MS2: Optimal Control in Applications

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ABSTRACT

Optimization problems subject to constraints given by partial differential equations (PDEs) with additional constraints on the control and/or state variables belong to the most challenging problem classes in natural sciences, engineering, and economics. Due to the complexities of the PDEs and the requirement for rapid solution pose significant challenges for the computational scientists. A particularly challenging class of PDE-constrained optimization problems in several applications is characterized by the need for real-time solution, i.e., in time scales that are sufficiently rapid to support simulation- based decision making. The main focus of this minisymposium is devoted to solve efficiently such large scale application problems which includes the design of preconditioners for KKT systems arising within the optimization, but also offer opportunities for storage management, subdomain model reduction and parallelization techniques.

SPEAKERS

1. Martin Weiser (Zuse Institute Berlin, Germany)
   Title: Data compression for parabolic optimal control problems with application to cardiac defibrillation

2. Armin Rund (Uni Graz, Austria)
   Title: Time Optimal Control of the monodomain model in cardiac electrophysiology

3. Federico Negri (EPFL SB MATHICSE CMCS, Lausanne)
   Title: Reduction strategies for PDE-constrained optimization with application in haemodynamics

4. Chamakuri Nagaiah (RICAM, Linz, Austria)
   Title: A parallel PDE-constrained optimization: an application to cardiac electrophysiology

5. Lorenz John (TU Graz Austria)
   Title: Optimal Dirichlet boundary control for arterial blood flow

6. Peng Chen (EPFL SB MATHICSE CMCS, Lausanne)
   Title: Weighted reduced basis method for stochastic optimal control problems with PDE constraints

7. Lars Lubkoll (Zuse Institute Berlin, Germany)
   Title: Optimal control in implant shape design

8. Henry Kasumba (Austrian Academy of Sciences, Linz, Austria)
   Title: A bilevel shape optimization problem for the exterior Bernoulli free boundary value problem

WEIGHTED REDUCED BASIS METHOD FOR STOCHASTIC OPTIMAL CONTROL PROBLEMS WITH PDE CONSTRAINTS

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Abstract: Optimal control problems governed by partial differential equations (PDEs) are commonly encountered in the optimal design, control and optimization of mathematical models for the underlying physical systems in many science and engineering fields. In practical applications, uncertainties may inevitably arise from various sources, e.g. the PDE coefficients, initial and boundary conditions, external loadings and computational geometries, leading to stochastic optimal control problems that require to solve the underlying PDEs at many realizations of the uncertainties. Whenever it is very heavy to solve the PDEs or the dimension of the uncertainties is too high, which are frequently faced in practice, the solution demand can easily go beyond any available computational power. In order to tackle these computational challenges, efficient combination of model reduction techniques and stochastic numerical methods have been recognized as one of the most promising approaches [1, 2, 3].

Adopting this approach, we have developed and analyzed an efficient computational strategy for solving stochastic optimal control problems with PDE constraints [4, 5, 6, 7]. We proposed a weighted algorithm based on reduced basis method (RBM) [8] to solve uncertainty propagation problems [5] and applied it to efficiently solve stochastic optimal control problems [6]. Based on constructive approximation theory, we have proven that the weighted RBM results in an approximation error converging exponentially fast as long as the solution is smooth in stochastic space, especially efficient for stochastic problems featuring various different probability distributions [5]. In analyzing the mathematical well-posedness of the stochastic optimal control problem, we first established a stochastic saddle point formulation for the optimal control problem and demonstrated that there exists a global and unique stochastic optimal solution for linear problems for the first time thanks to Brezzi's theorem [6, 7]. Regularity of the optimal solution in stochastic space was studied explicitly for the analysis of stochastic approximation error. For a complete discretization of the associated stochastic optimality system, we used finite element method (FEM) with optimal preconditioning techniques for deterministic approximation in physical space and applied the weighted RBM together with a stochastic collocation method (SCM) for stochastic approximation in probability space. A global error analysis of the FEM-wRBM-SCM strategy for solving the stochastic optimal control problems has been carried out in detail for linear problems and ongoing for nonlinear cases. Numerical experiments ranging from small-scale, low-dimensional problems to large-scale and high dimensional problems (with dimension $O(100)$) have been performed to illustrate the computational efficiency and accuracy of our method.

Keywords: optimal control problems, stochastic partial differential equations, uncertainty quantification, model order reduction, weighted reduced basis method, stochastic collocation method

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Optimal Dirichlet boundary control for arterial blood flow

Domain Decomposition Methods for Optimization with PDE Constraints, Monte Verita, Ascona, Switzerland, Sep 1–6, 2013

Lorenz John[1] Petra Pustejovska [2] Olaf Steinbach[3]

We consider an optimal Dirichlet boundary control problem for the Navier–Stokes equations. The control is considered in the energy space where the related norm is realized by the so called Steklov–Poincaré operator. We introduce a stabilized finite element method for the optimal control problem. Further we present some numerical results with emphasis on arterial blood flow.

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A BILEVEL SHAPE OPTIMIZATION PROBLEM FOR THE EXTERIOR BERNOULLI FREE BOUNDARY VALUE PROBLEM

H. KASUMBA, K KUNISCH, AND A. LAURAIN

ABSTRACT. A bilevel shape optimization problem with the exterior Bernoulli free boundary problem as lower-level problem and the control of the free boundary as the upper-level problem is considered. Using the shape of the inner boundary as the control, we aim at reaching a specific shape for the free boundary. A rigorous sensitivity analysis of the bilevel shape optimization in the infinite-dimensional setting is performed. The numerical realization using two different cost functionals is presented demonstrate the efficiency of the approach.

Optimal Control in Implant Shape Design

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Introduction

Today the design of implants is more dependent on the experience of medical scientists than on technical tools. In most cases the determination of an implant's shape is done by visually comparing CT scans with implant models and choosing one that seems to fit. This approach is very sensitive to the surgeon's skills and the geometry of the implant. Especially in the case of heavy fractures or natural deformations of the oral and maxillofacial bone structure it is often difficult to accurately predict the operation's outcome.

An automated implant design that considers the mechanical behaviour of the soft tissue would significantly improve this situation. Thus the goal of our project is the development of an algorithm that, given a desired outcome and under consideration of constraints given by the physician, computes an optimal implant shape.

Materials and Methods

The direct formulation of the shape design problem leads to a complicated MPEC (mathematical program with equality constraints) including a contact problem. For this reason we developed a formally equivalent formulation which considers the force exerted by the implant instead of its shape as design variable. This allows more natural combination with the mechanical descriptions of biological soft tissues and thus leads to a simpler control-contrained optimal control problem. The implant shape is indirectly determined by the soft tissue deformation.
In this setting constraints such as the fact that the soft tissue can glide over the implant as well as the requirement that voids between the implant soft tissue must not occur can be easily incorporated by interpreting the force exerted by the soft tissue as pressure boundary conditions.

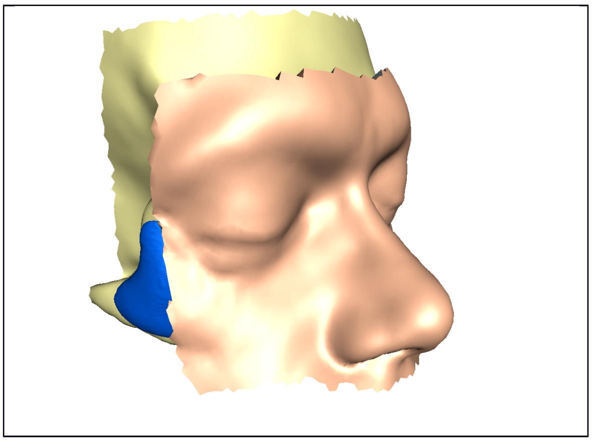

***Figure 2:** Zygomatic bone implant with soft tissue and bones.*

Results

The proposed model not only leads to smaller domains that must be discretized. It also allows a simpler, more natural formulation than the direct formulation als MPEC and avoids the inherent difficulties of contact problems. Its advantages are supported by first proof-of-concept computations in KASKADE7 [1,2].

In order to deal with the particular challenges of the efficient discretization of complicated soft tissue geometries we developed a mesh refinement strategy that is able to cheaply reconstruct complicated soft tissue geometries from coarse grids using convex combinations of local Hermite interpolation polynomials on the grids faces. Moreover this technique avoids strong refinements at artificial reentrant corners and thus leads to more efficient algorithms.

For the construction of efficient mesh hierarchies a goal-oriented error estimator has been developed that allows a better estimation of the influence of the discretization error on soft tissue shapes [3].

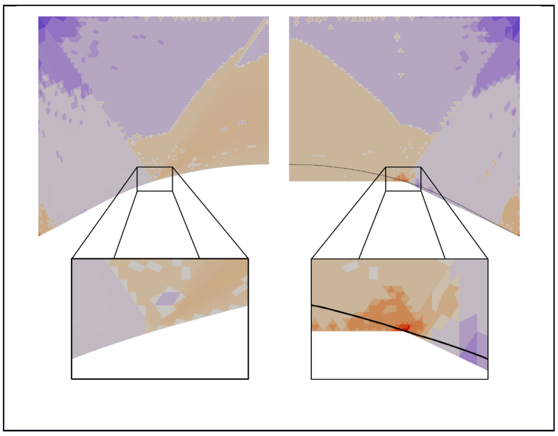

Figure 2: Hermite-Interpolation for smooth geometries avoids artifical mesh refinement at reentrant corners.

Discussion

While first computations have been realized for linear elastic constraints in general non-linear, polyconvex and compressible material models must be considered. For these problems the numerical solution of the optimization problem is more challenging. Therefore our current work focuses on the development of an efficient affine invariant composite-step method that is based on our derived mesh-refinement and error-estimation techniques.

Acknowledgments

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Reduction strategies for PDE-constrained optimization with application in haemodynamics.

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We present a reduced framework for the numerical solution of parametrized PDE-constrained optimization problems. This framework is based on a suitable *optimize-then-discretize-then-reduce* approach which takes advantage of the Reduced Basis method [2, 3] for the rapid and reliable solution of parametrized PDEs.
We mainly focus on control problems governed by advection-diffusion and Navier-Stokes equations involving infinite-dimensional control functions, thus requiring a suitable reduction of the whole optimization problem [1], rather than of the sole state equation. We discuss the stability of the reduced basis approximation and the convergence of a suitable Newton-SQP algorithm employed for the solution of both the underlying finite element approximation in the Offline stage and the RB approximation in the Online stage. Finally, by employing the Brezzi-Rappaz-Raviart theory, we derive a rigorous a posteriori error estimate.
We solve some problems arising from applications in haemodynamics, dealing with both data assimilation and optimal control of blood flows [4].

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A Parallel PDE-constrained Optimization: An Application to Cardiac Electrophysiology

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In this talk I will present domain decomposition techniques and their efficient implementation for PDE constrained optimization of bidomain model in cardiac electrophysiology. Anatomically realistic such multiscale models of torso embedded whole heart electrical activity are computationally expensive endeavor on its own right and solving optimal control of such models in an optimal manner is a challenging issue. The bidomain model consist of a system of elliptic partial differential equations coupled with a non-linear parabolic equation of reaction-diffusion type, where the reaction term, modeling ionic transport is described by a set of ordinary differential equations. An extra elliptic equation for the solution of an extracellular potential needs to be solved on the torso domain. The optimal control approach is based on minimizing a properly chosen cost functional depending on the extracellular current as input at the boundary of torso domain, which must be determined in such a way that wavefronts of transmembrane voltage in cardiac tissue are smoothed in an optimal manner. In parallel computations, the domain decomposition of such realistic geometry consists of heart surrounded by torso is not a trivial task. First, we partition the heart domain into p-subdomains and similarly partition the torso domain into p-subdomains and then we solve the PDEs as a decoupled system by expense of one additional communication at each time step. In this talk, a parallel finite element based algorithm is devised to solve an optimal control problem on such complex geometries and its efficiency is demonstrated not only for the direct problem but also for the optimal control problem. The computations realize a model configuration corresponding to optimal boundary defibrillation of a reentry phenomenon by applying current density stimuli.

Time Optimal Control of the Monodomain Model in Cardiac Electrophysiology

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Abstract

The electrical behavior of the cardiac tissue is described by the bidomain equations, a set of semilinear reaction-diffusion equations coupled with a set of ODE describing the cell level (e.g. of Hodgkin-Huxley type). The present work is concerned with time optimal control of the monodomain model, which is a simplification of the bidomain model, with the focus on cardiac arrhythmias. The aim is to determine effective and short defibrillation shocks.

Specifically, we look at a sample part of heart tissue that exhibits an undesired electrical behavior in the form of a reentry wave. By placing two electrode plates onto the heart tissue, the electrical behavior can be influenced by the current applied to the electrodes. The task is to find short and low-energy pulses, that allow for an effective termination of the reentry wave. The proper choice of the cost functional is crucial.

The time optimal control problem is reformulated as a bilevel optimization problem, where the terminal time is fixed in the lower level problem. The lower level problem itself is solved via second-order methods, in particularly a trust-region Newton method. The algorithmic and numerical solution of the bilevel problem is described in detail. The numerical experiments demonstrate that defibrillation pulses designed by the time optimal control approach influence and terminate reentry phenomena effectively.

Data compression for parabolic optimal control problems with applciation to cardiac defibrillation

M. Weiser, N. Chamakuri and S. Götschel

Solutions of the monodomain equations describing the propagation of cardiac excitation exhibit highly local features in their solutions, which has triggered the use of adaptive mesh refinement and time step selection. This talk addresses optimal control problems in defibrillation and focuses on techniques for spatiotemporal adaptivity to achieve a reduction of computation time and storage requirement. In particular we present adaptive lossy compression of state trajectory data for the adjoint computation of reduced gradients, storing both FE coefficients and adaptively refined meshes. A mixed a-priori/a-posteriori error estimator allows to choose the quantization tolerance such as not to impede the convergence of a Newton-CG optimization algorithm.

The decreased storage requirement allows to consider a longer time-horizon in the optimizations, which results in improved stability of the optimal solutions. The effectivity of the algorithm is illustrated on several numerical examples.