimension of the input space increase. When the input is a (suitably-discretized) field, and when the forward PDE requires hours to solve on a parallel computer, the MCMC framework collapses.

The central problem in scaling up conventional MCMC for large-scale forward simulations and high-dimensional input spaces is that this is a purely *black-box* approach, i.e. it does not exploit the structure of the input-output map $f(p)$. Several decades of work on algorithms for *deterministic* large-scale PDE-constrained optimization have taught us that making use of Hessian information can greatly speed up the search process for extremum points; we believe this information should prove valuable in addressing the curse of dimensionality in sampling methods as well. Using adjoint techniques, actions of Hessians on vectors can be computed at a cost of a pair of linearized forward solves, and this combined with specialized inexact Newton-CG solvers that exploit the fact that many ill-posed inverse problems have compact data misfit operators, often permits solution of deterministic inverse problems in a dimension-independent number of iterations (and thus forward solves).

Here, we build on the Langevin dynamics approach to sampling, which uses gradient information to accelerate sampling of a target density, e.g. [4]. The Langevin equation is a stochastic differential equation (SDE) with $\pi_{\text{post}}(p)$ as an invariant density:

$$d\boldsymbol{P}_t = \boldsymbol{A}\nabla \log \pi_{\text{post}}\, dt + \sqrt{2}\boldsymbol{A}^{1/2} d\boldsymbol{W}_t\ , \tag{2}$$

where $\boldsymbol{W}_t$ is the i.i.d. vector of standard Brownian motions. Preconditioning by a symmetric positive definite operator $\boldsymbol{A}$ preserves the invariance of the density. In practice, we discretize in time with timestep Δt, yielding (e.g. for explicit Euler) the update

$$\boldsymbol{p}_{k+1} = \boldsymbol{p}_k + \boldsymbol{A}\nabla \log \pi_{\text{post}} \Delta t + \sqrt{2\Delta t}\boldsymbol{A}^{1/2}\mathcal{N}(\boldsymbol{0}, \boldsymbol{I}) \tag{3}$$

where $\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$ is the i.i.d. standard normal density. Discretization in time can add bias, so typically we use the Langevin steps as proposals for MCMC. The form (3) shows immediately the connection with deterministic optimization methods: the gradient term $\nabla \log \pi_{\text{post}}$ is a steepest ascent direction for the posterior density. In its absence (and in the absence of preconditioning, i.e. $\boldsymbol{A} = \boldsymbol{I}$) we recover a Gaussian random walk. The addition of this term drives the samples in (the locally steepest) direction of higher probability. However, steepest descent is a poor choice for large-scale optimization (particularly for anisotropic problems), and we seek to improve on it.

Taking the preconditioner $\boldsymbol{A}$ as the inverse of the Hessian matrix of $\log \pi_{\text{post}}$, we obtain the stochastic equivalent of Newton's method. In the common case of Gaussian additive noise and prior, the (negative) log of the posterior density is simply the misfit objective (i.e. the sum of the data misfit and prior/regularization term) that deterministic inverse methods seek to minimize. Thus, similar to Newton's locally-quadratic approximation of the objective, the Hessian-preconditioned Langevin step makes a locally-Gaussian approximation of π_{post}. This endows the sampling process with curvature information for the posterior density surface, which is crucial in high dimensions. We expect this to result in a need for substantially fewer sampling points, just as deterministic Newton requires substantially fewer iterations to find the optimum compared to a derivative-free optimization method.

Moreover, it can be shown [1] that in the limiting case when the posterior density π_{post} is in fact Gaussian (such as when the inverse problem is linear and the noise is additive and Gaussian), this so-called *stochastic Newton* method not only samples the target density at long times, but accurately samples from π_{post} at *every time step*. This means that Metropolis-Hastings will accept all of the proposed sample points, and that a minimum number of points will be necessary to accurately sample from the given distribution. For densities that are not Gaussian, stochastic Newton will still provide a substantial speedup over a conventional random walk, since a local Gaussian approximation (based on a local quadratic approximation of $\log \pi_{\text{post}}$, or equivalently a linearized approximation of the inverse problem) will generally prove to yield more useful information on the behavior of π_{post} than a standard normal density approximation will. Indeed, our preliminary experience with stochastic Newton on a 1D (nonlinear) inverse medium scattering problem, with the medium parametrized by 65 layers, indicates just $\mathcal{O}(10^2)$ samples are necessary to adequately sample the (non-Gaussian) posterior density, while a state-of-the-art (but non-derivative) MCMC method (Delayed Rejection Adaptive Metropolis) is nowhere near converged after even $\mathcal{O}(10^5)$ samples [1].

Moreover, because the (inverse) Hessian captures the (local) covariance structure of the posterior density, this orders-of-magnitude speedup is expected to become even larger as the parameter dimension increases.

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Methods for Large-Scale Optimization Based on Iterative Solvers

Philip E. Gill

(joint work with Jennifer B. Erway)

Although a range of algorithms and software exist for *general-purpose* optimization by interior and SQP methods (see, e.g., [3, 7, 12, 21, 25, 26]), conventional methods are unable to take full advantage of the structure present in the huge finite-dimensional problems defined by the "discretize-then-optimize" paradigm of ODE- and PDE-constrained optimization. We consider large-scale finite-dimensional problems of the form:

$$\min_{x\in\Re^n} \quad f(x) \quad \text{subject to} \quad c(x) = 0\,, \quad x \geq 0\,, \tag{1}$$

where c denotes an m-vector of nonlinear functions that includes the discretized differential equations. (To simplify the discussion, we consider the bounds $x \geq 0$ in place of the more general form $\ell \leq x \leq u$.) The Lagrange multipliers associated with the constraints $c(x) = 0$ and $x \geq 0$ are denoted by y and z respectively. Following common practice, we refer to x as the *primal variables* and (y, z) as the *dual variables*. Our approach involves a class of primal-dual path-following methods based on the properties of the well-known augmented Lagrangian method, which solves the constrained problem as a sequence of unconstrained subproblems (see, e.g., [2, 10, 17]). Let μ be a small positive scalar and assume that y^e and z^e ($z^e \geq 0$) are estimates of the optimal dual variables y^* and z^*. Each subproblem involves finding an approximate minimizer of the function $\mathcal{M}_\mu(x, y, z)$ such that

$$\begin{aligned}\mathcal{M}_\mu(x,y,z) \,=\, f(x) - c(x)^T y^e + \frac{1}{2\mu}\|c(x)\|^2 + \frac{1}{2\mu}\|c(x)+\mu(y-y^e)\|^2 \\ - \mu\sum_{i=1}^{m} z_i^e \ln\left((x_i+\mu)^2 z_i\right) - \sum_{i=1}^{m}\left(\mu(z_i^e - z_i) - x_i z_i\right)\end{aligned} \tag{2}$$

(for further details, see [8,13,22]). Unlike the conventional augmented Lagrangian, $\mathcal{M}_\mu$ is minimized with respect to both the primal *and* dual variables. Moreover, the parameter μ need not go to zero to force convergence, but may be fixed at a small value that provides a *regularization* of each subproblem.

If $v = (x, y, z)$ denotes the vector of primal and dual variables, then each iteration of Newton's method for minimizing $\mathcal{M}(v) = \mathcal{M}(x, y, z)$ involves solving the linear equations $\nabla^2\mathcal{M}(v)\Delta v = -\nabla\mathcal{M}(v)$, where $\nabla\mathcal{M}$ and $\nabla^2\mathcal{M}(v)$ denote the gradient and Hessian of $\mathcal{M}$ with respect to x, y and z. These equations have fixed structure and are positive definite if the curvature of the underlying constrained problem is correct. The direction Δv is found by solving a related *generalized saddle-point problem* of the form:

$$\begin{pmatrix} H & -J^T & -I \\ J & \mu I & \\ I & & Z^{-1}(X+\mu I) \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \\ \Delta z \end{pmatrix} = - \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix},$$

where J is the Jacobian of c, H is the Hessian of the Lagrangian and X and Z are diagonal matrices with diagonal entries x_i and z_i. In [1,9] we describe efficient iterative methods for these equations based on the application of the conjugate-gradient method with certain structured preconditioners (also known as *constraint preconditioners*, see, e.g., [11, 14, 18–20]). The algorithm has the crucial property that the preconditioner equations need not be solved exactly, thereby allowing the use of multilevel preconditioners in the PDE context.

In order to ensure the convergence of each unconstrained minimization, we employ the trust-region modification of Newton's method. Trust-region methods define Δv as an approximate solution of the subproblem

$$\min_s \; q(s) = \nabla\mathcal{M}(v)^T s + \tfrac{1}{2} s^T \nabla^2\mathcal{M}(v) s \quad \text{subject to} \;\; \|s\| \le \delta \,, \tag{3}$$

where $\|\cdot\|$ is an inner-product norm and δ is a positive scalar that is updated as the iterations proceed (see, e.g., [3,21]). One of the most widely-used trust-region methods for the large-scale case is the Steihaug-Toint method [23,24], which uses the conjugate-gradient method to minimize $q(s)$ over a sequence of expanding subspaces until the iterates either converge to an interior point or cross the boundary of the constraint $\|s\| \le \delta$. However, if a preconditioner is used with the conjugate-gradient method, the Steihaug-Toint method requires that the trust-region norm be defined in terms of the preconditioning matrix. This implies that in the typical situation where a different preconditioner is used for each subproblem, the shape of the trust-region may change substantially from one subproblem to the next, which invalidates many of the assumptions on which standard methods for adjusting δ are based. To avoid this difficulty, we solve the inequality constrained trust-region subproblem (3) over a sequence of evolving low-dimensional subspaces. At the kth step, an estimate of Δv is given by

$$\Delta v_k = \operatorname*{argmin}_s \; \{\nabla\mathcal{M}(v)^T s + \tfrac{1}{2} s^T \nabla^2\mathcal{M}(v) s, \;\; \|s\| \le \delta, \;\; s \in \mathcal{S}_k\} \,,$$

where $\mathcal{S}_k$ is a subspace spanned by the previous iterate Δv_{k-1}, an estimate z_k of the leftmost eigenvector of $\nabla^2\mathcal{M}(v)$, and an "accelerator" direction s_k^a (see [4–6,15,16]).

The accelerator direction is obtained by applying a few iterations of a primal-dual interior method to the trust-region subproblem (3). A crucial property of this direction is that it is defined by applying the preconditioned conjugate-gradient method to a positive-definite system in both the primal and dual variables of the trust-region subproblem. This approach allows the trust-region norm to be defined independently of the preconditioner.

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Optimal Control Problems with Directional Sparsity

Roland Griesse
(joint work with Georg Stadler, Gerd Wachsmuth)

It is a feature of the 1-norm, both in $\mathbb{R}^n$ and function space, that it promotes sparsity of the solutions of optimization problems [1]. In particular, optimal control problems of the form

$$\text{minimize} \quad \frac{1}{2}\|\mathcal{S}u - y_d\|_H^2 + \frac{\alpha}{2}\|u\|_2^2 + \beta\,\|u\|_1$$

were considered by G. Stadler [2], where u is the control in $L^2(\Omega)$ and Ω is a bounded domain. These problems exhibit optimal controls which are zero on significant parts of the domain, but they do not provide any a priori information on the shape of the controls' support.

We consider here the following modification

$$\text{minimize} \quad \frac{1}{2}\|\mathcal{S}u - y_d\|_H^2 + \frac{\alpha}{2}\|u\|_2^2 + \beta\,\|u\|_{1(2)}\,, \tag{1}$$

where $\alpha, \beta \geq 0$ and the last term denotes the L^1-norm in some directions of the L^2-norm in the remaining directions of Ω. The coordinate directions are partitioned according to $\mathbb{R}^N = \mathbb{R}^n \times \mathbb{R}^{N-n}$ for some $1 \leq n < N$. The partition induces the sets

$$\Omega_1 = \{x_1 \in \mathbb{R}^n : \exists x_2 \in \mathbb{R}^{N-n} : (x_1, x_2) \in \Omega\}\,, \tag{2a}$$

$$\Omega_2(x_1) = \{x_2 \in \mathbb{R}^{N-n} : (x_1, x_2) \in \Omega\} \text{ for } x_1 \in \Omega_1\,, \tag{2b}$$

and Ω_1 can be interpreted as the projection of Ω onto $\mathbb{R}^n$, whereas $\Omega_2(x)$ is the cross section of Ω at position $x_1 \in \mathbb{R}^n$. Then $\|u\|_{1(2)}$ becomes

$$\|u\|_{1(2)} = \int_{\Omega_1} \left(\int_{\Omega_2(x_1)} u(x_1, x_2)^2 \,\mathrm{d}x_2 \right)^{1/2} \mathrm{d}x_1\,.$$

The "outer" direction x_1 is the one w.r.t. to which sparsity is promoted.

We assume that $\mathcal{S} \in \mathcal{L}(L^2(\Omega), H)$ is a bounded linear map into a Hilbert space H, and that $U_{ad} := \{u \in L^2(\Omega) : a \le u \le b \text{ a.e. in } \Omega\}$ with bounds $u_a, u_b \in L^2(\Omega)$. A function $\bar{u} \in U_{ad}$ is optimal for (1) if and only if

$$\langle u - \bar{u}, -\bar{p} + \beta\bar{\lambda} + \alpha\bar{u}\rangle \ge 0 \tag{3}$$

holds for all $u \in U_{ad}$, where $\bar{p} = \mathcal{S}^\star(y_d - \mathcal{S}\bar{u})$ is the optimal adjoint state and $\bar{\lambda} \in \partial\|\cdot\|_{1(2)}(\bar{u})$ is a subgradient.

In the presentation, we discuss algorithms of fixed-point and semismooth Newton type which address the solution of (3), and give some numerical results for elliptic and parabolic optimal control problems.

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From Simulation to Optimization with A Priori Bounded Retardation

Andreas Griewank

We consider the task of minimizing an objective function $f(y, u)$ with $(y, u) \in Y \times U$ the product of two Hilbert spaces subject to a state equation in fixed point form $G(y, u) = y$. The Jacobian $G_y = \partial G/\partial y$ is assumed to have a spectral radius $\rho < 1$ at all points of interest. Then feasible solutions $y = y(u)$ can be computed by the iteration $y_{k+1} = G(y_k, u)$ for $k = 1, \ldots$. We assume that the iteration function G is user supplied and may represent a simple local relaxation method or a sophisticated multigrid scheme [1]. The rate of convergence and thus the computational effort for resolving the state equation with a certain accuracy is determined by ρ or rather $1 - \rho$, which may be dependent on discretization parameters like for example the mesh width if the state equation is originally a PDE.

With $L(y, \bar{y}, u) \equiv f(y, u) + \bar{y}^\top(G(y, u) - y)$ the Lagrangian of the optimization problem we may append the primal iteration above with a dual iteration and an optimization loop to obtain the coupled system

$$\begin{aligned} y_{k+1} &= y_k + L_{\bar{y}}(y_k, \bar{y}_k, u_k) \\ \bar{y}_{k+1} &= \bar{y}_k + L_y(y_k, \bar{y}_k, u_k) \\ u_{k+1} &= u_k - B_k^{-1} L_u(y_k, \bar{y}_k, u_k) \ . \end{aligned}$$

The key ingredient of this one-shot approach is the design space preconditioner B_k, which must be selected as a symmetric positive definite $n \times n$ matrix in the practical situation $n \equiv \dim(U) < \infty$. Ideally B_k should be defined and computed such that the spectral radius $\hat{\rho}$ of the coupled system is below 1 and as close as possible to ρ.

We refer to the ratio $r \equiv (1-\rho)/(1-\hat{\rho})$ as the *retardation factor* of optimization relative to simulation. We believe that by chosing for a given state equation $G(y,u) = Y$ a family of more and more difficult objective functions the ratio can be made arbitrarily large. Moreover, we believe this conjecture to be true irrespective of the methodology in use for solving the primal. Naturally, there is the tacit assumption that the method for solving the dual is somehow 'naturally' related to that for solving the primal and in particular not much more sophisticated. In any case the retardation factor should be independent of incidental parameters like the discretization width.

Based on the theory developed in the papers [2–4] we have arrived at the tentative conclusion that a fairly optimal choice for B_k is given by

$$B \equiv \alpha G_u^\top G_u + \beta L_{uy} L_{yu} + L_{uu} .$$

Here the weighting coefficients are defined by

$$\alpha \equiv \frac{\|L_{yy}\|}{(1-\rho)^2} + \frac{q}{(1-\rho)} \quad \text{and} \quad \beta \equiv \frac{1}{q(1-\rho)}$$

where

$$q \equiv \max_{0 \neq v \in U} \frac{\|L_{yu} v\|}{\|G_u v\|} .$$

The ratio q quantifies the perturbation of the adjoint equation $L_y = 0$ caused by a design variation v relative to that in the primal equation $G - y = 0$. It can be shown that in the vicinity of a fixed point for this $B_k = B$ the coupled system cannot have real eigenvalues outside the open interval $(-1, 1)$. The modulus of complex eigenvalues is still under investigation.

The given preconditioner may be viewed and practically approximated as second order derivative with respect to the design u of the double augmented Lagrangian

$$L^a(y, \bar{y}, u) \equiv L(y, \bar{y}, u) + \frac{\alpha}{2}\|L_{\bar{y}}\|^2 + \frac{\beta}{2}\|L_y\|^2 .$$

Globally one can show that this merit function is consistently reduced by the coupled step defined above.

The one-dimensional case the the test problem proposed in [5] is given by

$$\min_{y,u} \int_0^1 0.5 \left[(y(t) - y^d(t))^2 + \mu u(t)^2 \right] dt \quad s.t. \; -y''(t) = u(t) \; , \; y(0) = 0 = y(1) .$$

Here we derived for our approach applied to Jacobi's method on a central difference discretization that the retardation factor r is proportional to the reciprocal of the regularization factor μ in the objective. We consider this to be a natural relation and are currently striving to derive a priori estimates of r for the general case, including nonseparable problems where L_{yu} does not vanish.

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Acoustic Optimization of Plates and Shells

Sean Hardesty
(joint work with Matthias Heinkenschloss)

We consider optimization of the radiated acoustic field produced by the vibrations of mechanically driven elastic shell structures. Changes in the radiated field are effected by variations in the structure geometry.

The structure occupies the domain $\Omega^- \subset \mathbb{R}^3$. We set $\Gamma = \partial\Omega^-$ and $\Omega^+ = \mathbb{R}^3 \setminus (\Gamma \cup \Omega^-)$. The model problem is formulated with 3D elasticity and the Helmholtz equation for the displacement vector u and the acoustic velocity potential φ:

$$\begin{aligned} -\omega^2\rho u &= \nabla\cdot\sigma(u) && \text{in } \Omega^- \\ \sigma(u) &= H : e(u) && \text{in } \Omega^- \\ \sigma(u)\cdot n &= f - i\omega\rho_0\varphi n && \text{on } \Gamma \\ \partial_n\varphi &= -i\omega u\cdot n && \text{on } \Gamma \\ \triangle\varphi + \kappa^2\varphi &= 0 && \text{in } \Omega^+ \\ |\nabla\varphi\cdot x/|x| - i\kappa\varphi| &= O\left(1/|x|^2\right) && \text{as } |x|\to\infty\,. \end{aligned}$$

Here f is an applied boundary traction. In the optimization problem we wish to modify the acoustic response φ over some frequencies ω in an observation region $\mathcal{O} \subset \Omega^+$ by varying the shape.

To model this problem, it is convenient to use Naghdi shell equations in conjunction with boundary integral equations so that the problem can be posed purely on a two-dimensional set of reference coordinates: it is thus possible to update the shape without modification of the mesh. To discretize the problem we apply MITC shell elements [9] and the piecewise-linear Galerkin boundary element formulation of [12]. In particular, the Duran-Libermann modification [4] of MITC3 plate elements is extended to Naghdi shells. The shell and boundary element equations are coupled using the thin boundary element method [11], which allows coupling at the shell mid-surface.

Existence and uniqueness theory for a problem that couples 3D elasticity with an integral equation formulation for exterior acoustics that is similar to ours is given in [2]. However, existence and uniqueness results for our coupled problem are not yet known.

Figure 1 shows numerical simulations of the acoustic response of a driven box that encloses the region $[-1,1]\times[-1,1]\times[0,1]$ with unit-circle hole in the top

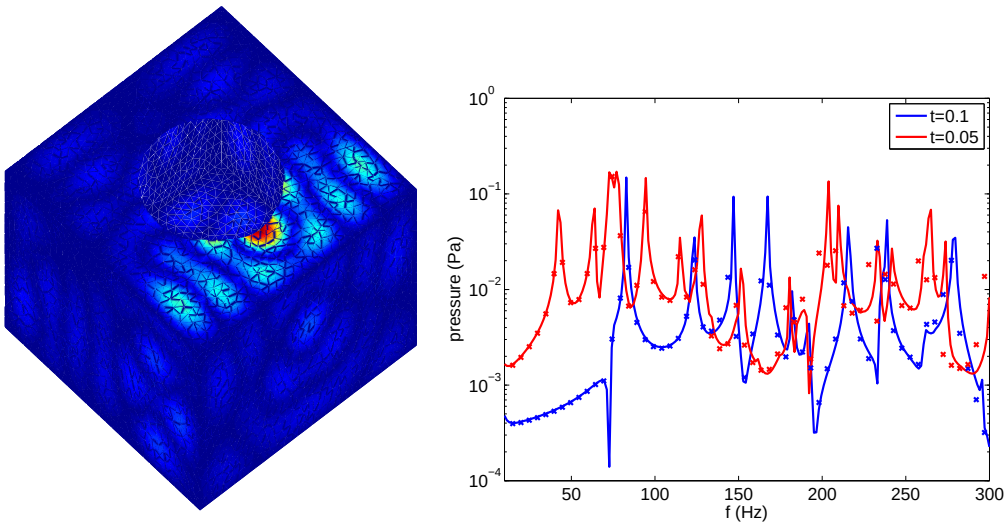

FIGURE 1. The driven box encloses the region $[-1,1] \times [-1,1] \times [0,1]$ with unit-circle hole in the top face. It is driven with a spatially Gaussian pulse, centered near the red spot at 200 Hz. The x-marks on the graph were computed on a refined mesh to test convergence.

face that is driven with a spatially Gaussian pulse. Simulations were done for two different thicknesses $t = 0.1$ and $t = 0.05$ of the box and two meshes for each thickness. The left plot shows the pressure for a spatially Gaussian pulse, centered near the red spot at 200 Hz. The right plot shows the pressure at a point outside the box for different frequencies. The right plot shows that the acoustic response can be modified by changing the thickness of Ω^-. It also indicates that the chosen mesh is sufficient to resolve the acoustic response at lower frequencies.

The next step is to apply optimization to find the best Ω^-, among a set of admissible shapes, so that the acoustic response matches a desired response. We can define the transfer function

$$T_\Gamma(\omega) = |\varphi_\omega(x^*)|/\|f_\omega\|_\Gamma \ .$$

Formally our optimization problem can be written as follows. We seek the solution over some admissible set of domain boundary shapes Γ_{ad} to

$$\min_{\Gamma \in \Gamma_{\text{ad}}} \|T_\Gamma - T^*\| \ ,$$

with T^* the desired transfer function. Formulation, analysis, and solution of this optimization problem is work in progress.

Optimization of similar problems has been done in [3,5,8], but with a variety of simplifying assumptions that limit the range of potential applications. In particular, it is often assumed that the structure is dense enough, that the air pressure loading can be neglected, or that the structural motions can be expanded in a basis of low-frequency eigenmodes of the elastic problem. Shape optimization has been done over a very targeted set of possible shape modifications using a small

parameter set, and without adjoint calculations. We aim to explore the possibilities of optimization using fully adjoint-based gradient calculation, and so to allow a wider variety of possible shapes. This is facilitated by choosing finite element schemes that make the coupling as simple as possible.

Thickness optimization of plates has been studied by [6,7], optimization of shells in [1]. Results on the existence of optimal solutions established in this papers are useful for the study of the optimization of our coupled problem.

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Recent Advances in the Numerical Solution of MPECs in Function Space

Michael Hintermüller

(joint work with Ian Kopacka, Moulay Hicham Tber)

In the recent past the problem class of *Mathematical Programs with Equilibrium Constraints* (MPECs) has received a considerable amount of attention in finite dimensions. In brief an MPEC is a constrained optimization problem where the

decision variables are related via the solution of a variational inequality, modeling an equilibrium process.

A general formulation of an MPEC is given by

$$\min J(y,u) \text{ subject to (s.t.) } (y,u) \in Z\,,\; y \in S(u)\,,$$

where Z is a joint upper-level feasible region of the pair (y,u) and $S(u)$ is the solution set of a variational inequality invoked by u. Many applications can, e.g., be found in economics (game theory, option pricing) or mechanics (lubrication problems, obstacle problems, elasto-plastic torsion).

From a mathematical point of view MPECs are especially interesting as they exhibit a number of challenging properties. Due to the nature of the constraints the feasible domain often exhibits structural intricacies, such as non-convexity or non-closedness. For some MPECs the feasible domain is not connected, or it might comprise of a finite union of sets giving rise to combinatorial issues. Furthermore classical constraint qualifications are generically violated for MPEC problems, hence the existence of Lagrange multipliers cannot be guaranteed using classical optimization theory. As a consequence a unique KKT-system cannot be defined for MPECs, rather a hierarchy of stationarity concepts has been developed for the problem class in finite dimensions (strong stationarity, M-stationarity, C-stationarity, W-stationarity, etc [6]).

In function space the MPEC theory is still significantly less researched. While additional difficulties, related to low multiplier regularity need to be taken into account, a theory in function space is appealing as numerical stability under refinement of the discretization can be expected for solution algorithms that allow a convergence analysis in function space. In our work we considered two approaches that enabled us to introduce counterparts of the finite dimensional stationarity concepts for a class of MPECs in function space, such as strong- and C-stationarity. Further weaker concepts, resulting from ambiguities due to low regularity, called $\mathcal{E}$-almost strong and $\mathcal{E}$-almost C-stationarity are introduced. The constructive nature of the proofs allows us to construct solution algorithms which admit function space based convergence analysis.

Relaxation/Regularization. We consider the following model problem, where the MPEC is governed by an elliptic variational inequality.

$$\begin{aligned} \min J(y,u) = \frac{1}{2}\|y-y_d\|_{L^2}^2 + \frac{\nu}{2}\|u\|_{L^2}^2 \text{ over } (y,u) \in H_0^1(\Omega)\times L^2(\Omega) \\ \text{s.t. } y \in K,\; a(y,v-y) \geq (u+f, v-y)_{L^2}\;\forall v \in K\,, \end{aligned} \tag{1}$$

where $\Omega \subset \mathbb{R}^n$, $n \leq 3$ is a bounded domain, $a(\cdot,\cdot) : H_0^1(\Omega)\times H_0^1(\Omega) \to H^{-1}(\Omega)$ is a bounded, coercive bilinear form, $y_d, f \in L^2(\Omega)$, $\nu > 0$ and the cone K is given by $K = \{v \in H_0^1(\Omega) : v \geq 0 \text{ a.e. in } \Omega\}$. If Ω and the coefficients of $a(\cdot,\cdot)$ are sufficiently smooth, the solution y of the variational inequality in (1) gains regularity and is in $H^2(\Omega)\cap H_0^1(\Omega)$. Hence introducing a slack variable $\xi \in L^2(\Omega)$ the variational inequality can equivalently be reformulated as a nonlinear complementarity

system and (1) is equivalent to

$$\begin{aligned} &\min J(y,u) \text{ over } (y,u,\xi) \in H_0^1(\Omega) \times L^2(\Omega) \times L^2(\Omega) \\ &\qquad \text{s.t. } \mathcal{A}y - u - f = \xi,\ y \geq 0,\ \xi \geq 0,\ (y,\xi)_{L^2} = 0\ , \end{aligned} \tag{2}$$

where $\mathcal{A} : H_0^1(\Omega) \to H^{-1}(\Omega)$ is the operator associated to the bilinear form $a(\cdot,\cdot)$.

The MPEC (2) is relaxed by introducing a *relaxation parameter* $\alpha > 0$ and replacing the product condition $(y,\xi) = 0$ by $(y,\xi) \leq \alpha$. Thus the feasible domain is artificially inflated and it turns out that constraint qualifications are satisfied for the relaxed problems. Due to the relaxation the bilevel structure of the problem is destroyed and boundedness of ξ has to be artificially ensured in order to guarantee the existence of a solution. This can either be done by adding a term of the form $\frac{\kappa}{2}\|\xi\|_{L^2}^2$ with $\kappa > 0$ to the cost functional or by adding an explicit constraint on the norm of ξ. The resulting problem resembles a state constrained optimal control problem, hence the problem of low multiplier regularity has to be dealt with. Introducing a further parameter $\gamma > 0$ the pointwise constraint on y is penalized using a Moreau-Yosida based regularization. The relaxed-regularized problem is then given by

$$\begin{aligned} &\min J(y,u) + \frac{\kappa}{2}\|\xi\|_{L^2}^2 + \frac{1}{2\gamma}\|\max(0, \bar{\lambda} - \gamma y)\|_{L^2}^2 \\ &\qquad \text{over } (y,u,\xi) \in H_0^1(\Omega) \times L^2(\Omega) \times L^2(\Omega) \\ &\qquad \text{s.t. } \mathcal{A}y - u - f = \xi,\ \xi \geq 0,\ (y,\xi)_{L^2} \leq \alpha\ , \end{aligned} \tag{3}$$

where $\bar{\lambda} \in L^q(\Omega)$, $q \geq 2$ is a shift parameter. Using standard Banach space theory, first order optimality conditions for (3) can be derived. The convergence behavior of stationary points for the relaxed-regularized problem (3) with respect to the parameters (α,κ,γ) is studied. If $\gamma \to \infty$ and $(\alpha,\kappa) \to 0$ with $\max\left((\alpha\sqrt{\gamma})^{-1}, \kappa\sqrt{\gamma}\right) \leq C$ it turns out that accumulation points of stationary points of (3) are $\mathcal{E}$-almost C-stationary for the MPEC (2); see [3]. Conditions are formulated that further ensure that the accumulation points are C- or strongly stationary.

Due to the nature of the approach a solution algorithm can be defined based on a continuation method with respect to the parameters (α,κ,γ). In each iteration a stationary point of (3) has to be computed. The optimality system is Newton-differentiable, hence a semismooth Newton method can be applied and local superlinear convergence can be expected. The theoretical results are verified by means of examples, including problems which lack strict complementarity, show degenerate behavior and utilize a nonsymmetric operator.

Application: Local volatility identification for American options. Given the price y_d of an American option, the objective is to recover the local volatility u. This

inverse problem can be formulated as the following MPEC:

$$\begin{aligned}
\min \quad & J(y,\,u) = \frac{1}{2}\|y - y_d\|^2_{L^2(Q)} + \frac{1}{2}\|y(T,\,\cdot) - y_T\|^2_{L^2(\Omega)} + \frac{\delta}{2}\|u\|^2_{\mathcal{U}} \\
\text{over} \quad & (y,\,u,\,\xi) \in W(0,T) \times U_{ad} \times L^2(Q) \\
\text{s.t.} \quad & u \in U_{ad}\ , \\
& \frac{\partial y}{\partial t} - u\frac{\partial^2 y}{\partial x^2} + f(u, y_0) - \xi = 0 \ \text{ in } L^2(0,\,T,\,H^{-1}(\Omega))\ , \\
& y(0) = 0 \text{ a.e. in } \Omega\ , \\
& y \geq 0 \text{ a.e. in } Q,\ \xi \geq 0 \text{ a.e. in } Q,\ (\xi, y)_{L^2(Q)} = 0\ ,
\end{aligned}$$

where Q is the time-space domain, U_{ad} is the admissible set for volatilities and f is a function depending on u and the pay-off y_0. The relaxed-regularized version of this problem reads

$$\begin{aligned}
\min \quad & J_\gamma(y,u) = J(y,u) + \frac{1}{2\gamma}\|\max(0,\,\overline{\lambda} - \gamma y)\|^2_{L^2(\Omega)} \\
\text{over} \quad & (y,\,u,\,\xi) \in W\,(0,T) \times \mathcal{U} \times L^2\,(Q) \\
\text{s.t.} \quad & u \in U_{ad}\ , \\
& \frac{\partial y}{\partial t} + A(u)y + f\,(u, y_0) - \xi = 0 \quad \text{in } L^2(0,\,T,\,H^{-1}(\Omega))\ , \\
& y(0) = 0 \text{ in } \Omega\ , \\
& \xi \geq 0 \text{ a.e. in } Q, \quad (\xi, y)_{L^2(Q)} \leq \alpha_\gamma\ , \\
& \frac{1}{2}\|\xi\|^2_{L^2(Q)} \leq R\ ,
\end{aligned}$$

with $\bar{\lambda} \geq 0$ fixed. In [5] a first order optimality system of C-stationarity type is derived. Moreover, an active-set-Newton with feasibility restoration solver is proposed. The stationary concept as well as the algorithmic approach used to solve this problem are supported by numerical results.

Smooth penalty. In the second approach the variational inequality in (1) is directly penalized using a max-operator, which is subsequently smoothed using a regularization $\max_\varepsilon$ which is at least C^1. This approach allows us to further consider pointwise constraints on the control variable u. The MPEC is hence approximated by the smooth penalty problem

$$\begin{aligned}
&\min J(y,u) \text{ over } (y,u) \in H^1_0(\Omega) \times L^2(\Omega) \\
&\qquad \text{s.t. } \mathcal{A}y - \gamma \max\nolimits_\varepsilon(0,-y) - u = f\ , \\
&\qquad\qquad a \leq u \leq b\ ,
\end{aligned} \tag{4}$$

where $\gamma > 0$ is a *penalty parameter* and $a, b \in L^2(\Omega) \cup \{-\infty, \infty\}$ with $b > a$. Again the penalization acts as a regularization of the feasible domain and optimality conditions of (4) can be derived using standard theory. As with the previous approach the convergence behavior of stationary points with respect to the parameters (γ, ε) is of interest. If $\gamma \to 0$ and $\varepsilon \to 0$ (depending on the nature of $\max_\varepsilon$) it is again shown that accumulation points of stationary points of (4) are

$\mathcal{E}$-almost C-stationary for the MPEC (1); see [4]. Based on these results a solution algorithm can again be formulated. The first order system of (4) is solved using nonlinear multigrid methods, such as the full approximation scheme (FAS) [1], where a smoother is designed utilizing a collective Gauss-Seidel scheme for which the scalar nonlinear equations are solved analytically in each grid point.

The theoretical results are verified by tests, where stability under mesh refinement and the typical convergence factors for FAS are shown.

Application: Lubrication problem. Estimating the film thickness in lubricated device when the cavitation phenomenon is taken into account by Reynolds model, gives rise to the following MPEC problem:

$$\begin{aligned} \text{minimize} \qquad & J(y,u) := \frac{1}{2}\|y-y_d\|_{L^2}^2 + \frac{\delta}{2}\|\nabla u\|_{L^2}^2 \qquad \text{over} \quad (y,u) \in K \times \mathcal{U}_{ad} \\ \text{s. t.} \qquad & y \in K,\ \langle -\mathrm{div}(u^3\nabla y), v-y\rangle \geq (\frac{\partial u}{\partial x_2}, v-y) \quad \forall v \in K\ , \end{aligned}$$

where y is the pressure, u is the film thickness, $K = \{v \in H_0^1(\Omega) =: V | v \geq 0\}$ and $\mathcal{U}_{ad} \subset H^1(\Omega)$. In [2] the variational inequality constraint is interpreted as a lower level optimization problem and a C-stationary optimality system is derived using the penalization approach. The penalized sub-problem reads

$$\begin{aligned} \text{minimize} \qquad & J(y,u) := \frac{1}{2}\|y-y_d\|_{L^2}^2 + \frac{\delta}{2}\|\nabla u\|_{L^2}^2 \qquad \text{over} \quad (y,u) \in V \times \mathcal{U}_{ad} \\ \text{s. t.} \qquad & \langle -\mathrm{div}(u^3\nabla y), v\rangle - (\frac{\partial u}{\partial x_2} + \max{}_\varepsilon(0, \overline{\lambda} - \gamma y), v) = 0 \quad \forall v \in V\ . \end{aligned}$$

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Numerical Analysis of Parabolic Control Problems with State Constraints

Michael Hinze
(joint work with Klaus Deckelnick)

In this talk we discuss parabolic optimal control problems with pointwise state constraints. The optimization problem is approximated using variational discretization combined with linear finite elements in space and a discontinuous Galerkin scheme in time for the discretization of the state equation. Error bounds for control and state are obtained both in two and three space dimensions. To achieve these bounds, uniform estimates for the discretization error of the state are proven which use natural regularity requirements on the optimal state. For the numerical analysis of the optimal control problem we use an approach which avoids error estimates for the adjoint state and which was developed in [2] for the analysis of elliptic optimal control problems with gradient constraints.

Let $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ be a bounded convex polygonal domain, $T > 0$ and $\Omega_T := \Omega \times (0, T)$. Let us consider the initial boundary value problem

$$y_t - \Delta y = f \quad \text{in } \Omega_T \tag{1}$$

$$\frac{\partial y}{\partial \nu} = 0 \quad \text{on } \partial\Omega \times (0, T) \tag{2}$$

$$y(\cdot, 0) = y_0 \quad \text{in } \Omega\ . \tag{3}$$

If $f \in L^2(0, T; H^1(\Omega))$ and

$$y_0 \in H^2(\Omega) \quad \text{with } \frac{\partial y_0}{\partial \nu} = 0 \quad \text{on } \partial\Omega\ , \tag{4}$$

then we have

$$y = \mathcal{G}(f) \in W := \{w \in C^0([0, T]; H^2(\Omega)) \mid w_t \in L^2(0, T; H^1(\Omega))\}\ . \tag{5}$$

Next, suppose that the functions $f_1, \ldots, f_m \in H^1(\Omega)$ are given and define $U := L^2(0, T; \mathbb{R}^m)$ as well as $B : U \to L^2(0, T; H^1(\Omega))$ by

$$Bu(x, t) := \sum_{i=1}^{m} u_i(t) f_i(x), \quad (x, t) \in \Omega_T\ .$$

Then $y = \mathcal{G}(Bu) \in W$ with

$$\max_{0 \le t \le T} \|y(t)\|^2_{H^2} + \int_0^T \|y_t(t)\|^2_{H^1} dt \le C\big(\|y_0\|^2_{H^2} + \int_0^T |u(t)|^2 dt\big)\ , \tag{6}$$

where the constant C depends in addition on the H^1–norms of $f_1, \ldots, f_m$.

We consider the optimization problem

$$(TP) \quad \begin{cases} \min_{u \in U} J(u) := \dfrac{1}{2} \displaystyle\int_0^T \|y(\cdot, t) - \bar{y}(\cdot, t)\|^2 dt + \dfrac{\alpha}{2} \int_0^T |u(t)|^2 dt \\ \text{s.t. } y = \mathcal{G}(Bu), \text{ and } y(x, t) \ge 0 \text{ in } \overline{\Omega_T}\ , \end{cases} \tag{7}$$

where $\bar{y} \in H^1(0,T;L^2(\Omega))$ and $\alpha > 0$ are given. From now on we shall assume (4) and that $\min_{x\in\bar{\Omega}} y_0(x) > 0$. It is not difficult to verify with the help of a comparison argument that

$$\mathcal{G}(0)(x,t) > 0 \text{ in } \overline{\Omega_T} \,. \tag{8}$$

Since the state constraints form a convex set and the set of admissible controls is closed and convex, one obtains the existence of a unique solution $u \in U$ to problem (7) by standard arguments. Moreover, using (8) combined with [1, Theorem 5.2] we have

Theorem 1. *Let $u \in U$ denote the unique solution to (7). Then there exist $\mu \in \mathcal{M}(\overline{\Omega_T})$ and a function $p \in L^s(0,T;W^{1,\sigma}(\Omega))$ for all $s,\sigma \in [1,2)$ with $\frac{2}{s}+\frac{d}{\sigma} > d+1$, such that with $y = \mathcal{G}(Bu)$ there holds*

$$\int_0^T (w_t - \Delta w, p) + \int_0^T \int_{\partial\Omega} \frac{\partial w}{\partial \nu} p = \int_0^T (y - \bar{y}, w) + \int_{\overline{\Omega_T}} w d\mu \;\; \forall w \in \tilde{W}_0 \,, \tag{9}$$

$$\alpha u_i(t) + (p(\cdot,t), f_i) = 0 \qquad \text{a.e. in } (0,T), i = 1,\dots,m \,, \tag{10}$$

$$\mu \le 0,\; y(t,x) \ge 0 \text{ in } \overline{\Omega_T} \qquad \text{and} \int_{\overline{\Omega_T}} y d\mu = 0 \,, \tag{11}$$

where $W_0 := W \cap \{w \in C^0(\overline{\Omega_T}) \,|\, w(\cdot,0) = 0 \text{ in } \bar{\Omega}\}$ and $\tilde{W}_0 := \{w \in W_0 \,|\, w_t \in L^\infty(\Omega_T)\}$.

1. Discretization

Let $\mathcal{T}_h$ be a quasi–uniform triangulation of Ω with maximum mesh size $h := \max_{S\in\mathcal{T}_h} \mathrm{diam}(S)$. Let us denote by $x_1,\dots,x_J$ the set of nodes of $\mathcal{T}_h$. We consider the space of linear finite elements

$$X_h := \{\phi_h \in C^0(\bar{\Omega}) \,|\, \phi_h \text{ is a linear polynomial on each } S \in \mathcal{T}_h\} \,.$$

Next, let $0 = t_0 < t_1 < \ldots < t_{N_1} < t_N = T$ a time grid with $\tau_n := t_n - t_{n-1}, n = 1,\dots,N$ and $\tau := \max_{1\le n\le N} \tau_n$. We set

$$W_{h,\tau} := \{\Phi : \bar{\Omega}\times(0,T) \,|\, \Phi(\cdot,t) \in X_h \text{ is constant in } t \in (t_{n-1},t_n), 1 \le t \le N\} \,.$$

For $Y, \Phi \in W_{h,\tau}$ we let

$$A(Y,\Phi) := \sum_{n=1}^N \tau_n (\nabla Y^n, \nabla \Phi^n) + \sum_{n=2}^N (Y^n - Y^{n-1}, \Phi^n) + (Y_+^0, \Phi_+^0) \,,$$

where $\Phi^n := \Phi_-^n, \Phi_\pm^n = \lim_{s\to 0^\pm} \Phi(t_n + s)$. Given $u \in U$, our approximation $Y \in W_{h,\tau}$ of the solution y of (1)–(3) is obtained by the following discontinuous Galerkin scheme:

$$A(Y,\Phi) = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} (Bu(t), \Phi^n) + (y_0, \Phi_+^0) \qquad \forall \Phi \in W_{h,\tau} \,. \tag{12}$$

The above solution will be denoted by $Y = \mathcal{G}_h(Bu)$. From here onwards it is convenient to suppose that $\tau \leq \gamma h^2$ for some $\gamma > 0$. We have the following uniform error estimate.

Lemma 1. *Let $u \in U, y = \mathcal{G}(Bu), Y = \mathcal{G}_h(Bu)$. Then*

$$\max_{1\leq n\leq N} \|y(\cdot,t_n) - Y^n\|_{L^\infty} \leq \left\{ \begin{array}{ll} Ch\sqrt{|\log h|}, & d=2, \\ C\sqrt{h}, & d=3. \end{array} \right\} \left(\|y_0\|_{H^2} + \|u\|_U\right) .$$

We use the variational approach of [3] in order to discretize our optimal control problem as follows:

$$(TP)_h \quad \left\{ \begin{array}{l} \min_{u\in U} J_h(u) := \dfrac{1}{2}\displaystyle\sum_{n=1}^{N} \tau_n \|Y^n - \bar{y}^n\|^2 + \dfrac{\alpha}{2}\int_0^T |u(t)|^2 dt \\ \text{s.t. } Y = \mathcal{G}_h(Bu) \text{ and } Y^n(x_j) \geq 0,\ 1 \leq j \leq J,\ 1 \leq n \leq N . \end{array} \right. \tag{13}$$

As a minimization problem for a quadratic functional over a closed and convex domain $(TP)_h$ admits a unique solution $u_h \in U$. Furthermore, for $h > 0$ small enough Lemma 1 ensures the Slater condition $\mathcal{G}_h(0) > 0$ in $\overline{\Omega_T}$, so that [1, Theorem 5.2] again yields that there exist $\mu_j^n \in \mathbb{R}, 1 \leq n \leq N, 1 \leq j \leq J$ as well as $P \in W_{h,\tau}$ such that

$$A(\Phi, P) = \sum_{n=1}^{N} \tau_n (Y^n - \bar{y}^n, \Phi^n) + \sum_{n=1}^{N}\sum_{j=1}^{J} \Phi^n(x_j)\mu_j^n \ \forall \Phi \in W_{h,\tau} , \tag{14}$$

$$\alpha u_{h,i}(t) + (P^n, f_i) = 0 \qquad \text{a.e. in } (t_{n-1}, t_n),\ i = 1, \ldots, m , \tag{15}$$

$$\mu_j^n \leq 0,\ Y^n(x_j) \geq 0 , \qquad \text{and } \sum_{n=1}^{N}\sum_{j=1}^{J} Y^n(x_j)\mu_j^n = 0 . \tag{16}$$

From this we infer

Lemma 2. *Let $u_h \in U$ be the optimal solution of (13) with corresponding state $Y = \mathcal{G}_h(Bu_h)$ and adjoint variables $P^n, 0 \leq n \leq N$ and $\mu_j^n, 1 \leq n \leq N, 1 \leq j \leq J$. Then there exists $h_0 > 0$ such that*

$$\sum_{n=1}^{N} \tau_n \|Y^n\|^2 + \int_0^T |u_h(t)|^2 dt + \sum_{n=1}^{N}\sum_{j=1}^{J} |\mu_j^n| \leq C \qquad \textit{for all } 0 < h \leq h_0 .$$

With the help of Lemma 1 and Lemma 2 we obtain our main result which reads

Theorem 2. *Let u be the solution of (TP), u_h the solution of $(TP)_h$ with corresponding states $y = \mathcal{G}(Bu)$ and $Y = \mathcal{G}_h(Bu_h)$. Then*

$$\sum_{n=1}^{N} \tau_n \|y(\cdot,t_n) - Y^n\|^2 + \int_0^T |u(t) - u_h(t)|^2 dt \leq \left\{ \begin{array}{ll} Ch\sqrt{|\log h|}, & \textit{if } d = 2 , \\ C\sqrt{h}, & \textit{if } d = 3 . \end{array} \right.$$

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Adaptive Discretization of Inverse Problems

Barbara Kaltenbacher

(joint work with Hend Ben Ameur, Anke Griesbaum, Boris Vexler)

Adaptive discretization in inverse problems especially in the context of PDEs is motivated by the need for high precision due to the inherent instability on one hand, and the by high computational effort on the other hand. The latter results from the fact that each regularized inversion involves several PDE solves, and it is necessary to repeatedly solve the regularized problem to determine the regularization parameter.

In this context we emphasize that for solving inverse problems it does not suffice to just make the residual (in the PDE) small as it is typically done by error estimator based adaptivity, but regularization has to be done by an appropriate tradeoff between smallness of the residual on one hand and stability on the other hand.

Among the recently increasing number of references on adaptivity for inverse problems, we wish to point out

- [Haber&Heldmann&Ascher'07]: Here Tikhonov regularization with a BV type regularization term is used and adaptive refinement is carried out for the state u such that the residual term is computed sufficiently precisely whereas adaptive refinement for the parameter q aims at computing the regularization term sufficiently precisely;
- [Neubauer'03, '06, '07]: The so-called moving mesh regularization and adaptive grid regularization are also based on Tikhonov regularization with a BV type regularization term: The grid is refined where the parameter q has jumps or large gradients;
- [Chavent&Bissell'98], [Ben Ameur&Chavent&Jaffré'02] propose to use refinement and coarsening indicators derived from Lagrange multipliers, see also [1] as well as below;
- Goal oriented adaptivity, see [2], [3], and below.

Refinement and coarsening indicators. Consider the example of identifying the piecewise constant spatially distributed transmissivity q from measurements of the hydraulic potential u in the PDE

$$s\frac{\partial u}{\partial t} - \text{div } (q \text{ grad } u) = f \text{ in } \Omega \subseteq \mathbb{R}^2 .$$

To identify the zonation for q as well as its values inside each zone, we minimize the misfit

$$J(q) := \|u(q) - u^\delta\|^2 = \min!$$

Starting from a coarse zonation, in order to decide whether and where to place zone interfaces, we consider the minimization problem for J under the constraint that the jump height across some tentative interface is equal to some value B. The Lagrange multiplier with respect to this constraint gives the sensitivity of the optimal misfit functional with respect to B and within a Taylor expansion around $B = 0$ (corresponding to the zonation without this interface) at first order indicates the potential decrease of the misfit by introducing this interface. The Lagrange multipliers can be cheaply evaluated for a large number of tentative interfaces and therewith serve as refinement indicators. Similarly, coarsening indicators can be defined. Confining the set of possible cuts to grid lines with a minimal mesh size h, we show convergence of the resulting refinement and coarsening algorithm in the following sense (for details on the assumptions, see [1]):

Theorem (Convergence with exact data to solution $q^\dagger$ as $h \to 0$):

$$\|q_h^* - q^\dagger\|_{L^2(\Omega)} = O(\sqrt{h}) \text{ and } \|q_h^* - q^\dagger\|_{L^\infty(\Omega)} = o(1)\ .$$

Theorem (Convergence with noisy data u^δ with $\|u - u^\delta\| \le \delta$ as $\delta \to 0$): $\quad h :\sim \delta^{\frac{2}{5}}$

$$\|q_{h(\delta)}^* - q^\dagger\|_{L^2(\Omega)} = O(\delta^{\frac{1}{5}}) \text{ and } \|q_{h(\delta)}^* - q^\dagger\|_{L^\infty(\Omega)} = o(1)\ .$$

Goal oriented error estimators. These were originally developed in the context of optimal control problems for PDEs, cf. [Becker&Kapp&Rannacher'00], [Becker&Rannacher'01], [Becker&Vexler '04, '05]. For PDE constrained minimization problems

$$\begin{aligned} &\text{Minimize} \quad J(q,u) \quad \text{over } q \in Q\,,\ u \in V \\ &\text{under the constraints} \ \ A(q,u)(v) = f(v) \quad \forall v \in V\,, \end{aligned}$$

they allow to estimate the error due to discretization with finite dimensional spaces $Q_h \subseteq Q$, $V_h \subseteq V$ in some *quantity of interest* I by means of (discrete) stationary points $x_h = (q_0, u_0, z_0)$ of an auxiliary functional

$$\mathcal{M}(q,u,z,p,v,y) = I(q,u) + \mathcal{L}'(q,u,z)[(p,v,y)] \quad (q,u,z,p,v,y) \in (Q \times V \times V)^2\,,$$

where $\mathcal{L}$ is the Lagrange functional. The error estimator η is a sum of *local* contributions due to *either q, u, z, p, v, or y*, which enables local refinement separately for $q \in Q_h$, $u \in V_h$, $z \in V_h$. A crucial question in the context of inverse problems such as parameter identification in PDEs formulated as operator equation

$$\text{solve} \ \ F(q) = g\,, \ \ \text{given} \ \ g^\delta \ \ \text{with} \ \|g - g^\delta\| \le \delta$$

is how to define appropriate quantities of interest there, since their number should be finite and low, therewith excluding control of high (i.e., discretized infinite dimensional) quantities like $\|F_h - F\|$ or $\|(F_h - F)q^\dagger\|$ for the discretized forward operator F_h. Our choice of I is based on the following convergence analysis results for Tikhonov regularization with the discrepancy principle (for details, see [2]

and [3])

Theorem *Let $\alpha_* = \alpha_*(\delta, g^\delta)$ and $Q_h \times V_h \times V_h$ be such that for $I(q,u) := \|F(q) - g^\delta\|_G^2$ there holds*

$$\underline{\underline{\tau}}^2\delta^2 \le I(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) \le \overline{\overline{\tau}}\delta^2 \,.$$

(i) If additionally

$$|I(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) - I(q^\delta_{\alpha_*}, u^\delta_{\alpha_*})| \le cI(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*})$$

for some sufficiently small constant $c > 0$, then $q^\delta_{\alpha_*} \longrightarrow q^\dagger$ as $\delta \to 0$.
Optimal rates are achieved under source conditions (logarithmic/Hölder).

(ii) If additionally for $I_2(q,u) := J(q,u)$

$$|I_2(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) - I_2(q^\delta_{\alpha_*}, u^\delta_{\alpha_*})| \le \sigma\delta^2$$

for some constant $C > 0$ with $\underline{\underline{\tau}}^2 \ge 1 + \sigma$, then $q^\delta_{h,\alpha_*} \longrightarrow q^\dagger$ as $\delta \to 0$.

as well as on the following convergence result for Newton's method for computing the regularization parameter

Theorem *Define*

$$i(\tfrac{1}{\alpha}) := I(q,u) := \|F(q) - g^\delta\|_G^2\,, \quad I_2(q,u) := i'(\tfrac{1}{\alpha})$$

$$\beta_* \text{ solution to } i(\beta_*) = \tau^2\delta^2 \text{ (discr.princ.)} \qquad \beta^{k+1} = \beta^k - \frac{i_h^k - \tau^2\delta^2}{{i'}_h^k} \text{ (Newton)}$$

for $k \le k_* - 1$ with $k_* = \min\{k \in \mathbb{N} \mid i_h^k - \tau^2\delta^2 \le 0\}$ with i_h^k, ${i'}_h^k$ satisfying

$$|i(\beta^k) - i_h^k| \le \varepsilon^k\,, \qquad |i'(\beta^k) - {i'}_h^k| \le {\varepsilon'}^k\,,$$

$\varepsilon^k, {\varepsilon'}^k$ sufficiently small.
Then β^k satisfies an asymptotically optimal quadratic convergence estimate and

$$(\tau^2 - \tilde\tau^2)\delta^2 \le i(\beta^{k_*}) \le (\tau^2 + \tilde\tau^2)\delta^2\,.$$

Consequently, the important quantities of interest for achieving fast convergence to the correctly regularized Tikhonov approximation are the squared residual, its derivative with respect to the regularization parameter, and the value of the Tikhonov functional. Efficient computation of the error estimators is enabled by

- computation of error estimators for $i(\beta)$ by to just one more SQP type step;
- direct extraction of $i'(\beta)$ from quantities computed for error estimators for $i(\beta)$;
- error estimators for $i'(\beta)$ that can be cheaply obtained from the stationary point of another auxiliary functional;

Similar conclusions can be drawn for regularization by discretization instead of Tikhonov's method, which has the additional advantage of a possible straightforward implementation in an iterative multilevel scheme.

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Calibration of Ground Water Models with POD

C. T. Kelley

(joint work with C. Winton, O. J. Eslinger, S. E. Howington, J. Pettway)

1. Introduction

We develop a version of proper orthogonal decomposition (POD) [3] for calibration of finite element models of three-dimensional steady state subsurface flow. We build the POD basis from the sensitivities, so only a single matrix assembly and factorization is needed for the entire optimization loop of the reduced model. After each optimization of the reduced model, we recompute the sensitivities and the reduced model, and then reoptimize the POD model. We present preliminary numerical results which indicate that the results can be as good as those obtained by putting the full three-dimensional simulator in the optimization.

We seek to identify a spatially-dependent conductivity K given measurements of the solution of the saturated flow equations

$$\operatorname{div}(K\nabla h) = f \tag{1}$$

with appropriate boundary conditions. In the context of the application, the inverse problem is regularized by assuming that the media consists of a finite (and small) number of zones, each composed of a single material. The unknowns are the conductivities in each zone.

These problems are naturally poorly scaled, with

$$10^{-7} \le K \le 10^{-2} \text{ and } 10 \le h \le 10,000\,.$$

The standard remedy is to fit the logarithms of K, and we do that here.

This project is a collaborative effort between our group at North Carolina State University and a group at the US Army Engineer Research and Development Center (ERDC). An important part of that collaboration was the need to integrate the solution of the inverse problem with the existing ERDC simulator ADH [7] and PEST [2], a nonlinear least squares solver which has been designed for hydrology problems. PEST is a well-designed bound-constrained Levenberg-Marquardt [4–6] code with an interface which has been developed with ERDC applications in mind.

The linear solvers in ADH assemble and store stiffness matrices, with a view toward using the matrix information either in a direct solver or as part of a domain-decomposition preconditioner. Hence we can assume that the stiffness matrix is available and we will use it to construct sensitivity vectors.

The zonal approximation to K is the piecewise constant approximation

$$K(x) = \sum_{i=1}^{N} p_i \chi_i(x) \ .$$

Here χ_i is the characteristic function of the ith zone and p_i is the hydraulic conductivity of that zone. Typically N, the number of zones, is small. We exploit the zones when we do matrix assembly. The finite element formulation of (1) has the form

$$Ah = f$$

where

$$A(p) = A_0 + \sum_i A_i p_i \text{ and } f = f_0 + \sum f_i p_i \ .$$

We need assemble the partial stiffness matrices A_i only once and then can rebuild $A(p)$ as needed when p changes. Given a solution h we then obtain the sensitivity vectors (the columns of the Jacobian) by solving

$$A(p)\frac{\partial h}{\partial p_i} = -A_i h + f_i \ ,$$

which requires no new matrix assembly or factorization.

The inverse problem is to find $p \in R^N$ which best fits measured pressure data with the computed pressure h. We let $d \in R^M$ denote the data, which are measurements of h at points in space $\{x_i\}_{i=1}^M$. Then if $h(p)$ is the output of the simulator, we define the vector $D(h(p))$ to be evaluations of $h(p)$ at the points $\{x_i\}$. With this in mind the nonlinear least squares problem is to minimize

$$f(p) = \frac{1}{2}\mathcal{R}(p)^T\mathcal{R}(p) \ ,$$

$\mathcal{R} : R^N \to R^M$ is

$$\mathcal{R}(p) = D(h(p)) - d \ .$$

The unconstrained Levenberg-Marquardt iteration is

$$p_+ = p_c - (\nu_c + \mathcal{R}'(p_c)^T\mathcal{R}'(p_c))^{-1}\mathcal{R}'(p_c)^T\mathcal{R}(p_c) \ ,$$

where p_c is the current value of the parameter vector, p_+ the updated value, and $\mathcal{R}'$ the Jacobian of $\mathcal{R}$. The Levenberg parameter ν_c depends on the status of the iteration in a standard way [1, 2, 4].

The cost of the optimization is mostly the evaluation of $\mathcal{R}$, which requires the computation of of h, *i. e.* matrix assembly and solving the differential equation. The matrix assembly is by far the most expensive part, and we see to use POD methods to take this out of the optimization.

In general terms POD begins with some vectors in the range of the solution operator for the differential equation, say $W = (w_1, \ldots w_L)$, takes a singular value

decomposition to obtain $U\Sigma V^T = W$, identifies a K for which σ_{K+1} is "small", and uses $\bar{U} = [u_1, \ldots, u_K]$ as a basis for the reduced order model. In time-dependent problems, W is typically built using "snapshots", *i. e.* solutions $u(x,t)$ of a differential equation sampled a discrete points in time.

Our problem is elliptic, so we must form W in a different way. We do this by using the sensitivities, which we would compute in any case to construct the Jacobian. We are currently setting $K = N$. The reduced order problem, which we put into the optimization loop instead of (1) is

$$\bar{A}\bar{h} = \bar{Q}^T A\bar{U}\bar{h} = \bar{f} = \bar{Q}^T f \ ,$$

where $\bar{Q}\bar{R} = A\bar{U}$ is the QR factorization of $A\bar{U}$.

2. Results

The results in this section are preliminary for a small model problem in three dimensions. We used direct solvers to solve (1) and compute the sensitivities for a give p. After that we solved a nonlinear least squares problem for the POD model

$$\min \|D(\bar{U}\bar{h}(p)) - d\|^2$$

to obtain a new p, for which we solved (1) and computed sensitivities until ∇f was sufficiently small.

As an example we use a column with three materials. The ADH discretization has roughly $6,000$ nodes and $31,000$ elements. The data are the exact solution perturbed by various levels of uniform noise. In Table 1 we report optimization statistics using the POD model for theses scenarios and compare them to optimization results using the fully resolved model. The important point is that the number of optimization iterations and the value of the objective function at the final results are roughly the same, but the number of calls to the full model is significantly reduced when the POD model is put into the optimization.

Table 1. Optimization Statistics

Noise	Full Model Calls	POD Model Calls	Final Residual
0%	38	N/A	8.1148E-03
	11	546	2.9348E-06
1%	60	N/A	8.3577E-03
	3	162	7.2897E-03
5%	63	N/A	1.0192E-01
	1	38	1.0651E-01
10%	30	N/A	3.2042E-01
	3	114	3.1953E-01

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Semi-smooth Newton Methods for Time Optimal Control for a Class of Linear Systems

Karl Kunisch

(joint work with Kazufumi Ito)

Consider the time-optimal control problem for a linear multi input system

$$\text{(P)} \qquad \begin{cases} \min_{\tau \geq 0} \int_0^\tau dt \\ \text{subject to} \\ \quad \frac{d}{dt}x(t) = Ax(t) + Bu(t),\ |u(t)|_{\ell^\infty} \leq 1,\ x(0) = x_0,\ x(\tau) = x_1\ , \end{cases}$$

where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $x_0 \in \mathbb{R}^n$, $x_1 \in \mathbb{R}^n$ are given, $u(t) \in \mathbb{R}^m$, u is measurable, and $|\cdot|_{\ell^\infty}$ denotes the infinity-norm on $\mathbb{R}^m$. It is assumed that x_1 can be reached in finite time by an admissible control. Then (P) admits a solution with optimal time denoted by τ^*, and associated state x^* and control u^*.

Under the assumption of strict transversality the first order optimality system for (P) can be expressed in terms of the adjoint p and the Hamiltonian

$$H(x, u, p_0, p) = p_0 + p^T(Ax + Bu)\ ,$$

as

$$\text{(1)} \qquad \begin{cases} \dot{x} = Ax + Bu,\ x(0) = x_0\ ,\ x(\tau) = x_1\ , \\ -\dot{p} = A^T p\ , \\ u = argmin_{|u|_{\ell^\infty}\leq 1} H(x, u, p)\ ,\ \text{a.e. in } (0, \tau)\ , \\ 1 + p(\tau)^T(Ax(\tau) + Bu(\tau)) = 0\ . \end{cases}$$

The non-differentiable operation involved in characterizing the optimal control,

$$u = -\sigma(p^T B) \ ,$$

where σ is defined as coordinate-wise operation, with

$$\sigma(s) \ \in \ \begin{cases} -1 & \text{if } \ s < 0 \\ [-1,\, 1] & \text{if } \ s = 0 \\ 1 & \text{if } \ s > 0 \end{cases} \tag{2}$$

prohibits the use of Newton-type methods for solving (1) numerically.

Therefore a family of regularized problems

$$(P_\varepsilon) \qquad \begin{cases} \min_{\tau \geq 0} \int_0^\tau (1 + \frac{\varepsilon}{2} \, |u(s)|^2) \, ds \\ \text{subject to} \\ \qquad \frac{d}{dt} x(t) = Ax(t) + Bu(t), \ |u(t)| \leq 1, \ x(0) = x_0, \ x(\tau) = x_1 \ , \end{cases}$$

with $\varepsilon > 0$ is considered.

Proposition 1. *For every $0 < \varepsilon_0 < \varepsilon_1$ and any solution $(\tau^*,\, u^*)$ of (P) we have*

$$\tau^* \leq \tau_{\varepsilon_0} \leq \tau_{\varepsilon_1} \leq \tau^*(1 + \frac{\varepsilon_1}{2}) \ , \tag{3}$$

$$|u_{\varepsilon_1}|_{L^2(0,\, \tau_{\varepsilon_1})} \leq |u_{\varepsilon_0}|_{L^2(0,\, \tau_{\varepsilon_0})} \leq |u^*|_{L^2(0,\, \tau^*)} \ . \tag{4}$$

If u^* is a bang-bang solution, then

$$0 \leq |u^*|^2_{L^2(0,\, \tau^*)} - |u_\varepsilon|^2_{L^2(0,\, \tau_\varepsilon)} \leq \ \mathit{meas}\, \{t \in [0, \tau^*] : |u_\varepsilon(t)| < 1\} \tag{5}$$

for every $\varepsilon > 0$.

Theorem 1. *For $\varepsilon \to 0^+$ we have $\tau_\varepsilon \to \tau^*$ and every convergent subsequence of solutions $\{(u_\varepsilon,\, x_\varepsilon)\}_{\varepsilon > 0}$ to (P_ε) converges in $L^2(0,\, \tau_\epsilon; \mathbb{R}^m) \times W^{1,2}(0,\, \tau_\epsilon;\, \mathbb{R}^n)$ to a solution $(u^*,\, x^*)$ of (P), where u^* is a minimum norm solution.*

We turn to the optimality condition for (P_ε). Let

$$\sigma_\varepsilon(s) \ \in \ \begin{cases} -1 & \text{if } \ s \leq -\varepsilon \\ \frac{s}{\varepsilon} & \text{if } \ |s| < \ \varepsilon \\ 1 & \text{if } \ s \geq \ 0 \ . \end{cases} \tag{6}$$

Theorem 2. *Assume that the pair (A, B) is normal and let $(x_\varepsilon, u_\varepsilon, \tau_\varepsilon)$ be a solution of (P_ε). If there exist α_i, $\delta > 0$, $\eta > 0$ such that*

$$|\, (\hat{u}_\varepsilon)_i(t)| \leq 1 - 2\eta \ \ \textit{for a.e. } \ t \in (\alpha_i, \alpha_i + \delta) \subset (0, 1), \ i = 1 \ldots, m \ , \tag{7}$$

then there exists an adjoint state p_ε such that

$$
(8)\qquad \begin{cases} \dot{x}_\varepsilon = Ax_\varepsilon + Bu_\varepsilon,\ x_\varepsilon(0) = x_0,\ x_\varepsilon(\tau_\varepsilon) = x_1 \\ -\dot{p}_\varepsilon = A^T p_\varepsilon \\ u_\varepsilon = -\sigma_\varepsilon(p_\varepsilon^T B) \\ 1 + \frac{\epsilon}{2}|u_\varepsilon(\tau_\varepsilon)|^2_{\mathbb{R}^m} + p_\varepsilon(\tau_\varepsilon)^T(Ax_\varepsilon(\tau_\varepsilon) + Bu_\varepsilon(\tau_\varepsilon)) = 0\,. \end{cases}
$$

We turn to the semi-smooth Newton method [2] for solving the regularized optimality system (8). For this purpose the system is transformed to the fixed time interval $(0, 1)$. We fix $\varepsilon > 0$ and denote by $(x_\varepsilon,\, u_\varepsilon,\, \tau_\varepsilon) \in W^{1,2}(0,1) \times L^2(0,1) \times \mathbb{R}$ a solution to (P_ε) with associated adjoint $p_\varepsilon \in W^{1,2}(0,\, 1)$. It is assumed that

$$
\text{(H1)}\qquad |b^T\, p_\varepsilon(1)| \neq \frac{1}{\varepsilon},\ \text{ and meas } \{|p_\varepsilon| < \frac{1}{\varepsilon}\} \neq 0\,.
$$

Here $\{|p_\varepsilon| < \frac{1}{\varepsilon}\}$ is shorthand for $\{t : |p_\varepsilon(t)| < \frac{1}{\varepsilon}\}$. With (H1) holding there exists a neighborhood $\mathcal{U}_{p_\varepsilon}$ in $W^{1,2}(0,1)$, $\bar{t} \in (0,1)$ and $\bar{c} > 0$ such that for $p \in \mathcal{U}_{p_\varepsilon}$ we have

$$
|b^T\, p(t)| \neq \frac{1}{\varepsilon} \text{ for all } t \in [\bar{t},\, 1]\,,
$$

and

$$
(9)\qquad \text{meas}\,\{|p| < \frac{1}{\varepsilon}\} > \bar{c}\,.
$$

We set $U = \{u \in L^2(0,\, 1) : u|[\bar{t},\, 1] \in W^{1,2}(\bar{t}, 1)\}$ endowed with the norm

$$
|u|_U = (|u|^2_{L^2(0,1)} + |\dot{u}|^2_{L^2(\bar{t},1)})^{\frac{1}{2}}\,,
$$

and introduce

$$
F : D_F \subset X \to L^2(0,1) \times L^2(0,1) \times U \times \mathbb{R}^2
$$

where

$$
D_F = W^{1,2}(0,1) \times \mathcal{U}_{p_\varepsilon} \times U \times \mathbb{R}\,,
$$

$$
X = W^{1,2}(0,\, 1) \times W^{1,2}(0,\, 1) \times U \times \mathbb{R},
$$

and

$$
(10)\qquad F(x,\, p,\, u,\, \tau) = \begin{pmatrix} \dot{x} - \tau Ax - \tau bu \\ -\dot{p} - \tau A^T p \\ u + \sigma_\varepsilon(b^T p) \\ x(1) - x_1 \\ 1 + \frac{\varepsilon}{2}u(1)^2 + p(1)^T\,(Ax(1) + bu(1)) \end{pmatrix}.
$$

For $(x,\, p,\, u,\, \tau) \in D_F$ we define $\mathcal{A} \in \mathbb{R}^{(n+1)\times(n+1)}$ by

$$
\mathcal{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & 0 \end{pmatrix},
$$

where

$$A_{11} = \varepsilon^{-1}\tau \int_0^1 e^{\tau A(1-t)} b b^T \chi_I \, e^{\tau A^T (1-t)} \in \mathbb{R}^{n\times n} \tag{11}$$

$$\begin{aligned} A_{12} = {} & \varepsilon^{-1}\tau \textstyle\int_0^1 e^{\tau A(1-t)} b b^T \chi_I \int_t^1 e^{-\tau A^T (t-s)} A^T p(s) ds\, dt \\ & - \textstyle\int_0^1 e^{\tau A(1-t)} (Ax + bu) dt \in \mathbb{R}^n \end{aligned} \tag{12}$$

$$A_{21} = (Ax(1) + bu(1))^T - (b^T p(1) + \varepsilon)\, \sigma_\varepsilon'(b^T p(1)) b^T \in (\mathbb{R}^n)^T \,, \tag{13}$$

where χ_I is the characteristic function of the set

$$I = I(p) = \{t : |b^T p| < \frac{1}{\varepsilon}\} \,,$$

which is nonempty for $p \in \mathcal{U}_{p_\varepsilon}$.

(H2) $\begin{cases} \text{there exists a bounded neighborhood } \mathcal{U} \subset D_F \subset X \text{ of } (x_\varepsilon,\, p_\varepsilon,\, u_\varepsilon,\, \tau_\varepsilon) \\ \text{and } c > 0 \text{ such that } |A_{21}\, A_{11}^{-1}\, A_{12}| \geq c \text{ for all } (x,\, p,\, u,\, \tau) \in \mathcal{U} \,. \end{cases}$

Theorem 3. *If (A, B) is normal,* (H1)*, and* (H2) *hold and $(x_\varepsilon,\, u_\varepsilon,\, \tau_\varepsilon)$ denotes a solution to (P_ε) with associated adjoint p_ε, then the semi-smooth Newton algorithm converges superlinearly, provided that the initialization is sufficiently close to $(x_\varepsilon,\, u_\varepsilon,\, \tau_\varepsilon)$.*

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On optimization of Materials and Processes

Günter Leugering

(joint work with Michael Stingl, Michal Kočvara)

We are generally concerned with optimization and control problems of the following type:

$$\begin{aligned} &\min \mathcal{J}(y, A, \rho, f, u) \quad \text{ s. t.} \\ &\rho \ddot{y} - \operatorname{div}(A \nabla y) = f \quad \text{ in } \Omega \\ &\partial_{\nu,A} y + \gamma y = u \quad \text{on } \Gamma \\ &y(0) = y_0, \quad \dot{y}(0) = y_1 \\ &(A, \rho, f, u) \in \mathcal{U}_{ad} \,. \end{aligned}$$

Applications are in context of Elastodynamics, structural optimization, Piezoelectricity, acoustics, and couplings. In particular, besides the more classical distributed and boundary controls, we focus on controls in the coefficients which is a widely open and challenging field of research. For the sake of brevity, we restrict ourselves to static problems that arise in material optimization [2–4]. To be even more specific, let us consider the following notation

Ω	:	Elastic body (design space),	$\Omega \subset \mathbf{R}^d$
$\partial\Omega$	:	Lipschitz boundary,	$\partial\Omega = \Gamma_0 + \Gamma$
f	:	surface force,	$f \in L^2(\Gamma)^d$,
u	:	displacement field,	$u \in \mathbf{H} := H^1(\Omega, \mathbf{R}^d)$
E	:	material tensor,	symmetric, pos. def.
e	:	(small) strain tensor,	$e(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$
σ	:	stress tensor,	$\sigma = E \cdot e(u)$

in particular

$$e = (e_{11}, e_{22}, \sqrt{2}e_{12})^\top, \quad \sigma = (\sigma_{11}, \sigma_{22}, \sqrt{2}\sigma_{12})^\top,$$

and

$$E = \begin{pmatrix} E_{1111} & E_{1122} & \sqrt{2}E_{1112} \\ & E_{2222} & \sqrt{2}E_{2212} \\ \text{symm.} & & 2E_{1212} \end{pmatrix}$$

and the corresponding problem in elasticity:
Find displacement field $u \in \mathcal{H}^1(\Omega; \mathbf{R}^N)$, such that

$$\begin{aligned} -\mathrm{div}(\sigma) &= g \text{ in } \Omega, \quad \text{(Equilibrium)} \\ \sigma \cdot n &= f \text{ in } \Gamma, \text{ (Neumann b. c.)} \\ u &= 0 \text{ in } \Gamma_0, \quad \text{(Dirichlet b. c.)} \\ \sigma &= Ee(u), \text{ (Hooke's law) .} \end{aligned}$$

The variational format is: Find $u \in \mathcal{V} := \{u \in \mathbf{H} | u_{\Gamma_0} = 0\}$, such that

$$\underbrace{\int_\Omega e(u)(x)^\top \cdot E \cdot e(v)(x)\mathrm{dx}}_{a_E(u,v)} = \underbrace{\int_\Gamma f(x)^\top v(x)\mathrm{dx}}_{l(v)} \quad \forall v \in \mathcal{V} .$$

The minimal compliance problem reads as:

$$\min_{E \in \mathcal{E}} c(E) := \int_\Gamma f(x)^\top u_E(x)\mathrm{dx} ,$$

where

$$u_E \text{ solves } a_E(u_E, v) = l(v) \quad \forall v \in \mathcal{V}$$

$$\mathcal{E} := \left\{ E \in \mathcal{L}^\infty(\Omega, \mathbf{S}^N) \mid E \succeq 0, \underline{\rho} \le \mathrm{tr}(E) \le \overline{\rho}, \int_\Omega \mathrm{tr}(E)\ \mathrm{dx} \le V \right\} .$$

The class of problems is considerably enlarged in this lecture. In order to obtain existence of solutions one may introduce various concepts of convergence of minimal sequences E_n. In fact for a general functional $J(E,u)$ we treat sequences of pairs $(E_n,u_n)_n$, where u_n solves state equation associated with E_n.
First trial: Can we show compactness in $\mathcal{L}^\infty(\Omega,S^N)\times\mathcal{V}$?
- $E_{n'} \overset{w-*}{\rightharpoonup} E^*$ in $\mathcal{L}^\infty(\Omega,S^N)$
- $u_{n'} \overset{w}{\rightharpoonup} u$ in $\mathcal{V}$

$$\dots \text{ but e.g. } \sigma_n = E_n e(u_n) \not\rightharpoonup E^* u$$

i.o.w. u is not necessarily a solution of state equation associated with E^*!(Counterexample by F. Murat 79'). We consider

$$\mathcal{E}^{\alpha,\beta} := \left\{E\in\mathcal{L}^\infty(\Omega,S^N) \mid 0<\alpha I_N \preccurlyeq E \preccurlyeq \beta I_N \text{ a. e. in } \Omega\right\} .$$

Definition (Murat, Tartar '79)**:** (E_n) in $\mathcal{E}^{\alpha,\beta}$ is said to H-converge to an H-limit $E^*\in\mathcal{E}^{\alpha,\beta}$ if, for any right hand side $g\in\mathcal{L}_2(\Omega;\mathbf{R}^N)$, the sequence u_n of solutions of $(*)$ with $E=E_n$ satisfies

$$\begin{aligned}(u_n) &\rightharpoonup u^* \text{ weakly in } \mathcal{V}\\ (\sigma_n):=(E_n e(u_n))_n &\rightharpoonup \sigma^*:=E^*e(u^*) \text{ weakly in } \mathcal{L}_2(\Omega;\mathbf{R}^{\bar N})\end{aligned}$$

where u^* is the solution of $(*)$ with $E=E^*$. It is well-known that $\mathcal{E}_{\alpha,\beta}$ is H-compact. We can prove
Lemma: [2] *The set*

$$\mathcal{E}^\epsilon := \left\{E\in\mathcal{L}^\infty(\Omega,S^N) \mid \epsilon I\preccurlyeq \underline{\rho} I\preccurlyeq E;\ \mathrm{tr}(E)\le\overline{\rho},\int_\Omega \mathrm{tr}(E)\ \mathrm{dx}\le V\right\}$$

is H-compact.

Consider cost functionals of the type

$$J:\mathcal{E}^{\alpha,\beta}\times\mathcal{V}\to\mathbf{R}$$

with the following property:

$$\left.\begin{aligned}(E_n)\overset{H}{\to}E \text{ in } \mathcal{E}^\varepsilon\\ (v_n)\rightharpoonup v \text{ in } \mathcal{V}\end{aligned}\right\}\Rightarrow \liminf_{n\to\infty} J(E_n,v_n)\ge J(E,v) .$$

Theorem: [2] *The regularized FMO problem*

$$\min_{E\in\mathcal{E}^\epsilon} C(E):=J(E,u_E)$$

has at least one solution.
Typical examples with property

$$\left.\begin{aligned}(E_n)\overset{H}{\to}E \text{ in } \mathcal{E}^\varepsilon\\ (v_n)\rightharpoonup v \text{ in } \mathcal{V}\end{aligned}\right\}\Rightarrow \liminf_{n\to\infty} J(E_n,v_n)\ge J(E,v)$$

are
- $J_1(E,u)=\int_\Gamma f\cdot u\ \mathrm{dx}$ or $J_2(E,u)=\|u-u_0\|^2_{\mathcal{L}_2(\Omega;\mathbf{R}^N)}$.

Even more importantly, we can handle some sort of state- and stress-constraints
• *Quadratic or tracking type displacement constraints* of the form

$$\int_\Omega (u(x)-u_0(x))^\top (u(x)-u_0(x)) \ \mathrm{dx} \le C \ ,$$

with here $u_0 \in \mathcal{V}$.
• *Integral stress constraints* of the form

$$\int_\omega \sigma(x)^\top M \sigma(x) \ \mathrm{dx} \le C \ ,$$

where $\omega \subset \Omega$ and M is either the unit or the von Mises matrix.
Theorem: [2]*Let g and h be weakly lower semicontinuous functions of the state variables u and σ, respectively. Then the set*

$$\mathcal{E}^{\varepsilon,g,h} := \{E \in \mathcal{E}^\varepsilon \mid g(u_E) \le C_u, \ h(\sigma_E) \le C_\sigma\} \ ,$$

with $u_E = S(E)$ and $\sigma_E = Ee(S(E))$ is H-compact.

We now consider approximations of the problem above. Let $\{\mathcal{T}_\kappa\}_{\kappa \to 0+}$ be a family of partitions of $\overline{\Omega}$ with $i = 1, 2, \ldots, N(\kappa)$ and

$$\overline{\Omega} = \bigcup_{i=1}^{N(\kappa)} \overline{\Omega}_i, \ \max_i \mathrm{diam}(\Omega_i) \le \kappa \ .$$

Associated with any $\mathcal{T}_\kappa$ we define an approximation of $\mathcal{E}^{\varepsilon,h,g}$ as

$$\mathcal{E}_\kappa^{\varepsilon,h,g} = \Big\{ E \mid E_i := E|_{\Omega_i} \in P_0(\Omega_i), E_i \succcurlyeq \underline{\rho} I_{\bar{N}}, \ \mathrm{tr}(E_i) \le \overline{\rho} \ , \\ i = 1, .., N(\kappa) \ , \\ \sum_{i=1}^{N(\kappa)} \mathrm{tr}(E_i) = \hat{v}, \ g(u_E) \le C_u, \ h(\sigma_E) \le C_\sigma \Big\} \ .$$

There exists $\kappa_0 > 0 : \mathcal{E}_\kappa^{\varepsilon,h,g}$ is non-empty for all $\kappa \le \kappa_0$. $(*)$
Lemma: [2]*Under assumption (*) the system $\left(\mathcal{E}_\kappa^{\varepsilon,h,g}\right)_{\kappa \le \kappa_0, \kappa \to 0+}$ is dense in $\mathcal{E}^{\varepsilon,h,g}$, i.e., for each $E \in \mathcal{E}^{\varepsilon,h,g}$ there exists $(E_\kappa) \in \left(\mathcal{E}_\kappa^{\varepsilon,h,g}\right)$ such that $E_\kappa \overset{H}{\rightharpoonup} E$.*

Define

$$(\mathcal{P}^\kappa) \qquad \inf_{E \in \mathcal{E}_\kappa^{\varepsilon,g,h}} J(E, u_E) \ .$$

Obviously: Problem $(\mathcal{P}^\kappa)$ admits a solution for each $\kappa \le \kappa_0$ Assume further (see also [1])

$$\left.\begin{array}{c} (E_\kappa) \overset{H}{\rightharpoonup} E \text{ in } \mathcal{E}^\varepsilon \\ (v_\kappa) \rightharpoonup v \text{ in } \mathcal{V} \end{array}\right\} \Rightarrow \lim_{\kappa \searrow 0} J(E_\kappa, v_\kappa) = J(E, v) \quad (**)$$

Theorem [2] *Let the cost functional J satisfy (**). Let further, for each $\kappa \le \kappa_0$, $E_\kappa \in \mathcal{E}_\kappa^{\varepsilon,g,h}$ be a solution of problem $\mathcal{P}^\kappa$ and u_κ the associated (unique) solution of the state problem. Then there exist subsequences (E'_κ) and (u'_κ) of (E_κ) and (u_κ) such that*

$$E'_\kappa \overset{H}{\rightharpoonup} E^* \text{ in } \mathcal{E}^\varepsilon, \ u'_\kappa \rightharpoonup u^* \text{ in } \mathcal{V} \quad \text{as } \kappa' \searrow 0 \ .$$

Moreover, E^* is an optimal solution of problem

$$(\mathcal{P}) \qquad \inf_{E \in \mathcal{E}^{\varepsilon,g,h}} J(E, u_E)$$

and u^* solves the associated state problem.

The state problem is approximated by FEM, u_E^h denotes the approximate solution of the state equation, π^h is a standard interpolation operator. We consider the fully discretized problem:

$$(\mathcal{P}^{\kappa,h}) \qquad \inf_{E \in \mathcal{E}_\kappa^{\varepsilon,g,h}} J\left(E, \pi^h(u_E^h)\right) \ .$$

$E^*_{\kappa_j,h_j}$ denotes the solution of $(\mathcal{P}^{\kappa,h})$ Then: We can find a diagonal sequence (κ_j, h_j) such that

$$\left(E^*_{\kappa_j,h_j}\right)_{\kappa_j,h_j} \overset{H}{\rightharpoonup} E^* \, .$$

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Optimal Control of a Special Class of State-Constrained Dynamical Systems with ODEs and PDEs

Hans Josef Pesch

(joint work with Armin Rund, Wolf von Wahl, and Stefan Wendl)

Realistic mathematical models of dynamical processes from scientific or engineering background may often have to consider different physical phenomena and therefore may lead to coupled systems of equations that include partial and ordinary differential equations as well as algebraic equations. Frequently, their numerical solution is only the first step. The identification of system parameters and the control of such systems are tackled subsequently. Mathematically one obtains optimization problems with constraints given by the underlying dynamical process. Because of their complexity, such optimization problems are not widely studied in literature, neither theoretically nor numerically.

The flight of a hypersonic aircraft under the objective of minimum fuel consumption may serve as a typical example. The flight trajectory is described, as usual, by a system of ordinary differential equations (ODE). This system is controlled by the usual control variables of flight path optimization under various control and

FIGURE 1. A detailed model of the lower stage of the German two-stage-to-orbit concept *Sänger II* [1], [5] provides the model for a hypersonic passenger aircraft, which gave the motivation for the "hypersonic car problem" investigated in [3], [4].

state variable inequality constraints. However, due to the hypersonic flight conditions, a thermal protection system is indispensable. A major additional goal of the optimization is the limitation of the heating of the thermal protection system. This additionally requires to take into account a quasi-linear heat equation with nonlinear boundary conditions, which is coupled with the ODE system through its coefficients and boundary conditions. Finally a pointwise state constraint enforces the limitaton of the heating of the thermal protection system. This constraint couples the PDE with the ODE reversely. See Ref. [1].

For our investigations, we take this challenging problem as motivation for a new class of optimal control problems with constraints in form of a coupled system of ordinary and partial differential equations. We call this class of problems hypersonic rocket car problems, since it is inspired, on the one hand, by the well-known rocket car problem, which often serves as a propaedeutic example in courses of optimal control, and, on the other hand, by the above mentioned recently investigated flight path trajectory optimization problem for a hypersonic aircraft. These problems mimic partly the coupling structure of the hypersonic aircraft problem and exhibit some intrinsic difficulties of such coupled systems.

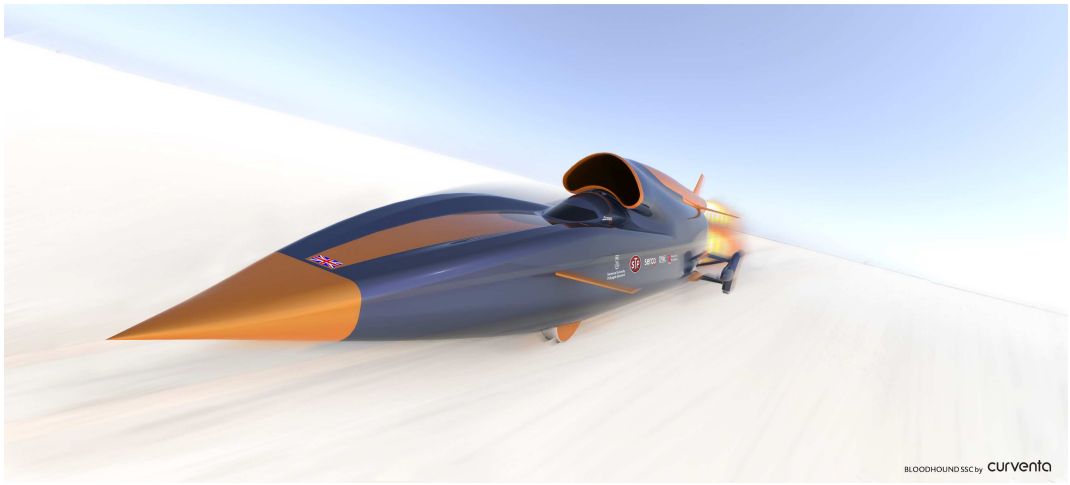

FIGURE 2. Although the hypersonic rocket car investigated in [3], [4] is virtually faster than the *Bloodhound Supersonic Car* of [2], this rocket car will most probably have a much better chance to be realized. Nevertheless, the hypersonic car problems of [3], [4] are an appealing challenge from the mathematical point of view.

Moreover, these problems can be considered as undressed abstract examples for a class of staggered state-constrained ODE-PDE-constrained optimal control problems that are typical for many current applications. The simplication allows to obtain analytical solutions to a certain extent which is normally prohibited by the enormous complexity of real-life problems.

Firstly, the analysis of structural questions concerning the existence of boundary arcs and touch points of state constraints is the aim of the talk. This is novel in the context of PDE-constrained optimal control. We obtain results, which are, at a first glance, similar to state-constrained ODE optimal control problems and show their relation to the differentiation index of the related partial differential algebraic equation system along state-constrained subarcs. At a second glance, new phenomena are observed caused by the non-local character of the state constraint in the ODE context and lead to additional hidden constraints on the ODE states from the beginning of the process on.

A crucial point namely is that the state constraint, which is pointwisely defined in the PDE context, looses its local character from the ODE point of view. This leads to new types of optimal control problems and new necessary conditions, both for the ODE and the PDE formulations of the hypersonic rocket car problems. In any case, integral relations between variables are present in certain necessary conditions making the application of adjoint based methods a challenge, if not almost impossible. In particular, new necessary conditions for unspecified terminal time and new jump conditions for certain state-constrained parabolic control problems are developed.

Investigations concerning the two essential numerical solution approaches, *first discretize, then optimize* (direct method) and *first optimize, then discretize* (indirect method) are carried out. It seems that only the first method can be performed with a passable effort. Nevertheless, many of the necessary conditions can be at least approximately verified on the basis of adjoint estimates from the direct method.

As outlook, an interesting approach could be based on the connection of state-constrained optimal control problems to free boundary value problems with the boundary (interface) between the active and inactive sets as optimization variable. This approach would contain the spirit of determining the junction points in ODE state-constrained problems as optimization parameters of a multi-point boundary value problem with jump conditions.

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Robust Solution Methods via Optimal Control Reformulation

Denis Ridzal

(joint work with Pavel B. Bochev)

We develop and analyze an optimization–based approach for robust and efficient solution of PDE problems consisting of multiple physics operators with fundamentally different mathematical properties. Our approach relies on three essential steps: decomposition of the original problem into subproblems for which robust solution algorithms are available; integration of the subproblems into an equivalent PDE–constrained optimization problem; and solution of the resulting optimization problem. The thrust of the work builds on the ideas of Lions on virtual control in the context of operator decomposition [4], and can be further related to the work of Gunzburger et al. [2].

Additive split of a model problem. We present the optimization–based approach using as an abstract model problem a strongly coercive variational formulation comprising a bilinear form $Q(\cdot,\cdot) : V \times V \mapsto \mathbb{R}$ and a data function $f \in V^*$: given $f \in V^*$ we seek $u \in V$ such that

$$Q(u,v) = (f,v)_H \qquad \forall\, v \in V\,, \tag{1}$$

where V and H are Hilbert spaces and V^* is the dual of V. We require that $Q(\cdot,\cdot)$ is V–elliptic and continuous. The *key idea* of the optimization–based approach for the solution of the model problem (1) rests on the assumption that the form $Q(\cdot,\cdot)$ can be written as a difference of two *component* bilinear forms

$$Q(\cdot,\cdot) = Q_1(\cdot,\cdot) - Q_2(\cdot,\cdot)$$

for which efficient solvers are available. We assume that $Q_1(\cdot,\cdot)$ and $Q_2(\cdot,\cdot)$ are V–elliptic and continuous. We derive an equivalent formulation of (1) in terms of its component problems. First, note that we can write (1) as *seek $u \in V$ such that*

$$\big\{Q_1(u,v) - (\theta,v)_V - (f,v)_H\big\} - \big\{Q_2(u,v) - (\theta,v)_V\big\} = 0 \quad \forall\, v \in V\,, \tag{2}$$

where $\theta \in V$ is arbitrary. To uncouple the component forms $Q_1(\cdot,\cdot)$ and $Q_2(\cdot,\cdot)$ we split the test function into a pair $\{v_1, v_2\} \in V \times V$ and consider the following weak problem: *seek $\{u,\theta\} \in V \times V$ such that*

$$\widetilde{Q}\big(\{u,\theta\},\{v_1,v_2\}\big) = (f,v_1)_H \quad \forall\, \{v_1,v_2\} \in V \times V\,, \tag{3}$$

where

$$\widetilde{Q}\big(\{u,\theta\},\{v_1,v_2\}\big) = \big\{Q_1(u,v_1) - (\theta,v_1)_V\big\} - \big\{Q_2(u,v_2) - (\theta,v_2)_V\big\}\,. \tag{4}$$

In contrast to (2), well–posedness of (3) and its equivalence with (1) is not immediately obvious. We address these issues first.

Theorem 1. *The bilinear form $\widetilde{Q}(\cdot,\cdot)$ defined in (4) is weakly coercive on $V \times V$: there exists a positive constant $\widetilde{\gamma}$ such that*

$$\sup_{\{v_1,v_2\} \in V \times V} \frac{\widetilde{Q}\big(\{u,\theta\},\{v_1,v_2\}\big)}{\|v_1\|_V + \|v_2\|_V} \geq \widetilde{\gamma}\big(\|u\|_V + \|\theta\|_V\big) \quad \forall\, \{u,\theta\} \in V \times V\,,$$

and

$$\sup_{\{u,\theta\} \in V \times V} \frac{\widetilde{Q}\big(\{u,\theta\},\{v_1,v_2\}\big)}{\|u\|_V + \|\theta\|_V} \geq 0 \quad \forall\, \{v_1,v_2\} \in V \times V\,.$$

Corollary 1. *The variational problem (3) has a unique solution $\{u,\theta\} \in V \times V$ for any $f \in V^*$ and that solution depends continuously on the data: $\|u\|_V + \|\theta\|_V \leq (1/\widetilde{\gamma})\|f\|_{V^*}$. The first component of the solution $\{u,\theta\}$ is the solution of (1).*

Reformulation into optimization problem. We replace (1) by the constrained optimization problem

$$(5)\qquad \begin{cases} \text{minimize} \qquad J^\varepsilon(u_1,u_2,\theta)=\dfrac{1}{2}\Big(\|u_1-u_2\|_H^2+\varepsilon\|\theta\|_V^2\Big) \\ \text{subject to} \begin{cases} Q_1(u_1,v_1)-(\theta,v_1)_V=(f,v_1)_H & \forall\, v_1\in V \\ -\big(Q_2(u_2,v_2)-(\theta,v_2)_V\big)=0 & \forall\, v_2\in V\,, \end{cases} \end{cases}$$

where $\varepsilon>0$ is a regularization parameter. Existence and uniqueness of optimal states and controls can be shown using standard techniques. The following key result estimates the error introduced by the optimization reformulation.

Theorem 2. *Let $\{u_1^\varepsilon,u_2^\varepsilon,\theta^\varepsilon\}\in V\times V\times V$ denote the solution of the optimization problem (5) and $u\in V$ the solution of (1). Then, there exists a positive constant C such that*

$$\|u_1^\varepsilon-u\|_V+\|u_2^\varepsilon-u\|_V\le\varepsilon C\|f\|_{V^*}\,.$$

The proof relies on the use of the intermediate variational problem (3), see [1].

Solution of the reformulated problem. We develop robust solution methods for (1). A finite element discretization of (5) typically yields

$$(6)\qquad \begin{cases} \underset{\vec{\boldsymbol{u}}_1,\vec{\boldsymbol{u}}_2,\vec{\boldsymbol{\theta}}}{\text{minimize}} \qquad \dfrac{1}{2}\Big((\vec{\boldsymbol{u}}_1-\vec{\boldsymbol{u}}_2)^T\mathbf{H}(\vec{\boldsymbol{u}}_1-\vec{\boldsymbol{u}}_2)+\varepsilon\,\vec{\boldsymbol{\theta}}^{\,T}\mathbf{V}\vec{\boldsymbol{\theta}}\Big) \\ \qquad\qquad \text{subject to} \begin{cases} \mathbf{Q}_1\vec{\boldsymbol{u}}_1-\mathbf{V}\vec{\boldsymbol{\theta}} &= \vec{\boldsymbol{f}} \\ -\mathbf{Q}_2\vec{\boldsymbol{u}}_2+\mathbf{V}\vec{\boldsymbol{\theta}} &= \vec{\boldsymbol{0}}\,. \end{cases} \end{cases}$$

Our approach is based on the premise that robust and efficient solution methods for linear systems involving the component operators $\mathbf{Q}_1$, $\mathbf{Q}_2$ are readily available. We solve (6) using the *reduced–space* approach, i.e. we solve the linear system

$$(7)\qquad \mathbf{H_{red}}\,\vec{\boldsymbol{\theta}}^{\,*}=-\vec{\boldsymbol{f}}_{\mathbf{red}}$$

where the reduced Hessian matrix $\mathbf{H_{red}}$ is given by

$$(8)\quad \mathbf{H_{red}}=\begin{pmatrix}\mathbf{V} & \mathbf{V}\end{pmatrix}\begin{pmatrix}\mathbf{Q}_1^{-T} & \mathbf{0}\\ \mathbf{0} & \mathbf{Q}_2^{-T}\end{pmatrix}\begin{pmatrix}\mathbf{H} & -\mathbf{H}\\ -\mathbf{H} & \mathbf{H}\end{pmatrix}\begin{pmatrix}\mathbf{Q}_1^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{Q}_2^{-1}\end{pmatrix}\begin{pmatrix}\mathbf{V}\\ \mathbf{V}\end{pmatrix}+\varepsilon\mathbf{V}$$

and the reduced right–hand side $\vec{\boldsymbol{f}}_{\mathbf{red}}$ is computed as follows,

$$(9)\qquad \vec{\boldsymbol{f}}_{\mathbf{red}}=\begin{pmatrix}\mathbf{V} & \mathbf{V}\end{pmatrix}\begin{pmatrix}\mathbf{Q}_1^{-T} & \mathbf{0}\\ \mathbf{0} & \mathbf{Q}_2^{-T}\end{pmatrix}\begin{pmatrix}\mathbf{H} & -\mathbf{H}\\ -\mathbf{H} & \mathbf{H}\end{pmatrix}\begin{pmatrix}\mathbf{Q}_1^{-1}\vec{\boldsymbol{f}}\\ \vec{\boldsymbol{0}}\end{pmatrix}\,.$$

Application to scalar advection–diffusion equation. As proof of concept, we offer evidence indicating that standard multigrid solvers lack robustness when applied to problems with complex advection fields and large Péclet numbers, and demonstrate that our approach offers a robust alternative. We consider the so–called *double–glazing problem*, see [3, p.119]. For this example, a generic discrete SUPG–stabilized $Q(\cdot,\cdot)$ form is given by (w.l.o.g. we assume $|\mathbf{b}|\approx 1$ and $|\mathbf{b}|\gg\nu$)

$$Q(u^h,v^h)=\nu\big(\nabla u^h,\nabla v^h\big)+\big(\mathbf{b}\cdot\nabla u^h,v^h+\delta\mathbf{b}\cdot\nabla v^h\big)-\big(\nu\Delta u^h,\delta\mathbf{b}\cdot\nabla v^h\big)_h\,.$$

To reformulate it using robust components we make the identification

$$\begin{aligned} Q_1(u^h, v^h) &= \big(\nabla u^h, \nabla v^h\big) + \big(\mathbf{b}\cdot\nabla u^h, v^h + \delta\mathbf{b}\cdot\nabla v^h\big) - \big(\nu\Delta u^h, \delta\mathbf{b}\cdot\nabla v^h\big)_h\,, \\ Q_2(u^h, v^h) &= (1-\nu)\big(\nabla u^h, \nabla v^h\big)\,, \end{aligned}$$

which makes $Q_1(\cdot,\cdot)$ and $Q_2(\cdot,\cdot)$ heavily *diffusion–dominated*.

For the solution of (1) we use multigrid solvers BoomerAMG (BAMG) and ML as preconditioners for GMRES. We note that the stated numerical results reflect the best solver settings that we could find for the example problem, and require expensive smoothing strategies. The optimization approach is denoted by OPT, and solves (7) using GMRES. Every optimization iteration involves four linear systems, see (8), which are solved efficiently using ML with a basic smoother. Only 5–8 iterations are required for the solution of each system within the optimization loop. The table below presents a comparison of the number of *outer* GMRES iterations for the optimization approach and the *total* number of GMRES iterations for multigrid solvers applied to the full problem. For the example problem, featuring a complex advection field and a large Péclet number ($\nu = 10^{-8}$), ML and BAMG show very strong mesh dependence, and fail to converge on the 256×256 mesh. In contrast, OPT is robust to mesh refinement, and successfully solves the problem for all mesh sizes. In addition, we show that while ML and BAMG are very sensitive to the size of the Péclet number, OPT's performance is affected only mildly. Overall, our optimization–based strategy provides a robust solution alternative for problems on which widely used multigrid solvers struggle.

	$\nu = 10^{-8}$			128×128		
	64×64	128×128	256×256	$\nu = 10^{-2}$	$\nu = 10^{-4}$	$\nu = 10^{-8}$
OPT	135	97	77	62	97	97
ML	71	196	—	9	96	196
BAMG	72	457	—	7	33	457

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Interior Point Methods in Function Space for State Constraints

Anton Schiela
(joint work with Andreas Günther, Michael Hinze)

The solution of PDE constrained optimal control problems with pointwise state constraints is a challenging and important issue. In the following we are going to sketch the main ideas of an interior point method in function space for its solution. To have an easy example at hand, consider the following problem, where u is the control and y is the state:

$$\begin{aligned} \min_{\substack{y\in H_0^1(\Omega),\\ u\in L_2(\Omega)}} J(y,u) &:= \frac{1}{2}\|y-y_d\|^2_{L_2(\Omega)}+\frac{\alpha}{2}\|u\|^2_{L_2(\Omega)} \\ \text{s.t. } a(y,v) &= (u,v)\ \forall v\in H_0^1(\Omega) \\ y &\geq \underline{y} \quad \text{on } \overline{\Omega}\,. \end{aligned} \tag{1}$$

Here $a(\cdot,\cdot)$ is a continuous and elliptic bilinear form with suitable regularity properties. We stress, however, that our algorithms and the corresponding analysis apply much more generally. The main requirement is that all feasible controls produce continuous states.

Interior point methods replace the inequality constraints by barrier functionals, so that our model problem is replaced by

$$\min_{\substack{y\in H_0^1(\Omega),\\ u\in L_2(\Omega)}} J(y,u)+\int_\Omega l(y(x);\mu)\,dx \ \text{ s.t. } a(y,v)=(u,v)\ \forall v\in H_0^1(\Omega)\,, \tag{2}$$

where l is either a *logarithmic* or a *rational barrier function*, which is scaled by a parameter μ, and $\lim_{\mu\to 0} l(y(x);\mu)=0$, if $y(x)>\underline{y}(x)$.

The idea is that for $\mu>0$ the smooth problem (2) is easier to solve than (1) and that the computation of a sequence of solutions of (2) for $\mu\to 0$ may yield an efficient algorithm for the solution of (1). Interior point methods for finite dimensional optimization are popular and well established in many variants, so the main challenge here is to analyse such a method in function space, and to construct an algorithm that exploits the particular structure of state constraints.

The following is a brief sketch of the results, achieved so far. Details can be found in the references, given below.

The Central Path [3,4]. The basis for the analysis of any path-following method is a systematic study of the corresponding homotopy path. Such a study consists of existence and uniqueness results, regularity considerations, and the study of analytic properties of the path, such as convergence, continuity and smoothness with respect to the homotopy parameter. In the context of optimization methods the characterization of points on the path via first order optimality conditions is an additional issue.

The homotopy path for interior point methods is traditionally called the *central path*. An analysis in function space has been performed for the state constrained

case with the expected positive results on existence, uniqueness and regularity. Furthermore, first order optimality conditions have been derived.

Interestingly, first order optimality conditions only look as expected, if the state is strictly feasible. This leads to the idea of using higher order barrier functionals, which guarantee strict feasibility of the state.

Analytically, the central path is well behaved. It is locally Lipschitz continuous with respect to the barrier parameter μ, and the Lipschitz constant behaves like $O(\mu^{-1/2})$ for $\mu \to 0$. A particular topological feature of barrier methods is already visible at this stage of analysis: the Lipschitz estimates can be shown for the *scaled norm*

$$\|(\delta y, \delta u)\|_{l''}^2 := \langle (1 + l''(y;\mu))\delta y, \delta y\rangle_{L_2(\Omega)} + \alpha \|\delta u\|^2 .$$

If the central path is strictly feasible, then it is also continuously differentiable. Further, the central path converges to the exact solution of the state constrained problem with a rate of convergence $O(\mu^{1/2})$, and the function values converge monotonically from above with a rate of convergence $O(\mu)$.

Path-following in Function Space [5]. The next step in the construction of path-following algorithms is a specification of a computational scheme for the solution of the homotopy subproblems. As usual we use a variant of Newton's method, applied to the *control reduced optimality system*, where the state and the adjoint state are the iteration variables and the control is eliminated. A special feature of the correction is a *pointwise damping* step, which guarantees feasibility of the iterates, exploiting the pointwise structure of the state constraints.

The resulting algorithm, which is still an algorithm in function space, can be shown to produce iterates, which converge to the solution of the original state constrained problem. So there is not only a convergence result for the homotopy *path* (see above), but also for a corresponding path-following *algorithm*.

Closely related to the analysis, a scheme for the update of the homotopy parameter has been constructed. It is based on computational estimates of the crucial quantities used in the convergence analysis. Here the use of the scaled norm $\|\cdot\|_{l''}$ turns out to be central. This observation corresponds to similar results in finite dimensional algorithms.

Discretization and Adaptivity [1, 6]. Up to now, we are equipped with an algorithm in function space, while actual computations only can solve discretized problems. So there is still a gap to be bridged.

First of all, a discretization scheme was established, and *a-priori error estimates* have been derived. State and adjoint state have been discretized - straightforwardly - by linear finite elements. As a detail of practical importance, it was shown that the evaluation of the barrier functionals and their derivatives can be performed simply by *quadrature* without losing convergence.

Second, an adaptive grid refinement procedure has been constructed to implement Newton steps in function space inexactly. This means that the *discretization error* of each Newton step is *controlled* by a-posteriori error estimation and adaptive grid refinement. This is performed with the aim to keep the iterates within

the radius of convergence of the Newton corrector in function space. For this an error estimator in the problem suited norm $\|\cdot\|_{l''}$ is desirable, and it turns out that such an estimator exists and can be evaluated inexpensively with techniques, known from goal oriented error estimation. Its construction exploits the special structure of the Jacobian matrix, which is the sum of a symmetric positive definite operator and a skew symmetric operator.

As first numerical test indicate, these techniques allow the solution of state constrained problems with an effort that is not much higher than the computation of the last Newton step on the finest grid.

Outlook. Some extensions and applications to related problems have been considered. The analysis of the central path also includes pointwise (upper and/or lower) control bounds and/or bilateral bounds on the states. Further, an application of interior point techniques to *gradient bounds* on the state [7] and *max-norm optimization* [2] has been considered.

So far, interior point methods have mostly been applied to elliptic problems in a convex setting. So it is straightforward to look for extensions to other types of partial differential equations and to non-convex non-linear problems. Some results can already be anticipated, but there are still several challenging problems to be solved.

Closely connected to these questions is the search for efficient *linear iterative solvers* for the computation of the Newton steps. Our algorithmic framework allows the inexact solution of these systems. Just as the a-posteriori error estimators an iterative solver should have the property to converge with respect to the scaled norm $\|\cdot\|_{l''}$.

Acknowledgment. The work of the speaker was supported by the DFG Research Center MATHEON "Mathematics for key technologies". The co-authors acknowledge support of the DFG Priority Program 1253 through grants DFG06-381 and DFG06-382.

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Robust Shape Optimization in CFD

Claudia Schillings
(joint work with Volker Schulz)

Recently, optimization has become an integral part of the aerodynamic design process chain. However, because of uncertainties with respect to the flight conditions and geometry uncertainties, a design optimized by a traditional design optimization method seeking only optimality may not achieve its expected performance. Robust optimization deals with optimal designs which are robust with respect to small (or even large) perturbations of the optimization setpoint conditions. That means, the optimal designs computed should still be good designs, even if the input parameters for the optimization problem formulation are changed by a non-negligible amount. Thus even more experimental or numerical effort can be saved. In this talk, we aim at an improvement of existing simulation and optimization technology, so that numerical uncertainties are identified, quantized and included in the overall optimization procedure, thus making robust design in this sense possible.
We consider the following aerodynamic shape optimization problem

$$\min_{y,p} f(y,p) \tag{1}$$

$$\text{s.t. } c(y,p) = 0\,, \tag{2}$$

$$h(y,p) \geq 0\,. \tag{3}$$

We think of the equation (2) as the discretized outer flow equation around, e.g., an airfoil described by geometry parameter $p \in \mathbb{R}^{n_p}$. The vector y is the state vector (velocities, pressure,...) of the flow model (2) and we assume that (2) can be solved uniquely for y for all reasonable geometries p. The objective in (1) $f : (y,p) \mapsto f(y,p) \in \mathbb{R}$ typically is the drag to be minimized. The restriction (3) typically denotes lift or pitching moment requirements. The general deterministic problem formulation (1-3) is influenced by stochastic perturbations described by a random variable s defined on a given probability space (Ω, Y, P) characterized by a probability density function $\varphi : \mathbb{R} \to \mathbb{R}_+$, or in the case of spatially distributed uncertainties, the perturbations are described by a random field. To compute a solution which is stable to stochastic variations in s, we introduce two robust formulations: the semi-infinite formulation and chance constraint formulation.
The semi-infinite formulation aims at optimizing the average objective function but maintaining the feasibility with respect to the constraints everywhere. Thus, it aims at an average optimal and always feasible robust solution. The ideal formulation is of the form

$$\min_{y,p} \int_{\Omega} f(y,p,\zeta) dP(\zeta) \tag{4}$$

$$\text{s.t. } c(y,p,\zeta) = 0\,,\ \forall \zeta \in \Omega\,, \tag{5}$$

$$h(y,p,\zeta) \geq 0\,,\ \forall \zeta \in \Omega\,. \tag{6}$$

This defintion of robustness can also be found in Ref. [3] and in Ref. [9]
Chance constraints leave some flexibility with respect to the inequality restrictions (cf. Ref. [5]) . The inequality restrictions are only required to hold with a certain probability P_0

$$\min_{y,p} \int_{\Omega} f(y,p,\zeta) dP(\zeta) \tag{7}$$

$$\text{s.t. } c(y,p,\zeta) = 0\,,\ \forall \zeta \in \Omega\,, \tag{8}$$

$$P(\{\zeta \,|\, h(y,p,\zeta) \geq 0\}) \geq P_0\ . \tag{9}$$

We will show some numerical results considering the velocity and the angle of attack as an uncertainty source and compare the two introduced robust formulations. The semi-infinite formulation leads to a better lift to drag ratio than the chance constraint formulation and seems most promising in our application. In order to obtain fast convergence, we have generalized the one-shot methods which are based on approximate reduced SQP iterations (cf. [2]) to the semi-infinite approach.
Beside the scalar valued uncertainties in the flight conditions we consider the shape itself as an uncertainty source and apply a Karhunen-Loève expansion to approximate the infinite-dimensional probability space. To overcome the curse of dimensionality an adaptively refined sparse grid is used in order to compute statistics of the solution. These investigations are part of the current German research program MUNA.

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Fast Non-Parametric Large Scale Aerodynamic Shape Optimization

Stephan Schmidt
(joint work with Caslav Ilic, Volker Schulz, Nicolas Gauger)

The talk focuses on structure exploitation for the aerodynamic shape optimization problem. Especially in three dimensions, the number of unknowns for both the fluid and the shape of the aircraft can be huge, requiring sophisticated numerics and analytic structure exploitation.

We present a Shape-OneShot method which combines the usual OneShot approach with the Hadamard-representation [2,6] of the shape derivative and a Hessian approximation based on the operator symbol of the pseudo-differential operator governing the shape Hessian, preventing any loss of regularity in the shape. The aircraft is treated like a submanifold, and the discretization of these two ingredients leads to an optimization procedure which operates on the surface of the "aircraft manifold" alone, which thus allows a huge deformation of the shape while being very fast for almost any number of design parameters.

We study the operator symbol of the Hessian similar to [1, 3] for the viscous energy dissipation problem:

$$\begin{aligned}
\min_{(u,\Omega)} J(u,\Omega) &:= \int_\Omega \nu \sum_{i,j=1}^{3} \left(\frac{\partial u_i}{\partial x_j}\right)^2 \, dA \\
\text{subject to} & \\
-\mu\Delta u + \rho u \nabla u + \nabla p &= 0 \quad \text{in} \quad \Omega \\
\operatorname{div} u &= 0 \\
u &= 0 \quad \text{on} \quad \Gamma \\
\operatorname{Vol}(\Omega) &= V_0 \, .
\end{aligned}$$

The speed of the fluid is given by $u = (u_1, u_2)^T$, μ is the absolute or dynamic viscosity, p denotes the pressure, and ρ is the density which is constant in an incompressible fluid. Also, $\Gamma_1 \subset \partial\Omega$, the no-slip surface of the flow obstacle, is the unknown to be found. The shape derivative for this problem is given by:

$$dJ(u,\Omega)[V] = \int_\Gamma \langle V, n\rangle \left[-\nu \sum_{k=1}^{3} \left(\frac{\partial u_k}{\partial n}\right)^2 - \frac{\partial u_k}{\partial n}\frac{\partial \lambda_k}{\partial n}\right] \, dS \, ,$$

where $\lambda = (\lambda_1, \lambda_2)^T$ and λ_p again satisfy the adjoint equation

$$\begin{aligned}
-\nu\Delta\lambda - \rho\lambda\nabla u - \rho\left(\nabla\lambda\right)^T u + \nabla\lambda_p &= -2\Delta u \quad \text{in } \Omega \\
\operatorname{div}\lambda_p &= 0 \quad \text{in } \Omega \\
\lambda &= 0 \quad \text{on } \Gamma \, .
\end{aligned}$$

In the limit of the Stokes-Problem, i.e. $\rho = 0$, it can be shown that an oscillation of the form

$$\tilde{\Gamma} := \{(x_1, x_2) \in \mathbb{R}^2 : x_2 \geq \tilde{q}(x_1)\}$$

where

$$\tilde{q}(x) = \hat{q}e^{i\omega x}$$

is mapped by the Hessian H as follows:

$$H\tilde{q} = |\omega|\tilde{q} \ .$$

Hence, the shape Hessian for this problem shares the same symbol as the Poincaré-Stecklov Operator. In the Navier-Stokes case, $\rho > 0$, the same can be shown discretely by comparing wave propagations numerically. More details can be found in [5].

Using such operator symbols, we employ the Shape-OneShot method to optimize a wing in three dimensions for a transonic and supersonic inviscid, compressible fluid modeled by the Euler equations:

$$\begin{aligned}
\min_{(U,\Omega)} F_{\text{drag}}(U,\Omega) &:= \int_\Gamma \langle p_d, n\rangle \, dS \\
\text{subject to} & \\
\sum_{i=1}^{3} A_i(V)\frac{\partial U}{\partial x_i} &= 0 \text{ in } \Omega \text{ (Euler equations)} \\
\langle u, n\rangle &= 0 \text{ on } \Gamma \text{ (Euler slip condition)} \\
F_{\text{lift}}(U,\Omega) := \int_\Gamma \langle p_l, n\rangle \, dS &\geq l_0 \text{ (lift force)} \\
L := \int_\Gamma dS &\leq L_0 \text{ (airfoil contour length, 2D only)} \\
I_x := \int_\Gamma (y - y_c)^2 \, dS &\geq I_{x_0} \text{ (airfoil bending stiffness, 2D only)} \\
V := \int_{\text{int } \Gamma} dA &\geq V_0 \text{ (airfoil volume, 2D and 3D) .}
\end{aligned}$$

A detailed derivation of the shape derivative and more numerical results can be found in [4]. The contour length and bending stiffness constraint are usually not both enforced at the same time. Also, they are substitute models not sophisticated enough for the structural loads in 3D.

The proposed Shape-OneShot method works extremely effective, tested by optimizing a 3D Onera M6 wing at $\alpha = 3.01°$ angle of attack and a reference Mach number of $M_\infty = 0.83$. A comparatively coarse mesh was used, resulting in $4,335,840$ unknowns for the state and $18,285$ unknowns for the shape. The state equation is solved using the DLR flow solver TAU. With an additional Laplace-Beltrami solve for the Hessian approximation, a single thread Intel Core2Duo E6600 needs about a minute per approximative SQP step in terms of CPU time. Each optimization step consists of roughly 10 primal solver time steps and 1 dual

time step for each of the adjoints. Note that due to the slower convergence of the adjoint solvers, this results in a retardation factor of ≈ 2, well below the expected retardation factor of 3 (primal solver and two adjoints).

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Towards Systematic Design of Metamaterials

Ole Sigmund

We describe a topology optimization approach for the systematic synthesis of dielectric based metamaterials. The procedure is based on repeated finite element analyses, S-parameter extractions, and gradient-based design updates. Examples include planar negative μ and ϵ materials.

Metamaterials are artificially designed materials with properties beyond those of naturally occurring materials. Lately a lot of attention has been devoted to electromagnetic metamaterials with negative indexes which may provide cloaking, perfect imaging and miniaturization of antennas [1] (see also Figure 1 for illustrations). Sofar practical realizations of metamaterials have been based on scientists' clever physical insight and intuition, and solutions depend strongly on wavelength (from microwaves to visible light).

The topology optimization method originally developed for mechanical systems design (see [2] for a review) and later extended to a range of other applications including photonic crystal design [3,4] may provide a basis for the systematic design of low-loss, isotropic metamaterials with desired properties. In this presentation we discuss initial results for dielectric-based planar metamaterial design using the topology optimization method.

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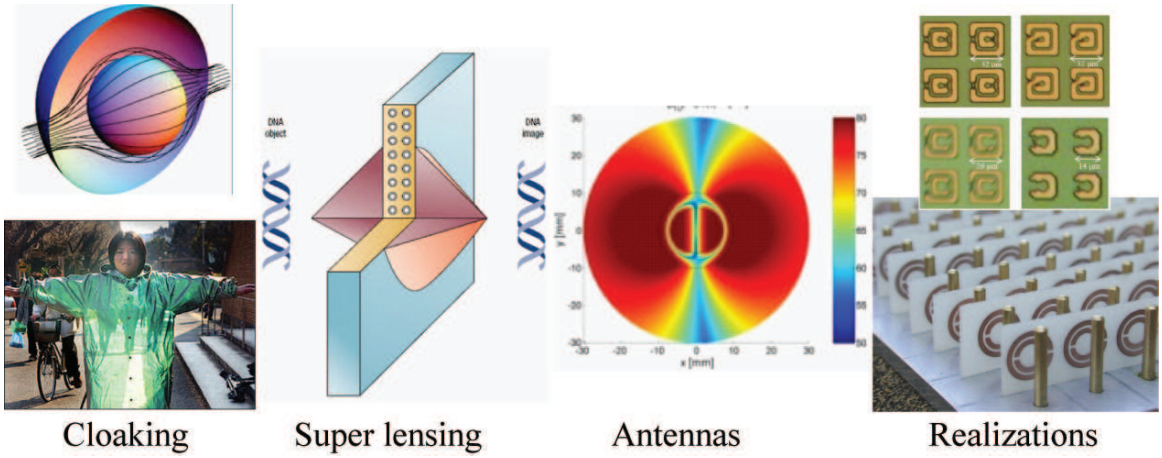

FIGURE 1. Applications and realizations of electromagnetic meta-materials from the literature.

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Modeling and Drag Minimization in Compressible Navier-Stokes Flows in Bounded Domains

JAN SOKOLOWSKI
(joint work with Pavel I. Plotnikov, Antoni Zochowski)

In the series of papers [1]-[8] the mathematical theory of shape optimization for compressible Navier-Stokes inhomogeneous boundary value problems is developed. The key part of the theory includes the new results on the existence and shape differentiability of the weak solutions to compressible Navier-Stokes equations. In particular, our results lead to the rigoruous mathematical framework for the drag minimization of an obstacle in the flow of gas with small adiabatic constant.

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. The velocity of the gas coincides with a given vector field $\mathbf{U} \in C^\infty(\mathbb{R}^3)^3$ on the surface Σ. The boundary of the flow domain Ω is divided into the three subsets, inlet $\Sigma_{\rm in}$, outgoing set $\Sigma_{\rm out}$ and the characteristic set Σ_0. The compact $\Gamma = \Sigma_0 \cap \Sigma$ splits the surface Σ into three disjoint parts $\Sigma = \Sigma_{\rm in} \cup \Sigma_{\rm out} \cup \Gamma$. The problem is to find the velocity field $\mathbf{u}$ and the gas density ϱ satisfying the following equations along with the boundary conditions

$$\Delta \mathbf{u} + \lambda \nabla \mathrm{div}\, \mathbf{u} = R\varrho \mathbf{u} \cdot \nabla \mathbf{u} + \frac{R}{\epsilon^2} \nabla p(\varrho) \text{ in } \Omega, \quad \mathrm{div}\,(\varrho \mathbf{u}) = 0 \text{ in } \Omega\,, \tag{1}$$

$$\mathbf{u} = \mathbf{U} \text{ on } \Sigma, \quad \mathbf{u} = 0 \text{ on } \partial S, \quad \varrho = \varrho_0 \text{ on } \Sigma_{\rm in}\,, \tag{2}$$

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

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

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

$$J_D(S) = \mathbf{U}_\infty \cdot \mathbf{J}(S), \tag{3}$$

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 describe briefly the numericals results given in Figures 1-4. The results are only preliminary, since they are obtained with few steps of the simple gradient method, with the shape gradient numerically evaluated according to the formulae given in [7]. Triangulation and computational domain are shown in Fig.1. The flow is from the left. Reynolds number $R = 0.01$, viscosity ratio $\lambda = 100$, the flow velocity is $U_1 = 1, U_2 = 0$ on outer boundary. The coefficient in gas law is $\gamma = 5/3$. The optimized shapes after few iterations are shown. In order to prevent moving the obstacle toward the boundary of the computational region, it is assumed that its gravity centre is fixed at the origin. The total volume of the obstacle is kept constant.

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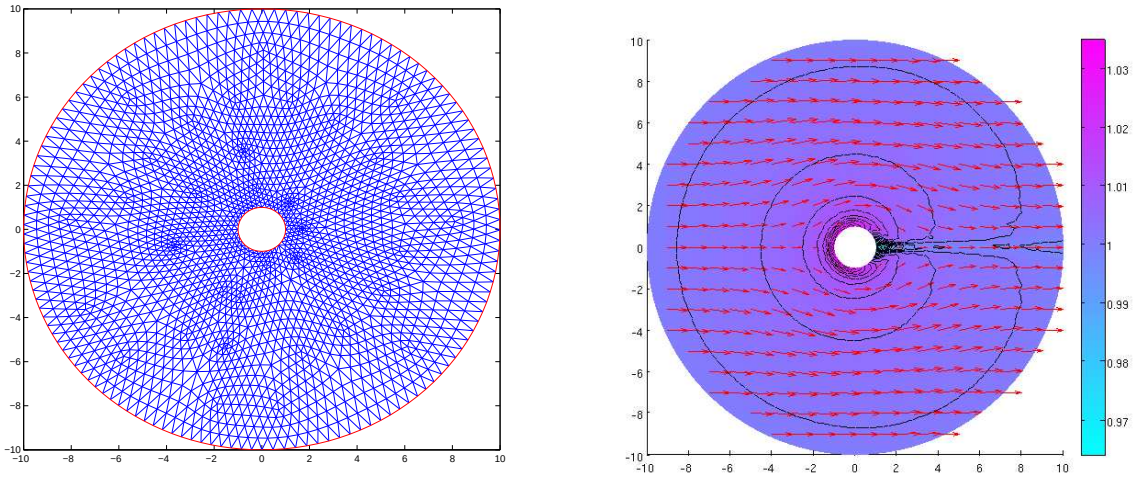

FIGURE 1. Initial computational domain with triangulation. Initial flow $\mathbf{u}$ and pressure p.

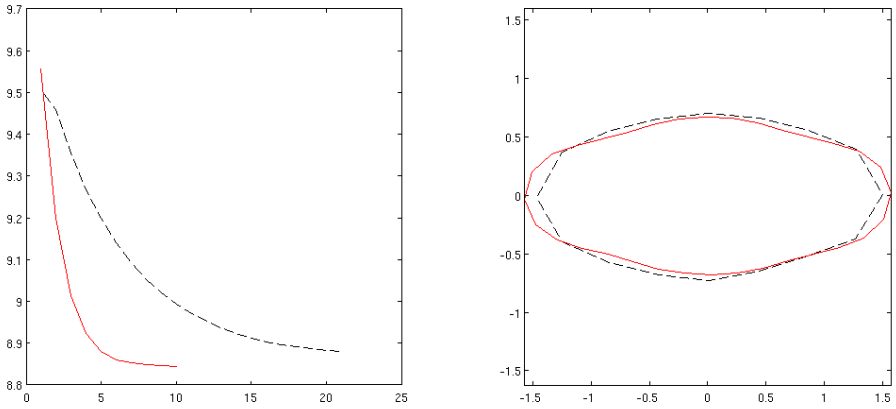

FIGURE 2. Shape of minimal drag for rough (dashed line) and finer discretizations. On the left history of optimization.

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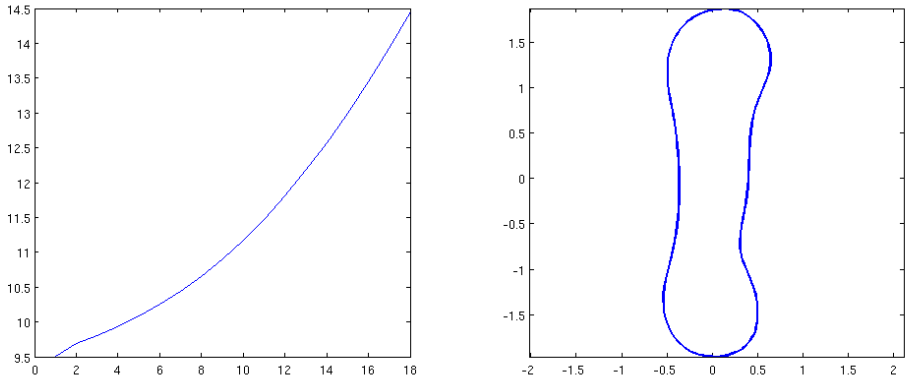

FIGURE 3. Shape after few steps of drag maximization and the history of drag values.

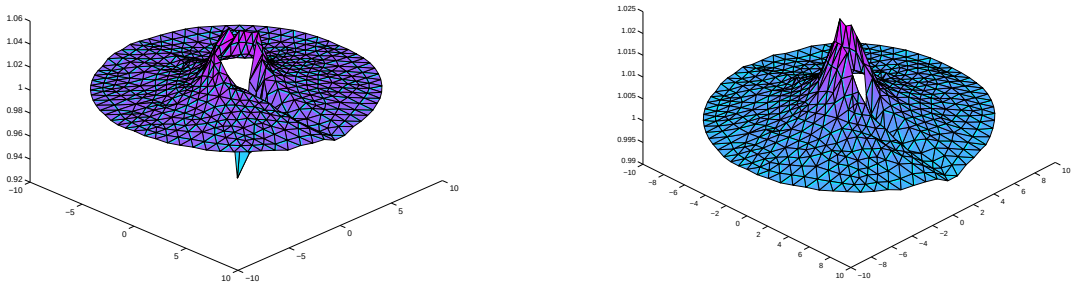

FIGURE 4. Pressure distribution around shapes of maximal (left) and minimal drag. The vertical range on the left is 0.96–1.06 input pressure, on the right 0.99–1.025.

Verification of Bang-bang Properties of Optimal Controls for Parabolic Boundary Control Problems

FREDI TRÖLTZSCH
(joint work with Vili Dhamo)

We discuss the parabolic optimal control problem

$$\min\ J(y,u) := \frac{1}{2}\int_0^1 (y(x,T) - y_d(x))^2\,dx \tag{1}$$

subject to the one-dimensional heat equation

$$
\begin{aligned}
y_t(x,t) &= y_{xx}(x,t)\,, \quad (x,t) \in (0,1)\times(0,T]\,,\\
y_x(0,t) &= 0\,, \qquad\qquad t \in (0,T]\,,\\
y_x(1,t)+\alpha y(1,t) &= \beta u(t)\,, \qquad t \in (0,T]\,,\\
y(x,0) &= 0\,, \qquad\qquad x \in (0,1)\,,
\end{aligned} \tag{2}
$$

and to the pointwise control constraints

$$
|u(t)| \le 1 \qquad \text{for almost all } \ t \ \text{ in } \ [0,T]\,, \tag{3}
$$

where $T > 0$, $\alpha > 0$, and $\beta > 0$ are fixed constants, and $y_d \in L^2(0,1)$ is given. The function $u \in L^\infty(0,T)$ is the unknown boundary control. We consider the cases $\alpha = \beta$ (Robin) or $\alpha = 0$, $\beta = 1$ (Neumann).

By Theorem 2, optimal boundary controls must be of bang-bang type, unless the optimal value $J(\bar y, \bar u)$ is zero. In other words, the optimal control is bang-bang, if the target state y_d is not reachable by admissible controls. Numerically computed optimal values of J are in general positive and it is difficult to decide if this holds also true for the exact value.

Using Theorem 3 together with numerical computations and careful estimations of Fourier series, we are able to verify bang-bang properties of optimal controls for concrete examples.

Let us first recall the known necessary optimality conditions for (1)–(3):

Theorem 1. *An admissible control $\bar u$ and its corresponding state $\bar y$ are optimal for the boundary control problem* (1)–(3)*, if and only if*

$$
\bar u(t) = \begin{cases} -1 & \text{when} \quad p(1,t) > 0 \\ +1 & \text{when} \quad p(1,t) < 0 \end{cases}
$$

holds for a.a. $t \in [0,T]$, where p is the adjoint state, defined as weak solution of the adjoint equation

$$
\begin{aligned}
-p_t(x,t) &= p_{xx}(x,t)\,, \qquad (x,t) \in (0,1)\times(0,T]\,,\\
p_x(0,t) &= 0\,, \qquad\qquad t \in (0,T]\,,\\
p_x(1,t)+\alpha p(1,t) &= 0\,, \qquad t \in (0,T]\,,\\
p(x,T) &= \bar y(x,T) - y_d(x)\,. \qquad x \in [0,1]\,.
\end{aligned}
$$

Therefore, the roots of $p_x(1,t)$ determine the form of $\bar u$. The following bang-bang principle is also well known:

Theorem 2 ([2])**.** *Let $\bar u$ be optimal for* (1)–(3) *and let $\bar y$ be the associated state. Suppose that $\|\bar y(\cdot,T) - y_d\|_{L^2(0,T)} > 0$. Then the function $t \mapsto p(1,t)$ has at most countably many zeros $0 < t_1 < t_2 < \ldots < t_i < \ldots < T$ in $[0,T]$, which can accumulate only at $t = T$. Therefore, either $\bar u(t) = (-1)^i$ or $\bar u(t) = (-1)^{i+1}$ holds a.e. on $[t_i, t_{i+1}]$ for all $i \in \mathbb{N}$.*

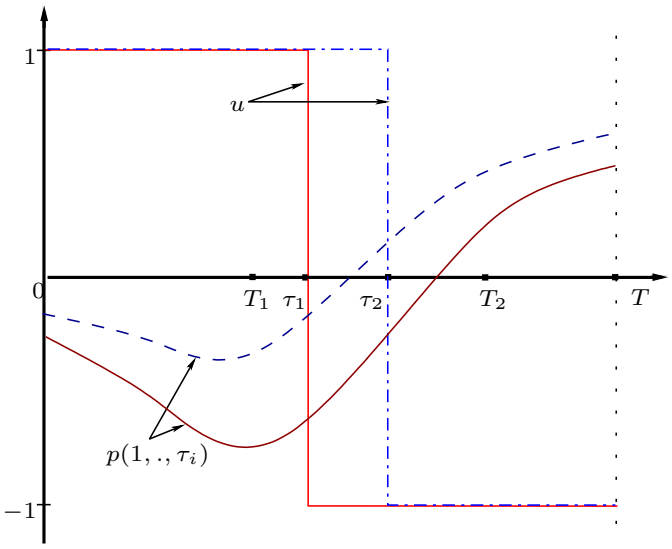

FIGURE 1. Illustration of the main idea

Our main idea is as follows. Assume that numerical optimization indicates an optimal control $\bar{u}$, which is bang-bang with exactly one switching point at an unknown value $\bar{\tau}, 0 < \bar{\tau} < T$. Assume w.l.o.g. that $\bar{u}$ is positive in $[0, \bar{\tau}]$. Then $\bar{u}$ should belong to the class of controls u having the form

$$u(t) = u(t, \tau) := \begin{cases} 1 & \text{for } t < \tau \\ -1 & \text{for } t > \tau\,. \end{cases}$$

Therefore, we try to verify that among those bang-bang controls there is really one that satisfies the optimality conditions.

Let $u_i = u(\cdot, \tau_i)$, $i = 1, 2$, be two controls of this form, with switching points $\tau_1 < \tau_2$. Assume that the associated adjoint state $p(1, \cdot, \tau_1)$ has exactly one zero at $t_1 = t(\tau_1)$ located right of τ_1. Let analogously the adjoint state $p(1, \cdot, \tau_2)$ have a single root $t_2 = t(\tau_2)$ located left of τ_2. The situation is shown in Figure 1. In the application, these relations must be verified by careful estimations. For this purpose, we used Fourier expansions of y and p.

It turns out that the associated root $t(\tau)$ of $p(1, t, \tau)$ defines a strongly monotone decreasing and continuous function of τ on $[\tau_1, \tau_2]$. Increasing the switching point τ will decrease the zero $t(\tau)$ of p. We have $t(\tau_1) - \tau_1 > 0$ and $t(\tau_2) - \tau_2 < 0$ so that the intermediate value theorem ensures the existence of a value $\bar{\tau} \in [\tau_1, \tau_2]$, where $\bar{\tau} = t(\bar{\tau})$. This root of $p(1, \cdot, \bar{\tau})$ coincides with the switching point $\bar{\tau}$. Our idea leads to the following result:

Theorem 3. *Assume the existence of values* $0 \le T_1 \le \tau_1 < \tau_2 \le T_2 \le T$ *with the following properties:* $p(1, \cdot, \cdot)$ *is continuously differentiable on* $D := (T_1, T_2) \times [\tau_1, \tau_2]$, $p(1, \tau_1, \tau_1) < 0$, $p(1, T_2, \tau_1) > 0$, $p(1, T_1, \tau_2) < 0$, $p(1, \tau_2, \tau_2) > 0$, *and* $p(1, t, \tau)$ *is strongly monotone increasing w.r.t.* t *and* τ, *for all* $(t, \tau) \in D$.

Then, for all $\tau \in [\tau_1, \tau_2]$, the function $t \mapsto p(1, t, \tau)$ has a single root $t(\tau)$ between $t(\tau_1)$ and $t(\tau_2)$. There exists a unique fixed point $\bar{\tau}$ of the mapping $\tau \mapsto t(\tau)$ in (τ_1, τ_2).

If we show in addition that the function $t \mapsto p(1, t, \bar{\tau})$ does not have any other root in $(0, T)$ and is negative on $(0, \bar{\tau})$, then $u(\cdot, \bar{\tau})$ satisfies the optimality conditions and is optimal. To check this requires extensive and very precise estimates, which cannot be obtained on using finite element or finite difference methods. We again used Fourier expansions of p. For the details, the reader is referred to [1].

Example 1. We applied our technique for the Neumann problem with $T = 1$ and

$$y_d(x) = \frac{1}{2}(1 - x^2) \, .$$

To verify the assumptions of Theorem 3, we took $\tau_1 = 0.66$, $\tau_2 = 0.6665$, $T_1 = 0$, $T_2 = T$. In this way, we were able to prove that the optimal control is bang-bang with exactly one switching point $\bar{\tau} \in (0.66, 0.6665)$. Numerically we found $\bar{\tau}$ at 0.66639. Moreover, we verified that the optimal value of J is positive so that y_d is not reachable under our restrictions.

Example 2. For the Robin problem with $T = 1.58$, $\alpha = 1$ and the same y_d as in Example 1, we proved that the optimal control is bang-bang with exactly one switching point $\bar{\tau} \in (1.329, 1.3294)$. To this end, we used $\tau_1 = 1.329$, $\tau_2 = 1.3294$, $T_1 = 1.2$ and $T_2 = 1.42$. Also here, y_d cannot be reached, as we showed by further estimates. This example was introduced by Schittkowski [3] and it was open since that time, if the optimal control is bang-bang or not. It was even not known, if the number of switching points is finite.

While these results concern the case of single switching points, an application of a theorem by Miranda permits to discuss also problems with more switching points, we refer to [1].

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A New Mesh-Independence Result for Semismooth Newton Methods

Michael Ulbrich

We investigate the mesh-independence properties of semismooth Newton methods for bound-constrained variational inequalities of the form

$$u \in L^2(\Omega), \ \alpha \le u \le \beta, \quad (V(u), \hat{u} - u)_{L^2(\Omega)} \ge 0 \quad \forall \ \hat{u} \in L^2(\Omega), \ \alpha \le \hat{u} \le \beta \, .$$

Here, $-\infty \leq \alpha < \beta \leq +\infty$ are constant (for simplicity) bounds, $\Omega \subset \mathbb{R}^n$ is a measurable set with $0 < \mathrm{meas}(\Omega) < \infty$, and $V : L^2(\Omega) \to L^2(\Omega)$ is a continuously Fréchet differentiable operator. It is a well-known approach to reformulate the variational inequality as a nonsmooth equation of the form

$$F(u) := u - P_{[\alpha,\beta]}(u - \sigma V(u)) = 0$$

by using the pointwise projection $P_{[\alpha,\beta]}(t) = \min(\max(\alpha, t), \beta)$ and to apply semismooth Newton methods to it. Under the frequently encountered structural assumption that $V(u) = \lambda u + A(u)$, where $\lambda > 0$ and $A : L^2(\Omega) \to L^p(\Omega)$, $p \in (2, \infty]$, is a locally Lipschitz continuous operator that is continuously Fréchet differentiable from $L^2(\Omega)$ to $L^2(\Omega)$, it is known [3, 5] that for the choice $\sigma = 1/\lambda$ the operator $F : L^2(\Omega) \to L^2(\Omega)$,

$$F(u) = u - P_{[\alpha,\beta]}(u - \sigma V(u)) = u - P_{[\alpha,\beta]}(-(1/\lambda)A(u))$$

is semismooth. For convenience, we focus on the unilateral case $\alpha = 0$, $\beta = \infty$, i.e., $F(u) = u - \max(0, -(1/\lambda)A(u))$. In this case, the variational inequality is equivalent to the complementarity problem

$$u \geq 0, \quad V(u) \geq 0, \quad uV(u) = 0 \quad \text{in } \Omega\,.$$

We start by examining the order of semismoothness of the operator F in detail, which under a regularity condition on the generalized derivatives determines the order of local q-superlinear convergence of the semismooth Newton's method. Here, defining the residual

$$R_F(u, d) := F(u + d) - F(u) - M_F(u + d)d\,,$$

with $M_F(u + d) \in \partial F(u + d)$ denoting an element of the (suitably defined, see [3, 5]) generalized differential of F, F is semismooth of order $\alpha > 0$ at u if $\|R_F(u, d)\|_{L^2} = O(\|d\|_{L^2}^{1+\alpha})$ for $\|d\|_{L^2} \to 0$. It was already observed in [4] that the size of $R_F(u, d)$ compared to d is not stable with respect to perturbations of u and d. This makes mesh-independence proofs different to the smooth case, where, e.g., local Lipschitz continuity of the Fréchet derivative of the underlying operator is a typical assumption [1], which is not transferable to the semismooth case in general.

If the operator A is sufficiently well-behaved (e.g., if A' is locally Lipschitz continuous), the order of semismoothness of the nonsmooth reformulation turns out to be dominated by the order of semismoothness of the superposition operator $G : L^p(\Omega) \to L^2(\Omega)$, $G(z) = \max(0, z)$. We show that the order of semismoothness of this operator at $\bar{z} \in L^p(\Omega)$ is given by $\frac{\gamma(p-2)}{2(p+\gamma)}$, where $\gamma > 0$ quantifies the growth rate of the measure of the set where $|\bar{z}|$ is small:

$$\mathrm{meas}(\{x \in \Omega\,;\, 0 < |\bar{z}(x)| < t\}) \leq Ct^\gamma \quad \forall\ 0 < t \leq t_0 \tag{1}$$

with constants $C > 0$ and $t_0 > 0$. If $\bar{u}$ solves $F(\bar{u}) = 0$ and if $\bar{z} = -(1/\lambda)A(\bar{u})$, then it is not difficult to see that $|\bar{z}(x)| > 0$ is equivalent to $|\bar{u}(x)| + |V(\bar{u})(x)| > 0$ and thus $|\bar{z}|$ can be interpreted as a measure of strict complementarity.

We now consider the reformulated complementarity problem $F(u) = 0$ and corresponding discretizations $F_h(u_h) = 0$ with

$$F_h(u_h) := u_h - \max(0, -(1/\lambda)A_h(u_h)) = u_h - G(-(1/\lambda)A_h(u_h))$$

of the discrete complementarity problems

$$u_h \geq 0, \quad V_h(u_h) \geq 0, \quad u_h V_h(u_h) = 0 \quad \text{in } \Omega\,.$$

Here, $h > 0$ measures the accuracy of the discretization, $u_h \in U_h \subset L^2(\Omega)$ is a suitable discrete approximation of u (e.g., by piecewise constant finite elements as it is often used for control discretizations), and $V_h(u_h) = \lambda u_h + A_h(u_h)$, where $A_h : U_h \to U_h$ is a suitable discrete approximation of A. The aim is to derive mesh-independence results for the semismooth Newton iteration for $F(u) = 0$ in a neighborhood of the solution $\bar{u}$ and for the corresponding discrete semismooth Newton iterations for $F_h(u_h) = 0$ in neighborhoods of the discrete solutions $\bar{u}_h$, $0 < h \leq h_0$. For compact notation, we let $h = 0$ correspond to the original problem, i.e., $A_0 = A$, $F_0 = F$, $\bar{u}_0 = \bar{u}$, etc.

The first mesh-independence result for this setting was presented by M. Hintermüller and the author [4]. They proved under suitable assumptions on the solution $\bar{u}$, the problem data, and the discretization that for every given q-linear rate $0 < \eta < 1$ there exist $\delta > 0$ and $h_1 \leq h_0$ such that the semismooth Newton methods started at initial points u_h^0 lying in δ-neighborhoods $B_\delta(\bar{u}_h)$, $0 \leq h \leq h_1$, generate sequences (u_h^k) that converge at least q-linearly with rate η to $\bar{u}_h$, $0 \leq h \leq h_1$.

The contribution of the present work is to extend this mesh-independence result to a mesh-independent order of q-superlinear convergence. Under suitable assumptions, our above investigations of the order of semismoothness of G show that the q-superlinear orders of convergence of the semismooth Newton processes are determined by the orders of semismoothness of G at $\bar{z}_h = -(1/\lambda)A_h(\bar{u}_h)$, $0 \leq h \leq h_0$. From this, we can derive the following first version of a mesh-independent order of convergence result:

If there exist $\gamma > 0$, $C > 0$, $t_0 > 0$, and $h_1 \leq h_0$ such that (1) is satisfied for all $\bar{z}_h = -(1/\lambda)A_h(\bar{u}_h)$, $0 \leq h \leq h_1$, then there exists $\delta > 0$ such that for all initial points $u_h^0 \in B_\delta(\bar{u}_h)$, $0 \leq h \leq h_1$, the semismooth Newton iterates (u_h^k) converge q-superlinearly to $\bar{u}_h$, $0 \leq h \leq h_1$, with order $1 + \frac{\gamma(p-2)}{2(p+\gamma)}$.

Next, we investigate if the growth condition on the continuous and all discrete solutions can be replaced by a condition on the continuous solution alone. An example, however, shows that the order of semismoothness of G at $\bar{z}$ is *not* stable with respect to perturbations, even if strict complementarity holds at $\bar{z}$ in the sense that $\mathrm{meas}(\{x \in \Omega\,;\, \bar{z}(x) = 0\}) = 0$.

An escape from this difficulty is provided by the observation that, for the constructed example, the orders of $\|R_G(\bar{z}, s)\|_{L^2}$ and of $\|R_G(\bar{z}_h, s)\|_{L^2}$ in terms of $\|s\|_{L^p}$ differ significantly only if $\|s\|_{L^p}$ is much smaller than the discretization error $\|\bar{z}_h - \bar{z}\|_{L^p}$. Motivated by this observation we are able to prove that, under a growth condition (1) only for $\bar{z}$, strict complementarity of $\bar{z}$, and further suitable

assumptions, there holds

$$\|R_G(\bar{z}_h, s)\|_{L^2} \le C_1 \max(\|\bar{z}_h - \bar{z}\|_{L^p}, \|s\|_{L^p})^{\frac{\gamma(p-2)}{2(p+\gamma)}} \|s\|_{L^p} \quad \forall\, 0 \le h \le h_1,\ \|s\|_{L^p} \le \varepsilon$$

with appropriate constants $C_1 > 0$, $h_1 \le h_0$, and $\varepsilon > 0$. From this, we can derive that under appropriate assumptions, there exist $h_1 \le h_0$, $\delta > 0$, and $C_2 > 0$ (depending, in particular, on λ), such that for all initial points $u_h^0 \in B_\delta(\bar{u}_h)$, $0 \le h \le h_1$, the semismooth Newton iterates (u_h^k), satisfy

$$\|u_h^{k+1} - \bar{u}_h\|_{L^2} \le C_2 \max(\|A_h(\bar{u}_h) - A(\bar{u})\|_{L^p}, \|u_h^k - \bar{u}_h\|_{L^2})^{\frac{\gamma(p-2)}{2(p+\gamma)}} \|u_h^k - \bar{u}_h\|_{L^2}$$

for all $k \ge 0$, $0 \le h \le h_1$. This shows that the full order of convergence is achieved as long as there exists $c > 0$ with $\|u_h^k - \bar{u}_h\|_{L^2} \ge c\|A_h(\bar{u}_h) - A(\bar{u})\|_{L^p}$. If this condition is not satisfied for reasonably sized c, it is preferable to try to detect this situation by appropriate error estimators and to adapt the discretization instead of performing a further Newton step on the current discretization level.

Using results from [2, 4], we can verify our assumptions for a class of semilinear elliptic optimal control problems. Numerical tests are presented that support the theoretical results. A preprint containing the full details of the presented mesh-independence results is in preparation.

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Convergence of Linearised and Adjoint Approximations for Discontinuous Solutions of Conservation Laws

Stefan Ulbrich

(joint work with Michael B. Giles)

In this talk, which is based on [3], we analyse the convergence of discrete approximations to the linearised and adjoint equations arising from optimal control problems governed by an unsteady one-dimensional hyperbolic equation with a convex flux function. As control the initial data are considered. A simple modified Lax-Friedrichs discretisation is used on a uniform grid, and a key point is that the numerical smoothing increases the number of points across the nonlinear discontinuity as the grid is refined. It is proved that this gives convergence

in the discrete approximation of linearised output functionals, and pointwise convergence almost everywhere for the solution of the adjoint discrete equations. In particular, the adjoint approximation converges to the correct uniform value in the region in which characteristics propagate into the discontinuity. As a consequence, the discrete reduced gradient converges to the correct gradient of the continuous problem.

More precisely, we consider objective functionals

$$J(u) = \int_{\mathbb{R}} \gamma(x) G(u(x,T))\,\mathrm{d}x$$

where $u = u(u_0)$ is the entropy weak solution of the conservation law

$$N(u) \equiv u_t + f(u)_x = 0\,, \quad \text{on } \Omega_T := \mathbb{R} \times (0,T)\,,$$
$$u(\cdot,0) = u_0\,, \quad \text{on } \mathbb{R}\,.$$

We assume that $\gamma \in C_c^\infty(\mathbb{R})$, $G \in C^\infty(\mathbb{R})$ and that the flux function $f \in C^\infty(\mathbb{R})$ is convex. Consider the case that (which will be generalised below)

(A1) apart from a discontinuity at $x_s(0)$, $u_0(x)$ is C^∞ with all derivatives in L^1,
(A2) the discontinuity has finite strength for the entire time interval $[0,T]$ and no other discontinuity is formed during this time interval.

Let $\widetilde{u}_0 \in C_c^\infty(\mathbb{R})$ be a perturbation of u_0. The corresponding linear perturbation $\widetilde{J}$ of J is [2,6]

$$\widetilde{J} \;=\; \int_{\mathbb{R}\setminus\{x_s(T)\}} \gamma(x)\; G'(u(x,T))\; \widetilde{u}(x,T)\,\mathrm{d}x \;-\; \widetilde{x}_s(T)\,\gamma(x_s(T))\;[G(u)]_T\,,$$

where $[G(u)]_T$ is the jump in $G(u(x,T))$ across the shock, $\widetilde{x}_s(T)$ is the linear perturbation of the shock position and $\widetilde{u}$ is outside of the shock governed by the linear PDE

$$L(u)\,\widetilde{u} \equiv \widetilde{u}_t + (f'(u)\widetilde{u})_x = 0\,, \quad \widetilde{u}(\cdot,0) = \widetilde{u}_0\,. \tag{1}$$

With the appropriate definiton of $\widetilde{u}$ as duality solution of (1) in the sense of [1,4,5], which is a measure, since it develops a Dirac measure along the shock, one obtains the representation

$$\widetilde{J} \;=\; \int_{\mathbb{R}} w_T(x)\;\widetilde{u}(\mathrm{d}x,T)$$

where

$$w_T(x) = \begin{cases} \gamma(x)G'(u(x,T)), & x \neq x_s(T)\,, \\ \gamma(x_s(T))[G(u)]_T/[u]_T, & x = x_s(T)\,. \end{cases}$$

It can be shown that the adjoint representation of $\widetilde{J}$ is [2,6,7]

$$\widetilde{J} \;=\; \int_{\mathbb{R}} w(x,0)\,\widetilde{u}_0(x)\,\mathrm{d}x\,,$$

where w is the reversible solution of the adjoint equation

$$w_t + f'(u)w_x = 0\,, \quad w(\cdot,T) = w_T$$

with w_T as above. Here, the reversible solution is defined along generalised backward characteristics and satisfies automatically the interior boundary condition $w(x_s(t),t) = \gamma(x_s(T))[G(u)]_T/[u]_T$, see [7].

The aim of this talk is to show the convergence of discretised approximations $\widetilde{J}_h$ for the linearised objective function and w_h of the adjoint state, if a numerical scheme with sufficiently large viscosity together with its discrete linearised and adjoint scheme is used. More precisely, we consider a modified Lax-Friedrichs scheme

$$\begin{aligned} &U_j^{n+1} - U_j^n + \tfrac{1}{2}\, r\, \big(f(U_{j+1}^n) - f(U_{j-1}^n)\big) - \varepsilon\, d\, \big(U_{j+1}^n - 2U_j^n + U_{j-1}^n\big) = 0\,, \\ &U_j^0 = u_0(x_j)\,, \end{aligned}$$

with timestep k, meshsize h in space, and

$$k = \frac{T}{N}\,, \quad r \equiv \frac{k}{h}\,, \quad d \equiv \frac{k}{h^2}\,, \quad \varepsilon = h^\alpha\,, \quad \varepsilon\,\frac{k}{h^2} = c$$

for some fixed constants $2/3 < \alpha < 1$, $0 < c < 1/2$. Hence, the scheme has numerical viscosity $O(\varepsilon) = O(h^\alpha)$, which is essential to approximate the influence of the shock sensitivity $\widetilde{x}_s(T)$ on $\widetilde{J}$ correctly.

The objective functional is approximated by

$$J_h \equiv h \sum_j \gamma(x_j) G(U_j^N)\,.$$

Then the linearised objective functional reads

$$\widetilde{J}_h = h \sum_j \gamma(x_j) G'(U_j^N) \widetilde{U}_j^N\,,$$

where $\widetilde{U}_j^n$ is given by the linearised scheme

$$\begin{aligned} &\widetilde{U}_j^{n+1} - \widetilde{U}_j^n + \tfrac{1}{2} r \left(f'(U_{j+1}^n)\, \widetilde{U}_{j+1}^n - f'(U_{j-1}^n)\, \widetilde{U}_{j-1}^n\right) - \varepsilon\, d\, \left(\widetilde{U}_{j+1}^n - 2\widetilde{U}_j^n + \widetilde{U}_{j-1}^n\right) = 0 \\ &\widetilde{U}_j^0 = \widetilde{u}_0(x_j)\,. \end{aligned}$$

The adjoint representation has the form

$$\widetilde{J}_h = h \sum_j W_j^0\, \widetilde{U}_j^0\,,$$

where W_j^n is given by the discrete adjoint scheme

$$\begin{aligned} W_j^{n-1} &= W_j^n + \tfrac{1}{2}\, r\, f'(U_j^{n-1}) \left(W_{j+1}^n - W_{j-1}^n\right) + \varepsilon\, d\, \left(W_{j+1}^n - 2W_j^n + W_{j-1}^n\right), \\ W_j^N &= \gamma(x_j)\; G'(U_j^N)\,. \end{aligned}$$

To show the convergence of $\widetilde{J}_h$ and w_h as $h \to 0$ we use the technique of matched inner (i.e. close to the shock) and outer asymptotic expansions to construct approximations to both U_j^n and $\widetilde{U}_j^n$. Discrete stability estimates are used to bound the errors in the asymptotic approximations.

Assume that assumptions (A1), (A2) hold. Then we show the following by using the structure of the constructed approximations and the error estimates.

(1) For smooth initial perturbations $\widetilde{u}_0$ and corresponding approximations $\widetilde{U}_j^0 = \widetilde{u}_0(x_j)$ one has $|\widetilde{J} - \widetilde{J}_h| = O(h^\alpha)$.
(2) For Dirac initial perturbations $\widetilde{u}_0$ with support apart from the extreme characteristics confining the shock region, the error is $|\widetilde{J} - \widetilde{J}_h| = O(h^\alpha)$.
(3) Outside of the extreme backward characteristics the error in the discrete adjoint is $|w(0,x) - w_h(0,x)| = O(h^\alpha)$. The discrete adjoint within the shock region (more precisely, within any subdomain bounded away from its two bounding characteristics) is constant to within $o(h^q)$, for any $q > 0$.

The results can be extended to the essentially more general case, where (A1), (A2) are replaced by the requirement on u_0 that no new shocks form at time T, pre-existing shocks have a smooth behaviour in an open neighbourhood of T, and between the shocks the solution $u(x,T)$ is smooth. Numerical results are presented that confirm the obtained convergence results and that show the necessity of a numerical viscosity $O(h^\alpha)$, $2/3 < \alpha < 1$. For details we refer to [3].

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A Priori Error Estimates for Finite Element Discretization of State Constrained Optimal Control Problems Governed by Parabolic Equations

Boris Vexler

(joint work with Dominik Meidner, Rolf Rannacher)

In this talk we present an a priori error analysis for finite element discretization of an optimal control problem, which is governed by a linear parabolic equation and is subject to state constraints. The problem under consideration is formulated as follows:

$$(1)\quad \text{Minimize}\quad J(q,u) = \frac{1}{2}\int_0^T \int_\Omega (u(t,x) - \hat{u}(t,x))^2\, dx\, dt + \frac{\alpha}{2}\int_0^T \int_\Omega q(t,x)^2\, dx\, dt$$

for the control $q \in Q = L^2(0,T;L^2(\Omega))$ and the state $u \in W(0,T)$ subject to

$$\begin{aligned} u_t - \Delta u &= q && \text{in } (0,T)\times\Omega\,, \\ u &= 0 && \text{on } (0,T)\times\partial\Omega\,, \\ u &= u_0 && \text{in } \{0\}\times\Omega\,, \end{aligned} \tag{2}$$

with control constraints

$$q_a \le q(t,x) \le q_b \quad \text{a.e. in } (0,T)\times\Omega \tag{3}$$

and state constraints

$$(Gu)(t) \le b \ \text{ in } \ [0,T]\,, \tag{4}$$

where $G\colon L^2(\Omega)\to\mathbb{R},\ G(v)=\int_\Omega v\,\omega\,dx$ and $\omega\in L^2(\Omega)$. The last inequality is a state constraint, which is formulated pointwise in time, see, e. g., [3] for an analysis of optimal control problems with this type of state constraints.

The main difficulty in the analysis of optimal control problems with state constraints is the lack of regularity caused by the fact that the Lagrange multiplier corresponding to state constraint (4) is a Borel measure $\mu \in C([0,T])^*$. The optimality system for the problem under consideration consists of the state equation (2), an adjoint equation, a variational inequality, and complementarity conditions. The adjoint state z lies in the space $L^2(0,T;H_0^1(\Omega))$ and is in general discontinuous in time. From the regularity of the adjoint solution, one can deduce a regularity result for the optimal control $\bar q \in L^2(0,T;H^1(\Omega))\cap L^\infty((0,T)\times\Omega)$. The lack of temporal regularity is one of the challenges in deriving a priori error estimates for finite element discretization of this problem.

For the numerical solution of this optimal control problem we consider the discretization of the state equation (2) in time using the discontinuous Galerkin methods dG(0) and in space using usual conforming linear finite elements. The control variable q is discretized by cellwise constant functions in space and time. We refer to [6,7] for an error analysis of this type of discretization for unconstrained optimal control problems and for problems with control constraints.

We denote by k the maximal step size in the temporal discretization and by h the maximal cell size of the spatial mesh. For the optimal solution $\bar q_\sigma$ of the discrete optimal control problem we prove the following error estimate:

Theorem 4 (see [5]). *Let $\Omega\subset\mathbb{R}^d$ $(d=2,3)$ be a convex polygonal domain, $\hat u\in L^2(0,T;L^2(\Omega))$, $u_0\in H^2(\Omega)\cap H_0^1(\Omega)$ and $\alpha>0$. Then there holds*

$$\|\bar q-\bar q_\sigma\|_{L^2(0,T;L^2(\Omega))} \le \frac{C}{\sqrt{\alpha}}\,|\log k|^{\frac14}(k^{\frac12}+h)\,,$$

where the constant C depends on u_0, $\hat u$, Ω and T.

To our knowledge, this is the first error estimate for the discretization of a state constrained optimal control problem governed by a parabolic PDE. In the talk of M. Hinze at this Oberwolfach workshop, he presented error estimates for the optimal control problem in a different setting. Error estimates for state constrained elliptic problems can be found for example in [1, 8].

The proof of Theorem 4 is divided in two steps. In the first step we discretize the state equation in time and provide estimates for the error between optimal control $\bar{q}$ and the optimal solution $\bar{q}_k$ of the semi-discrete problem. Due to the fact that the control variable stays undiscretized in this step, the temporal regularity of $\bar{q}$ is not required. From the optimality system of the semi-discrete problem one can deduce that the optimal solution $\bar{q}_k$ is piece-wise constant in time. In the second step the state variable and the control variable are discretized in space and one proves an error estimate for $\bar{q}_k - \bar{q}_\sigma$. The essential tools for our proof are error estimates with respect to the $L^\infty(0,T;L^2(\Omega))$-norm for the state equation. Denoting by $u(q)$ the solution of the state equation (2) for a fixed control $q \in L^\infty(0,T;L^2(\Omega))$, by $u_k(q)$ the corresponding solution of the semi-discretized equation and $u_{kh}(q)$ the solution of the discretized state equation, we provide the following estimates:

$$\|u(q) - u_k(q)\|_{L^\infty(0,T;L^2(\Omega))} \le c|\log k|^{\frac{1}{2}}\, k \left(\|u_0\|_{H^2(\Omega)} + \|q\|_{L^\infty(0,T;L^2(\Omega))}\right)$$

and

$$\|u_k(q) - u_{kh}(q)\|_{L^\infty(0,T;L^2(\Omega))} \le c|\log k|^{\frac{1}{2}}\, h^2 \left(\|u_0\|_{H^2(\Omega)} + \|q\|_{L^\infty(0,T;L^2(\Omega))}\right).$$

The derivation of these estimates is based on techniques from [2, 4, 9].

As a byproduct of our error estimate in Theorem 4, we derive a new regularity result for the optimal control,

$$\bar{q} \in H^s(0,T;L^2(\Omega)) \quad \text{for all } \ 0 \le s < \frac{1}{2}\,,$$

see [5] for details.

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On Goal-Oriented Error Estimation for Optimal Control Problems

Martin Weiser

Goal-oriented error estimation and mesh refinement for optimal control problems with PDE constraints has been proposed by Becker, Kapp, and Rannacher [1]. Quite naturally, the quantity of interest in optimization problems is the value of the cost function to be minimized, whereas the distance of the approximate solution to the exact one measured in some general norm is of less importance. This is different from parameter identification problems written as optimization problems, where the natural quantity of interest is the value of the parameter to be identified [7] or the data mismatch in case a regularization parameter needs to be determined from a discrepancy principle [3].

For simplicity of presentation we consider linear problems of the form

$$\min_{y\in Y,u\in U} J(y,u) = \langle y, \frac{1}{2}H_{yy}y - b_y\rangle + \langle u, \frac{1}{2}H_{uu}u - b_u\rangle \tag{1}$$

subject to the equality constraint

$$Ay + Bu - b_\lambda = 0\ . \tag{2}$$

Here, Y and U are Banach spaces, $H_{yy} : Y \to Y^*$ and $H_{uu} : U \to U^*$ are symmetric and positive semidefinite, and $A : Y \to Y^*$ has a bounded inverse. $B : U \to Y^*$ is merely continuous, and clearly $b_y, b_\lambda \in Y^*$ and $b_u \in U^*$ hold. In this setting, the state is determined by a given control as $y(u) = A^{-1}(b_\lambda - Bu)$.

For any approximate solution (y^h, u^h), the quantity of interest proposed in [1] and subsequently used throughout the literature (see the survey [6] and recent work on inequality constrained problems [2, 4, 5, 8]) is the *all-at-once error*

$$E(y^h, u^h) = J(y^h, u^h) - J_{\text{opt}}\ .$$

However, if the aim of optimization is to compute a control that is to be applied in a physical system, the discretized state y^h is of little interest. All that matters is the control u^h and the resulting state $y(u^h)$ of the physical system (here we neglect modelling erros, which are a completely different topic). In this setting, the relevant quantity of interest is the *black-box error*

$$\tilde{E}(u^h) = J(y(u^h), u^h) - J_{\text{opt}}\ .$$

Even though the formal difference is small, since both concepts capture the error in the cost functional, the quantitative difference and the impact on mesh refinement can be significant.

Error representation. We introduce the reduced cost function $\tilde{J}(u) = J(y(u), u)$ and the reduced Hessian $\tilde{H} = \tilde{J}'' = B^*A^{-*}H_{yy}A^{-1}B + H_{uu}$, which we assume is positive definite such that (1) has a unique minimizer $(\bar{y}, \bar{u})$. Due to $\tilde{J}'(\bar{u}) = 0$ we have $\tilde{E}(u^h) = \frac{1}{2}\langle \delta u, \tilde{H}\delta u\rangle$ for $\delta u = \bar{u} - u^h$.

We assume that (1) is solved numerically by a Galerkin discretization of the KKT system. Elementary calculation reveals the error representation in terms of

the residuals r_y, r_u, and r_λ of the adjoint equation, optimality equation, and state equation, respectively:

$$\tilde{E}(u^h) = \frac{1}{2}\left(\langle w_y, r_y\rangle + \langle w_u, r_u\rangle + \langle w_\lambda, r_\lambda\rangle\right)$$

with the weight functions $\tilde{w}_y = -A^{-1}B\delta u$, $\tilde{w}_u = \delta u$, and $\tilde{w}_\lambda = -A^{-*}H_{yy}\tilde{w}_y$.

Hierarchical error estimation. The Galerkin approximation $x^h = (y^h, u^h, \lambda^h) \in X^h \subset Y \times U \times Y$ satisfies $H^{hh}x^h = b^h$, where H^{hh} is the Galerkin representation of the Hessian of the Lagrangian $L = J(y,u) + \langle \lambda, Ay + Bu - b_\lambda\rangle$. The remaining residual $r = b - Hx^h$ is then polar to X^h. For approximating δu and computing the weight functions $\tilde{w}$ we extend the Galerkin ansatz space X^h with an extension space $X^e \subset Y \times U \times Y$ such that $X^h \cap X^e = \{0\}$. On the extended ansatz space, the error $\delta x = \bar{x} - x^h$ can be approximated by solving

$$\begin{bmatrix} H^{hh} & H^{eh} \\ H^{he} & H^{ee} \end{bmatrix} \begin{bmatrix} \delta x^h \\ \delta x^e \end{bmatrix} = \begin{bmatrix} 0 \\ r^e \end{bmatrix}. \tag{3}$$

As is usual in hierarchic error estimators, only local defect problems are solved by dropping all off-diagonal entries in the blocks of H^{ee}. Moreover, H^{he} is neglected in (3), such that δx^h and δx^e can be computed sequentially. It is important not to drop H^{eh}, because otherwise $\delta x^h = 0$ results and since only local defect problems are solved in X^e, the pollution error would be neglected. The same considerations lead to the computation of the weight functions as

$$\begin{bmatrix} A^{hh} & \\ A^{he} & \hat{A}^{ee} \end{bmatrix} \begin{bmatrix} \tilde{w}_y^h \\ \tilde{w}_y^e \end{bmatrix} = \begin{bmatrix} B^{hh} & B^{eh} \\ B^{he} & B^{ee} \end{bmatrix} \begin{bmatrix} \delta u^h \\ \delta u^e \end{bmatrix}$$

and

$$\begin{bmatrix} A^{hh} & A^{eh} \\ & \hat{A}^{ee} \end{bmatrix}^* \begin{bmatrix} \delta w_\lambda^h \\ \delta w_\lambda^e \end{bmatrix} = \begin{bmatrix} H_{yy}^{hh} & H_{yy}^{eh} \\ H_{yy}^{he} & H_{yy}^{ee} \end{bmatrix} \begin{bmatrix} \tilde{w}_y^h \\ \tilde{w}_y^e \end{bmatrix}.$$

Finally, the error estimate can be computed as

$$\tilde{E}(u^h) \approx \frac{1}{2}\left(\langle w_y^e, r_y^e\rangle + \langle w_u^e, r_u^e\rangle + \langle w_\lambda^e, r_\lambda^e\rangle\right).$$

Illustrative example. The following example with scalar control is tailored to highlight the differences between all-at-once error and black-box error:

$$\min_{y\in H^1(\Omega), u\in\mathbb{R}} \frac{1}{2}\|y-1\|^2_{L^2(\Omega)} \quad \text{s.t.} \quad \begin{aligned} -\Delta y &= 3 + \chi_{\Omega_c} u && \text{in } \Omega\,, \\ y &= 0 && \text{on } \partial\Omega\,, \\ \partial_n y &= 0 && \text{on } \partial\Omega_N\,. \end{aligned}$$

The control acts on a subset Ω_c of the domain Ω that is separated from the corner singularity by the narrow neck of the domain. Linear finite elements with quadratic bubbles for error estimation have been used. Figure 1 shows adaptively refined meshes for both error concepts as well as the actual and estimated error values. The black-box error is smaller than the all-at-once error by orders of mag-

nitude, which makes an important difference in case a desired accuracy is used as termination criterion. Moreover we observe that the generated meshes are quite different. The result is that the actually computed value of the cost functional is worse by a factor of up to 100 when using the black-box error for mesh refinement, but the value of the reduced cost functional is indeed better by a factor of up to 4.

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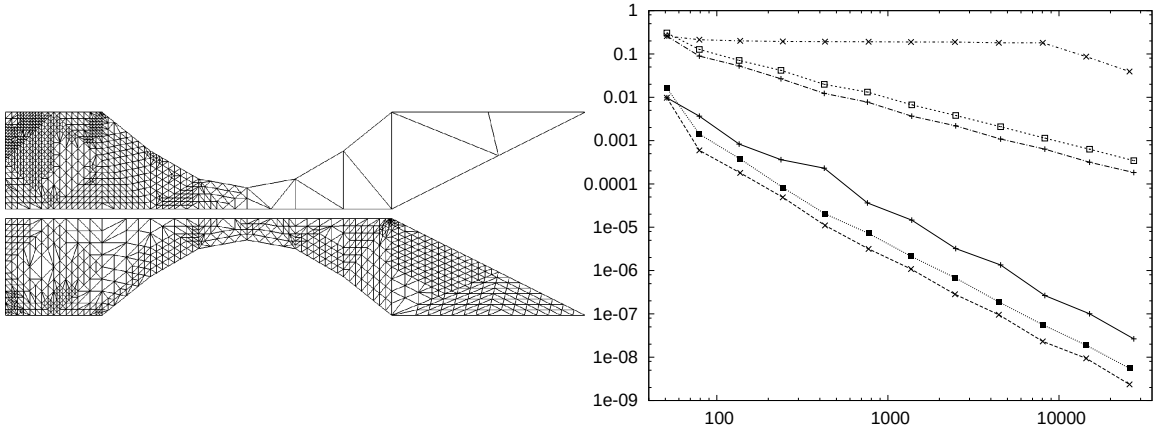

FIGURE 1. Left: Meshes obtained by refining six times towards $\tilde{J}(u^h)$ (top, 1365 dofs) and $J(y^h, u^h)$ (bottom, 1417 dofs). Right: Error versus total number of degrees of freedom. Top lines: errors $E(y^h, u^h)$ for both refinement strategies and estimated error E ($\square$) for ($+$). Bottom lines: errors $\tilde{E}(u^h)$ for both refinement strategies and estimator $\tilde{E}^h$ ($\blacksquare$) for ($\times$). Refinement according to E is shown as $+$, according to $\tilde{E}$ as $\times$.

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Modelling of Signal Processing in Neurons

Gabriel Wittum

The crucial feature of neuronal ensembles is their high complexity and variability. This makes modelling and computation very difficult, in particular for detailed models based on first principles. The problem starts with modelling geometry, which has to extract the essential features from those highly complex and variable phenotypes and at the same time has to take in to account the stochastic variability. Moreover, models of the highly complex processes which are living on these geometries are far from being well established, since those are highly complex, too, and couple on a hierarchy of scales in space and time. Simulating such systems always puts the whole approach to test, including modeling, numerical methods and software implementations. In combination with validation based on experimental data, all components have to be enhanced to reach a reliable solving strategy.

To handle problems of this complexity, new mathematical methods and software tools are required. In recent years, new approaches such as parallel adaptive multigrid methods and corresponding software tools have been developed allowing to treat problems of huge complexity.

In the lecture we present a three dimensional model of signaling in neurons. First we show a method for the reconstruction of the geomety of cells and subcellular structures as three dimensional objects. With this tool, NeuRA, complex geometries of neuron nuclei were reconstructed. We present the results and discuss reasons for the complicated shapes. To that end, we present a model of calcium signaling to the nucleus and show simulation results on reconstructed nuclear geometries. We discuss the implications of these simulations.

We further show reconstructed cell geometries and simulations with a three dimensional active model of signal transduction in the cell which is derived from the Maxwell equations and uses generalized Hodgkin-Huxley fluxes for the description of the ion channels.

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