Workshop

on

PDE Constrained Optimization

Center for International Mathematics

Thematic term on Optimization

July 26-29, 2005
Tomar, Portugal

http://www.mat.uc.pt/tt2005/pde

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Scope: Optimization problems governed by partial differential equation (PDE) constraints arise in many important applications. Progress in computational and applied mathematics combined with the availability of rapidly increasing computer power steadily enlarges the range of applications that can be simulated numerically and for which optimization tasks, such as optimal design, parameter identification, and control are being considered. For most of these optimization problems, simple approaches combining off-the-shelf PDE solvers and optimization algorithms often lack robustness or can be very inefficient.

Successful solution approaches have to overcome challenges arising from, e.g., the increasing complexity of applications and their mathematical models, the influence of the underlying infinite dimensional problem structure on optimization algorithms, and the interaction of PDE discretization and optimization.

This workshop will combine a wide range of topics important to PDE constrained optimization in an integrated approach, fusing techniques from a number of mathematical disciplines including functional analysis, optimal control theory, numerical optimization, numerical PDEs, and numerical analysis and application specific structures.

A short course will be offered on the first day of the workshop.

Invited and contributed presentations will be scheduled during the remaining three days.

Organizers

Luís Merca Fernandes (ESTT, Tomar, Portugal)
Matthias Heinkenschloss (Rice Univ., USA)
Luís Nunes Vicente (Univ. Coimbra, Portugal)

Sponsors

Centro Internacional de Matemática

Centro de Matemática da Universidade de Coimbra

Escola Superior de Tecnologia de Tomar

Fundação Calouste Gulbenkian

Fundação para a Ciência e a Tecnologia

Other Events

Workshop on Optimization in Finance
School of Economics, University of Coimbra, July 5-8, 2005
`http://www.mat.uc.pt/tt2005/of`

Summer School on Geometric and Algebraic Approaches for Integer Programming
Faculty of Science, University of Lisbon, July 11-15, 2005
`http://www.mat.uc.pt/tt2005/ss`

Workshop on Optimization in Medicine
IBILI, University of Coimbra, July 20-22, 2005
`http://www.mat.uc.pt/tt2005/om`

PROGRAM AT GLANCE

Tuesday 26	
9:00-9:45	Registration
9:45-10:00	Opening Remarks
10:00-12:30	Tutorial T1
12:30-14:00	Lunch
14:00-16:30	Tutorial T2
17:00	Visit to Convento de Cristo
Wednesday 27	
9:00-10:00	Invited Speaker I1
10:00-10:30	Coffee Break
10:30-12:30	Session OS1
12:30-14:00	Lunch
14:00-15:00	Invited Speaker I2
15:00-15:30	Coffee Break
15:30-16:50	Session S1
17:00	Visit to Castelo de Bode (dinner included)
Thursday 28	
9:00-10:00	Invited Speaker I3
10:00-10:30	Coffee Break
10:30-12:30	Session OS2
12:30-14:00	Lunch
14:00-15:00	Invited Speaker I4
15:00-15:10	Break
15:10-16:10	Invited Speaker I5
16:10-16:40	Coffee Break
16:40-18:00	Session S2
18:00-18:10	Break
18:10-19:10	Session S3
20:00	Conference Dinner
Friday 29	
9:00-10:00	Invited Speaker I6
10:00-10:30	Coffee Break
10:30-12:30	Session OS3
12:30-14:00	Lunch
14:00-15:00	Invited Speaker I7
15:00-15:30	Coffee Break
15:30-16:50	Session S4

Tuesday 26

9:00-9:45 **Registration** – Room Cruzada

9:45-10:00 **Opening Remarks** – Room Convento

Tutorial T1 – Room Convento

10:00-12:30 **Matthias Heinkenschloss**, Rice Univ., USA
Fredi Tröltzsch, Tech. Univ. Berlin, Germany
Introduction to the theory and numerical solution of PDE constrained optimization problems

12:30-14:00 **Lunch**

Tutorial T2 – Room Convento

14:00-16:30 **Matthias Heinkenschloss**, Rice Univ., USA
Fredi Tröltzsch, Tech. Univ. Berlin, Germany
Introduction to the theory and numerical solution of PDE constrained optimization problems

17:00 **Visit to Convento de Cristo**

Wednesday 27

Invited Speaker I1 – Room Convento

9:00-10:00	**Max Gunzburger**, Florida State Univ., USA *Reduced-order modeling of complex systems*

10:00-10:30	**Coffee Break**

Applications of PDE Constrained Optimization – OS1 – Room Convento

Organizer: **Bijan Mohammadi**, Univ. Montpellier, France

10:30-11:00	**Laurent Dumas**, Univ. Paris VI, France *Global optimization methods and applications in CFD*
11:00-11:30	**Mohamed Masmoudi**, CNRS, Univ. Paul Sabatier, Toulouse, France *Topological shape optimization, imaging and image processing*
11:30-12:00	**François Jouve**, CMAP, École Polytechnique, France *Level set method and topological gradient in structural optimization*
12:00-12:30	**Ivorra Benjamin**, Univ. Montpellier, France *A new semi-deterministic global optimization method*

12:30-14:00	**Lunch**

Invited Speaker I2 – Room Convento

14:00-15:00	**Rolf Rannacher**, Univ. Heidelberg, Germany *On the discretization of optimization problems by adaptive finite element methods*

15:00-15:30	**Coffee Break**

Time Dependent Problems – S1 – Room Convento

15:30-15:50	**Dominik Meidner**, Univ. Heidelberg, Germany *Adaptive solution of nonstationary optimal control problems*
15:50-16:10	**Andrea Walther**, Tech. Univ. Dresden, Germany *Online checkpointing for adjoint computation in PDEs: Application to goal oriented adaptivity and flow control*
16:10-16:30	**Kostas Chrysafinos**, Univ. Bonn, Germany *Error estimates for discontinuous Galerkin approximations of distributed optimal control problems*
16:30-16:50	**Jens Saak**, Tech. Univ. Chemnitz, Germany *An LQR approach to tracking control for parabolic systems*

17:00 **Visit to Castelo de Bode (dinner included)**

Thursday 28

Invited Speaker I3 – Room Convento

9:00-10:00 **Günter Leugering**, Univ. Erlangen-Nürnberg, Germany
Modelling, control and optimization of distributed parameter systems on networked domains

10:00-10:30 **Coffee Break**

Approximation of PDE Constrained Optimization – OS2 – Room Convento

Organizer: **Eduardo Casas**, Univ. Cantabria, Spain

10:30-11:00 **Michael Hinze**, Tech. Univ. Dresden, Germany
Discrete concepts in PDE constrained optimization

11:00-11:30 **Mariano Mateos**, Univ. Oviedo, Spain
Error estimates for the numerical approximation of Neumann control problems

11:30-12:00 **Jean-Pierre Raymond**, Univ. Paul Sabatier, Toulouse, France
Error estimates for the numerical approximation of distributed control problem of the steady Navier-Stokes equations

12:00-12:30 **Eduardo Casas**, Univ. Cantabria, Spain
Error estimates for the numerical approximation of Dirichlet boundary control problems

12:30-14:00 **Lunch**

Invited Speaker I4 – Room Convento

14:00-15:00 **Ronald Hoppe**, Univ. Ausgburg, Germany; Univ. Houston, USA
Adaptive finite element methods for optimally controlled elliptic problems with control constraints

15:00-15:10 **Break**

Invited Speaker I5 – Room Convento

15:10-16:10 **Karl Kunisch**, Univ. Graz, Austria
Optimal control with state constraints: theory and numerical methods

16:10-16:40 **Coffee Break**

Elliptic Control Problems – **S2** – Room Convento

16:40-17:00 **Angela Kunoth**, Univ. Bonn, Germany
Wavelet schemes for an elliptic control problem with Dirichlet boundary control

17:00-17:20 **Carsten Burstedde**, Univ. Bonn, Germany
Wavelet methods for linear-quadratic elliptic optimal control problems

17:20-17:40 **Boris Vexler**, RICAM, Austrian Academy of Sciences, Austria
Finite element discretization of Dirichlet optimal control problems

17:40-18:00 **Alexandra Gaevskaya**, Univ. Augsburg, Germany
Error majorants for distributed optimal control problems with control constraints

18:00-18:10 **Break**

Optimization Algorithms – **S3** – Room Convento

18:10-18:30 **Anton Schiela**, Konrad Zuse Inst. Berlin, Germany
A control reduced interior point method for PDE constrained optimization

18:30-18:50 **Jan Christoph Wehrstedt**, Tech. Univ. München, Germany
All-at-once bundle methods for state constrained optimization

18:50-19:10 **Amos Lawless**, Univ. Reading, UK
Approximate Gauss-Newton methods for data assimilation in numerical weather prediction

20:00 **Conference Dinner** – Hotel dos Templários

Friday 29

Invited Speaker I6 – Room Convento

9:00-10:00	**Anthony T. Patera**, MIT, USA *Certified reduced-basis methods for reliable rapid solution of parameterized partial differential equations: Application to real-time parameter estimation, adaptive design, and optimal control*

10:00-10:30 **Coffee Break**

Efficient Solution Techniques in Constrained Optimal Control and Shape Optimization – OS3 – Room Convento

Organizer: **Michael Hintermueller**, Univ. Graz, Austria

10:30-11:00	**Sebastian Singer**, Univ. Ulm, Germany *Efficiency optimization of the Voith-Schneider-propeller*
11:00-11:30	**Juan-Carlos de los Reyes**, Tech. Univ. Berlin, Germany; EPN Quito, Ecuador *A semi-smooth Newton method for state-constrained optimal control of the Navier-Stokes equations*
11:30-12:00	**Gunther Peichl**, Univ. Graz, Austria *Variational approach to shape derivatives for a class of Bernoulli problems*
12:00-12:30	**Michael Hintermueller**, Univ. Graz, Austria *Shape sensitivity and level set methods in constrained minimization*

12:30-14:00 **Lunch**

Invited Speaker I7 – Room Convento

14:00-15:00	**Ekkehard W. Sachs**, Univ. Trier, Germany; Virginia Poly. Inst., USA *Preconditioning techniques for optimal control problems*

15:00-15:30 **Coffee Break**

Applications – S4 – Room Convento

15:30-15:50	**Cecília S. Pinto**, Inst. Politécnico Viseu, Portugal *Shape differentiability for a contact bone remodelling rod model*
15:50-16:10	**Rui Manuel Pinto**, Inst. Politécnico Leiria, Portugal *Nonlinear Schrödinger equation (with magnetic field) instability of stationary states with cylindrical symmetry*
16:10-16:30	**Norbert E. Ligterink**, Univ. Twente, Netherlands *Controlling the energy in distributed systems*
16:30-16:50	**Shahlar Maharramov**, Nat. Acad. Sciences, Azerbaijan Republic *Optimization of the discrete control system with varying structure*

Title and Abstract – Tutorial

Introduction to the theory and numerical solution of PDE constrained optimization problems

Matthias Heinkenschloss and Fredi Tröltzsch

Optimization problems governed by partial differential equations (PDEs) arise in many science and engineering applications. The development and analysis of efficient methods for the solution of such problems and their successful application to practical problems requires techniques from a number of mathematical disciplines including functional analysis, optimal control theory, numerical optimization, numerical PDEs, and numerical analysis. This tutorial will provide an integrated introduction to the theory and numerical solution of PDE constrained optimization problems.

Among the topics covered are the existence and characterization of solutions to PDE constrained optimization problems. Optimality conditions and their role in optimization algorithms. Discretization of PDE constrained optimization problems. Gradient and second order methods for PDE constrained optimization problems. Challenges arising in and methods for handling control and state constraints.

Titles and Abstracts – Invited Talks

Reduced-order modelling of complex systems

Max Gunzburger

The computational approximation of solutions of complex systems such as the Navier-Stokes equations is often a formidable task. For example, in feedback control settings where one often needs solutions of the complex systems in real time, it would be impossible to use large-scale finite element or finite-volume or spectral codes. For this reason, there has been much interest in the development of low-dimensional models that can accurately be used to simulate and control complex systems. We review some of the existing reduced-order modeling approaches, including reduced-basis methods and especially methods based on proper orthogonal decompositions techniques. We also discuss a new approach based on centroidal Voronoi tessellations. We discuss the relative merits and deficiencies of the different approaches and also the inherent limitations of reduced-order modeling in general. We also discuss the use of design of experiment strategies for helping to construct effective reduced bases.

Adaptive finite element methods for optimally controlled elliptic problems with control constraints

Ronald Hoppe

We are concerned with the development and analysis of adaptive finite element methods for optimally controlled elliptic PDEs with constraints on the control. In the unconstrained case, such methods have been considered previously (cf., e.g., [Bangerth and Rannacher 2003] and the references therein), whereas in the presence of control constraints some results have been obtained in [Li, Liu, Ma, and Tang 2002] and [Liu and Yan 2003]. The methods presented in this contribution provide an error reduction and thus guarantee convergence of the adaptive loop which consists of the essential steps SOLVE, ESTIMATE, MARK, and REFINE. Here, SOLVE stands for the efficient solution of the finite element discretized problems which is taken care of by appropriate active set strategies (cf., e.g., [Hintermüller, Ito, and Kunisch 2003]). The following step ESTIMATE is devoted to the a posteriori error estimation of the global discretization errors in the state, the co-state, and the control by easily computable local quantities. A greedy algorithm is the core of the step MARK to indicate selected elements for refinement, whereas the final step REFINE deals with the technical realization of the refinement process itself. The analysis is carried out for the lowest order P1 conforming finite elements. Important tools in the convergence proof are the reliability of the estimator, a strong

discrete local efficiency, and quasi-orthogonality properties (see, e.g., [Carstensen and Hoppe 2005] and [Morin, Nochetto, and Siebert 2000] for various finite element approximations of elliptic PDEs). The proof does not require regularity of the solution nor does it make use of duality arguments.
Joint with: Alexandra Gaevskaya and C. Iyyunni

Optimal control with state constraints: Theory and numerical methods

Karl Kunisch

First a brief summary on the existence and structure of Lagrange multipliers for state constrained optimal control problems is given. Then two rather recent numerical solution techniques are discussed. One approach involves the use of level sets describing the interfaces between active and inactive sets of the constrained state variables. The other one is based on semi-smooth Newton methods in functions spaces. Here, in particular, a new path-following algorithm for proper increase of a penalty parameter will be introduced.

Modelling, control and optimization of distributed parameter systems on networked domains

Günter Leugering

We consider modelling, analysis, optimization and control of transport processes and problems of wave propagation on multi-dimensional networks. Transport processes in networks are of importance in the control-management of water-, gas- and electrical power systems, as well as in the simulation and the control of blood- and traffic flow, while waves propagating within networked domains occur in flexible structures, mechanical microstructures, macromolecules and seismic problems. The mathematical modelling along with its analysis requires model hierarchies, multiple joint conditions, homogenization, domain decomposition or substructuring and hybrid systems approaches. The optimization and control problems are formulated for the entire network problem followed by a reduction to tractable subproblems via homogenization and domain decomposition. As for domain decomposition methods, a posteriori estimates will also be discussed, and numerical examples will be provided.

Certified reduced-basis methods for reliable rapid solution of parameterized partial differential equations: Application to real-time parameter estimation, adaptive design, and optimal control

Anthony T. Patera

Engineering analysis requires the prediction of selected "outputs" s relevant to ultimate component and system performance. These outputs are functions of "input" μ that serve to identify a particular configuration of the component or system. In many cases, the output is best articulated as a (say) linear functional ℓ of a field variable $u(\mu)$ that is the solution to an input-parametrized (μ-parametrized) partial differential equation. System behavior is thus described by an input-output relation $s(\mu) = \ell(u(\mu))$ the evaluation of which requires solution of the underlying partial differential equation. Characterization, design, optimization, and control typically require *thousands of evaluations* $\mu \to s(\mu)$ — and often in effectively *real-time*.

Most classical numerical approaches consider effectively "dense" approximation subspaces: the computational requirement for a *particular* value of μ is thus typically measured in minutes, hours, or even days. This has two distinct but related implications. First, we can not adequately explore the parameter domain: thus we can not determine which parts of the parameter domain are indeed "representative"; and hence we can not rationally decide which expensive "next experiment" should be accorded highest priority. Second, we can not address the many "design" and "operations" applications that require either *real-time response* to — or simply *very many* — queries $\mu \to s(\mu)$: thus we can not perform optimization of components and processes, robust parameter estimation of properties and state, or adaptive design and control of assets and missions.

The goal of our work is to address this deficiency: we present a technique for the rapid and reliable prediction of (linear-functional) outputs of partial differential equations with approximately affine parameter dependence. The method is applicable to a wide variety of coercive and noncoercive, linear and nonlinear, and elliptic and parabolic equations.

The essential components of our approach are threefold: (i) rapidly and uniformly convergent reduced-basis approximations — Galerkin projection onto a space W_N spanned by solutions of the governing partial differential equation at N optimally selected points in parameter space; (ii) *a posteriori* error estimation — relaxations of the residual equation that provide inexpensive yet sharp and rigorous bounds for the error in the outputs of interest; and (iii) offline/online computational procedures — strategies that accept increased initial preprocessing (offline) expense in exchange for greatly reduced subsequent (online) *marginal cost*.

The method is ideally suited to the many-query and real-time contexts (in which marginal cost is clearly the critical computational metric): the operation count for the online, or "deployed," stage depends only on N — typically very small — and the parametric complexity of the problem. We can thus provide predictions that are *certifiably* as good as classical "truth" approximations but literally *several or-*

ders of magnitude less expensive. Online factors of improvement of $O(100\text{–}1000)$ are often observed: two-dimensional Navier-Stokes natural convection at moderate Grashof number — from prescribed input to output and error bound in 0.01 seconds on a Pentium 1.6GHz; three-dimensional exterior Dirichlet acoustic Helmholtz (albeit in relatively simple geometry) — from input to output and error bound in 0.04 seconds.

The advantages of our approach can be further leveraged in service of parameter estimation, optimization, and adaptive design. In particular, not only can we rigorously accommodate numerical uncertainty, but — through the extensive exploration of parameter space afforded by our rapid evaluation technology — we can also accommodate (some) model uncertainty. Real-time applications may thus be considered: we can quickly arrive at conclusions which will be feasible, optimal, and robust. Of particular interest are "assess-act" scenarios: real-time parameter "assess" followed by fail-safe optimal "act".

We draw our examples from heat transfer, elasticity, incompressible fluid flow (Navier-Stokes), and quantum mechanics, with application to robust parameter estimation — nondestructive crack assessment, acoustic inverse scattering for mine detection, material properties from quantum models; adaptive design — maximal safe load prediction, vehicle stealth, thermal managment; and optimal control — contaminant remediation, heat treatment, reactor design.
Joint with: K. Veroy, N.C. Nguyen, M.A. Grepl, G. Pau, G.R. Liu, and Y. Maday

On the discretization of optimization problems by adaptive finite element methods

Rolf Rannacher

In this talk we summarize recent developments in a posteriori error estimation and mesh adaptation for the discretization of optimization problems. In the context of the finite element Galerkin method we describe the Dual Weighted Residual (DWR) method exploiting "Galerkin orthogonality", "residual evaluation" and "dual stability". The applications discussed range from simple boundary control over parameter identification and model callibration to first steps towards experimental design.

Preconditioning techniques for optimal control problems

Ekkehard W. Sachs

In this talk we consider the preconditioning for linear systems arising in problems of optimal control that are governed by partial differential equations. We address first the infinite dimensional problem and apply some classical results to these cases. In the sequel we refine the approach by looking at discretized problems and derive results including the mesh size parameters. This is applied to some examples of optimal control problems.

Titles and Abstracts – Talks

A new semi-deterministic global optimization method

Ivorra Benjamin

Most deterministic minimization algorithms can be seen as discrete dynamical systems coming from the discretization of first or second order Cauchy problems. On the other hand, global optimization can be considered as an over-determined Boundary Value Problem (BVP) for these problems. We study the mathematical characteristics of these dynamic systems and exhibit a second order dynamic system with friction suitable for discretization and development of minimization algorithm. In particular, we propose one possible solution where the over determination is removed by considering initial conditions as new variables to be found by the minimization of a new functional involving the infimum of the original one. Hence, we propose an original Semi-Deterministic Algorithm (SDA) for global optimization.

The algorithm is applied to various academic and industrial applications. In particular, two industrial applications is considered: the design of multichannel filters based on optical fibers and shape optimization of a Fast-Microfluidic-Mixer for protein folding. The results are compared to those obtained with an Hybrid Genetic Algorithm.

Joint with: Bijan Mohammadi, J. Santiago, and D. Hertzog

Wavelet methods for linear-quadratic elliptic optimal control problems

Carsten Burstedde

Using the wavelet framework, fractional Sobolev norms for the state and the control become numerically accessible. While fractional norms of general functions are represented up to equivalence, we present a scheme which captures the norms exactly for selected special cases. We transform the optimality system into an equivalent well-conditioned infinite-dimensional system in wavelet coordinates which permits the fast solution for both uniform and adaptive discretizations, and present selected numerical results.

Error estimates for the numerical approximation of Dirichlet boundary control problems

Eduardo Casas

We study the numerical approximation of boundary optimal control problems governed by semilinear elliptic partial differential equations with pointwise constraints on the control. The control is the trace of the state on the boundary of the domain, which is assumed to be a convex, polygonal, open set in $\mathbb{R}^2$. Piecewise linear finite elements are used to approximate the control as well as the state. We prove that the error estimates are of order $o(h^{1/2})$, which is consistent with the $H^{\varepsilon+1/2}(\Gamma)$-regularity of the optimal control.

Error estimates for discontinuous Galerkin approximations of distributed optimal control problems

Kostas Chrysafinos

We analyze the classical discontinuous Galerkin (DG) method for a distributed optimal control problem related to parabolic PDEś. The class of DG schemes we consider, are classical in the sense that the discrete solutions may be discontinuous in time but are conforming in space. The DG scheme allows different discrete subspaces to be used in each time step. Fully-discrete error estimates are presented in the natural energy norms. Our error estimates are posed in terms of suitable projections and are valid under minimal regularity assumptions on the given data.

Global optimization methods and applications in CFD

Laurent Dumas

New global optimization methods are constructed in order to be able to design optimal shapes in various aero or hemodynamic contexts. All the methods consist in improving the well known genetic algorithm method, either by coupling it with a deterministic local search procedure or by incorporating a fast but approximated evaluation process. The efficiency of these methods is shown, first on analytical test functions, then on various realistic application, such as a 3D drag reduction problem in the automotive industry or an stent shape optimization in micro-surgery. In all these problems, the use of such methods has permitted to reduce the computational time of a genetic algorithm by a factor ranging from 2 to 10 while keeping all its advantages.

Error majorants for distributed optimal control problems with control constraints

Alexandra Gaevskaya

In this talk, we introduce a new approach to the numerical analysis of distributed optimal control problems for PDEs. It is based on functional type a posteriori estimates that provide guaranteed upper bounds for the difference between the exact solution of a boundary-value problem and any trial function from the respective energy class. By applying these estimates, we derive computable majorants for the cost functional that can be used for the direct solution of the optimal control problem.

Shape sensitivity and level set methods in constrained minimization

Michael Hintermueller

In many optimal control problems for PDEs or inverse problems one faces states which have to satisfy (pointwise) inequality constraints or coefficients in underlying differential operators which exhibit jumps. In the first case, the regularity of Lagrange multipliers may be poor, and in the second case an efficient solution procedure dealing with jumps in the coefficients has to be found. The combination of shape sensitivity analysis and level set methods provides a new iterative solver paradigm where geometrical objects replace the functional quantities as the iterates. This talk focuses on the reformulation of the original problem as a shape optimization problem, shape sensitivity aspects, the combination with level set methods in a descent framework, and aspects of the numerical realization. Finally, numerical results are discussed.

Discrete concepts in PDE constrained optimization

Michael Hinze

In my talk I will discuss a new discretization concept for abstract control problems with control constraints which extends the common discrete approaches. Discretization only is applied to the state variables, which in turn implicitly yields a discretization of the control variables by means of the first order optimality condition. For discrete controls obtained in this way an optimal error estimate in terms of the state-discretization parameter is presented.

Applied to control of partial differential equations combined with finite element discretization of the state the key features of the new control concept include

- Decoupling of finite element grid and discrete active set

- Numerical implementation requires only small additional overhead compared to commonly utilized methods (discretization of state and of admissible controls)
- Approach applicable in 1,2 and 3 spatial dimensions, and also for Galerkin type discretization schemes of time dependent state equations
- Numerical analysis seriously simplifies compared to the common approach

As numerical solution algorithms primal-dual active set strategies and semismooth Newton methods are discussed. Several numerical examples will be presented that confirm the theoretical investigations.

Level set method and topological gradient in structural optimization

François Jouve

A numerical coupling of two recent methods in shape and topology optimization of structures is proposed. On the one hand, the level set method, based on the classical shape derivative, is known to easily handle boundary propagation with topological changes. However, in practice it does not allow for the nucleation of new holes (at least in 2-d). On the other hand, the bubble or topological gradient method is precisely designed for introducing new holes in the optimization process. Therefore, the coupling of these two method yields an efficient algorithm which can escape from local minima in a given topological class of shapes. Both methods rely on a notion of gradient computed through an adjoint analysis, and have a low CPU cost since they capture a shape on a fixed Eulerian mesh. The main advantage of our coupled algorithm is to make the resulting optimal design largely independent of the initial guess.
Joint with: G. Allaire, F. De Gournay, and A.M. Toader

Wavelet schemes for an elliptic control problem with Dirichlet boundary control

Angela Kunoth

This talk will be concerned with numerical schemes based on wavelet expansions for control problems with Dirichlet boundary control constrained by a linear elliptic partial differential equation. The constraints will be formulated as a saddle point problem. Striving for efficiency and optimal complexity, I will address preconditioning issues, the selection of appropriate norms in the control functional, and adaptive methods for the resolution of singularities. A convergence proof and convergence rates for an adaptive algorithm for the system of optimality conditions will be presented, which can be shown to be asymptotically optimal compared with the wavelet-best N-term approximation of the state, the adjoint and the control. I will conclude with some numerical results.

Approximate Gauss-Newton methods for data assimilation in numerical weather prediction

Amos Lawless

Variational data assimilation is a technique for retrieving the state of a system using observed data, through the minimization of a cost function constrained by a numerical model. The method is used in numerical weather prediction to obtain the initial conditions for a weather forecast. In practice this leads to a very large nonlinear optimization problem, of several million variables, which must be solved in real-time. In order to solve this problem efficiently, operational forecasting centres have implemented what is called an "incremental" version, whereby the solution to the full minimization problem is approximated by the minimization of a sequence of linear quadratic cost functions, each of which is constrained by the linearization of the full nonlinear numerical model. This procedure can be shown to be equivalent to applying a standard Gauss-Newton iteration method to minimize the original nonlinear problem.

In practice this procedure is too expensive to apply exactly in operational weather forecasting and various approximations must be made. Here we examine two types of approximation used commonly in data assimilation. Firstly, we examine "truncated" Gauss-Newton methods, where the inner linear problem is not solved exactly, and secondly we examine "perturbed" Gauss-Newton methods where the true linearized inner problem is approximated by a simplified linear problem. We establish conditions which ensure that these approximate methods converge and derive rates of convergence for the iterations. The results are illustrated with a numerical example.

Joint with: S. Gratton and N.K. Nichols

Controlling the energy in distributed systems

Norbert E. Ligterink

Controlled systems described by PDE's are systems with varying boundary conditions. Energy balance is useful maintain stability. Furthermore, the proper separation of conservation laws from energy storage allows one to retain handles on the simulation, even in the case of nonlinear systems. The general principles of such analysis, called port-based modelling, are discussed, and energy-flux and the corresponding interconnection structure between energy storage, energy dissipation, and boundary energy flow is derived. If time permits, a structural example is discussed.

Optimization of the discrete control system with varying structure

Shahlar Maharramov

In this study the optimal control with several objects and their consecutive working is considered. The starting conditions for any next object depend on the final conditions of the previous one. The union of all these objects is called a step control system. For example, in a rocet there are two types of engines that work consecutively. The work of the second engine depends on the first one. Moreover, the rocet moves from one controlling area to a second one that changes all the structure (controls, functions, conditions).

Topological shape optimization, imaging and image processing

Mohamed Masmoudi

Topological optimization is a 0-1 optimization problem. Determining an optimal domain is equivalent to finding its charachteristic function. At first sight, this is a non differentiable problem. But there are three ways to make it differentiable: - In the relaxation method, the discrete characteristic function is replaced by a material density taking its values between zero an one (Kikuchi, Bendsoe, Allaire, ...), - In the level set method, the unknown is a level set function (Osher, Santosa, Sethian, Allaire, Ě); this regular function is positive inside the domain, negative inside and equal to zero on its boundary, - Using the topological asymptotic expansion, it is possible to calculate the variation of a cost function if we switch the characteristic function from one to zero or from zero to one in a small area. The topological asymptotic expansion has a fundamental property: at convergence, the positiveness of the topological gradient (the leading term) is a necessary and even a sufficient local optimality condition.

We will focus this talk on the basic concepts of the topological asymptotic expansion and the related algorithms. Then we will present some real life applications in topological shape optimization, imaging, and image processing.

Error estimates for the numerical approximation of Neumann control problems

Mariano Mateos

We discuss error estimates for the numerical analysis of Neumann boundary control problems. Continuous piecewise linear functions are used to discretize the control. Both a general functional and a quadratic one are studied. In the first case, the L^2 error is of order $o(h)$, while in the second it is of order $h^{3/2}$. We also check what happens when the problem is only semidiscretized. Finally we obtain error estimates in the uniform norm.

Adaptive solution of nonstationary optimal control problems

Dominik Meidner

We consider nonstationary optimal control problems governed by parabolic partial differential equations. The state equation is discretized by space-time finite element method, using continuous Galerkin (cG) or discontinuous Galerkin (dG) methods for the time discretization. We present error estimators for the time and space discretization errors with respect to the cost functional. These error estimators are used for quantitative error control and for successive improvement of the accuracy by appropriate refinement of the spacial meshes and the step size in the time discretization. Numerical examples for nonlinear parabolic equations demonstrate the behavior of our method.
<u>Joint with:</u> Boris Vexler

Variational approach to shape derivatives for a class of Bernoulli problems

Gunther Peichl

The shape derivative of a functional related to a Bernoulli problem is derived without using the the shape derivative of the state. Instead we only employ Hölder continuity of the state with respect to perturbations of the domain. The gradient information is combined with level set ideas in a steepest descent algorithm. Numerical examples show the feasibility of the approach.

Shape differentiability for a contact bone remodelling rod model

Cecília S. Pinto

We consider a bone remodeling model, for a rod that may come into contact without friction with a rigid obstacle, due to the action of external loads. We characterize the conical differentiability of the solution to this model, with respect to small variations of the geometry of the rod's cross section.This perturbation is associated to a small parameter denoted by s .

The bone remodeling rod model that we consider is the elastic adaptive reduced rod model derived by [Figueiredo and Trabucho 2004], but with different boundary conditions and additional contact constraints. The model is characterized by a variational inequality, coupled with an ordinary differential equation with respect to time, where the unknowns are the vector field u^s, which represents the displacement of the rod and the scalar field d^s, that is the measure of change in volume fraction of the rod's material. The unknowns are interdependent, the displacement u^s is the solution of the variational inequality and depends on d^s and the unknown d^s depends on u^s and it is the solution of the ordinary differential equation with respect to time.

We prove the differenciability of u^s and d^s with respect to the geometric parameter s [Figueiredo, Leal, and Pinto 2005], using a technique described in [Sokolowski and Zolesio 1992].

Joint with: Isabel N. Figueiredo and Carlos F. Leal

Nonlinear Schrödinger equation (with magnetic field) instability of stationary states with cylindrical symmetry

Rui Manuel Pinto

Instability properties of solutions of the well known Schrödinger equation in the presence of a uniform magnetic field. Its proved that exist instability by the flow of the evolution equation in some conditions, and the trajectories used to exhibit instability are global and uniformly bounded.

Error estimates for the numerical approximation of distributed control problem of the steady state Navier-Stokes equations

Jean-Pierre Raymond

A constrained distributed control problem governed by the stationary Navier-Stokes equations is studied. First and second order optimality conditions are obtained. The numerical approximation is performed and error estimates are derived. We do not assume that the data of the Navier-Stokes equations are small. We assume that the local solution we want to approximate is a non singular solution to the Navier-Stokes equations.

A semi-smooth Newton method for state-constrained optimal control of the Navier-Stokes equations

Juan-Carlos de los Reyes

We study semi-smooth Newton methods for the numerical solution of pointwise state-constrained optimal control problems governed by the Navier-Stokes equations. After deriving an appropriate optimality system, a class of regularized problems is introduced and the convergence of their solutions to the original optimal one is proved. For each regularized problem a semi-smooth Newton method is applied and its convergence verified. Finally, selected numerical results illustrate the behavior of the method.

An LQR approach to tracking control for parabolic systems

Jens Saak

We present a linear-quadratic regulator design for tracking reference states of parabolic systems. It is shown that the solution strategy is closely related to an earlier approach where the LQR approach was used to achieve asymptotic zero stabilization. That means, here we want to regulate the state to a given stationary state. We discuss theoretical extensions to the earlier approach needed to complete this task and compare numerical results for both approaches.

A control reduced interior point method for PDE constrained optimization

Anton Schiela

A primal interior point method for control constrained optimal control problems with PDE constraints is considered. Pointwise elimination of the control leads to a homotopy in the remaining state and dual variables, which is addressed by a short step pathfollowing method. The algorithm is applied to the continuous, infinite dimensional problem, where discretization is performed only in the innermost loop when solving linear equations. The a priori elimination of the least regular control permits to obtain the required accuracy with comparatively coarse meshes. Moreover, the method shows superlinear local convergence. We present an outline of the corresponding theory and illustrate our results at numerical examples.

Efficiency optimization of the Voith-Schneider-propeller

Sebastian Singer

In efficiency optimization of the Voith-Schneider-Propeller constraints and objective function depend on cfd, i.e. the solution of the instationary incompressible Navier-Stokes equations. Several cfd codes (self-made and commercial) have been used in conjunction with direct search methods and a significant improvement has been achieved for the steering of the blades. Characteristics of the problem are local non-differentiability, the existence of several local maxima and –depending on the cfd code– high computational costs or inexactness of solutions of the underlying pde. At present studies are undertaken to incorporate the shape of blades as control variables, the use of approximation models to combine different cfd-codes in the optimization process and the use of model reduction techniques. The project is a joined venture of Voith Turbo Marine Heidenheim (Germany) and the Department of Numerical Analysis of Ulm University.

Finite element discretization of Dirichlet optimal control problems

Boris Vexler

We develop a priori and a posteriori error analysis for finite element Galerkin discretization of elliptic Dirichlet optimal control problems. The state equation is given by an elliptic partial differential equation and the finite dimensional control variable enters the Dirichlet boundary conditions. The direct discretization of the optimality system leads in general only to a reduced order of convergence, i.e. $O(h)$ for (bi)linear elements. We present another discretization concept, prove the optimal order of convergence, i.e. $O(h^2)$, and show numerical examples confirming our results.

Online checkpointing for adjoint computation in PDEs: Application to goal oriented adaptivity and flow control

Andrea Walther

The computation of derivatives for optimizing time-dependent PDE-based problems usually requires the integration of the adjoint differential equation. For this purpose, the knowledge of the complete forward trajectory is needed. In the area of flow control, especially for three dimensional problems, it is usually impossible to keep track of the full forward solution due to the lack of storage capacities. Furthermore, quite often adaptive time-stepping procedures are needed to ensure efficient integration schemes in time. Therefore, standard optimal offline checkpointing strategies are usually not well-suited or can simply not be applied.

In this talk we present a new approach for an online checkpointing procedure that determines the checkpoint distribution on the fly. Complexity estimates are derived. The proposed method allows an efficient gradient computations even for situations where the standard approach of recording everything fails due to the enormous amount of memory required.

The resulting optimal checkpointing approach is integrated in HiFlow, a multipurpose Finite-Element package with a strong emphasis in computational fluid dynamic, reactive flows and related subjects. Numerical experiments for prototypical flow control problems demonstrate the efficiency of the proposed approach.

Joint with: Vincent Heuveline

All-at-once bundle methods for state constrained optimization

Jan Christoph Wehrstedt

In this talk we introduce an all-at-once proximal bundle method for optimization problems with a parameter-dependent variational inequality as constraint (infinite dimensional MPEC). Such problems arise for example in the context of shape optimization problems for contact problems. In contrast to the implicit programming approach, where the in general nonsmooth reduced problem is solved, the proposed algorithm is an all-at-once method, i.e., the variational inequality and the optimization problem are solved simultaneously. The algorithm belongs to the class of composite step trust region methods. In every iteration we calculate an approximation of the solution of the variational inequality for example with some iterative solver and we compute approximately an element of the subgradient. During the iteration the feasibility of the iteration points as well as the accuracy of the subgradients are improved. In case of exact evaluation this bundle method behaves like well-established bundle methods for non-convex problems. However, its all-at-once character offers the potential of considerably reduced computational costs.

Joint with: Stefan Ulbrich

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