Mathematisches Forschungsinstitut Oberwolfach

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Numerical Techniques for Optimization Problems with PDE Constraints

February 16th – February 22nd, 2003

This workshop was organized by Matthias Heinkenschloss (Rice University, Houston), Ronald H. W. Hoppe (Universität Augsburg and University of Houston) and Volker Schulz (Universität Trier). Forty-four participants from six countries contributed to the stimulating atmosphere of the workshop.

Optimization problems with partial differential equation (PDE) constraints arise in many science and engineering applications, e.g., in form of optimal control, optimal design or parameter identification problems. The robust and efficient solution of these problems presents many mathematical challenges and requires a tight integration of properties and structures of the underlying problem, of fast numerical PDE solvers, and of numerical nonlinear optimization. This workshop has brought together some of the leading experts as well as future leaders in the above subdisciplines to exchange the latest research developments, discuss open questions, and to foster interactions between these subdisciplines. The talks were focussed on the following themes: Adaptive methods for PDE constraint optimization, discretization effects and discretization error estimates for the optimization problem, fast solvers for optimization subproblems, optimization algorithms tailored to problems with PDE constraints, all in the context of current applications in science and engineering.

Abstracts

Optimization and PDEs

Randolph E. Bank and Philip E. Gill
University of California, San Diego

We wish to study the interactions between adaptive meshing algorithms, multilevel iterative methods, and interior-point optimization algorithms in the context of parallel computation. In this talk, we focus on the optimization algorithms and parallel computation. We consider three model problems involving optimization with inequality constraints and PDEs—an obstacle problem, a parameter identification problem, and an optimal control problem. We describe how these problems fit into an adaptive feedback loop and how the required linear systems may be solved using the multigraph method. We then describe parallelization using the Bank-Holst paradigm and give some numerical illustrations using the finite element package PLTMG.

Adaptive Finite Elements for Optimal Control

Roland Becker
Universität Heidelberg

We present the different a posteriori error estimates for optimal control and parameter estimation problems. The state equation is given by a partial differential equation with controls/parameters acting in various forms. The first order optimality system which is discretized by the finite element method. We derive a posteriori error estimates for a) the value of the cost functional, b) a functional of the controls, and c) a natural norm of the control, which is related to the nature of the optimization problem via the second order condition. Such error estimators are used in order to assess the accuracy of a computation and to increase it by local mesh refinement in an iterative manner. Different examples are given.

Discretize Then Optimize

John T. Betts
The Boeing Company, Seattle

Computational techniques for solving optimal control problems typically require combining a discretization technique with an optimization method. One possibility is to *Discretize Then Optimize*, that is first discretize the differential equations and then apply an optimization algorithm to solve the resulting finite dimensional problem. Conversely one can *Optimize Then Discretize*, that is write the continuous optimality conditions first and then discretize them. The goal of this paper is to compare the two alternatives and assess the relative merits.

NLP Strategies for PDE Models: An Application to Pressure Swing Adsorption (PSA) for Air Separation

Lorenz T. Biegler
Carnegie Mellon University, Pittsburgh

Pressure swing adsorption systems have become a key technology for gas separation, but have resisted the application of efficient optimization approaches. The talk describes the formulation of models and algorithms for the solution of design optimization problems for PSA systems. The resulting PDEs have dominant hyperbolic characteristics along with periodic boundary conditions. For design optimization, a number of standard integration and sensitivity tools are applied along with the development of a specialized reduced Hessian SQP method. The optimization strategy is an order of magnitude faster than conventional approaches and yields significant improvements over existing designs. Future work and extensions to larger PSA systems are also outlined.

State Estimation via Real-Time Optimization Based on Wavelet Techniques

Luise Blank
Universität Regensburg

In chemical engineering complex dynamic optimization problems have to be solved on-line. The need of a fast solution of the optimization problem is additionally restricted by the a priory unknown available computation time. Therefore, we propose a multiscale approach based on wavelets. It shall provide a coarse approximation after a very short time and upgrades iteratively the initial solution in each refinement step. The refinement costs shall be in relation to a given error improvement. Therefore, the information and solutions gained on coarser grids have to be exploited in each refinement step and on all levels of the optimization solver. Moreover, each discrete problem has to be solved only with an accuracy comparable to the current approximation error. Hence, we use an iterative solver also for the arising systems of linear equations, where problem adapted preconditioning is necessary. We will introduce the iterative wavelet based multiscale concept and will present numerical results as well as open questions.

Theory and Practice of Geometric and Algebraic Multigrid Methods for Elliptic Optimality Systems

Alfio Borzi
Karl-Franzens-Universität, Graz

An important class of efficient and robust solvers for optimization is represented by multigrid methods. We report our contribution to convergence theory for multigrid schemes applied to elliptic optimality systems and provide a link to our numerical experience with geometric and algebraic multigrid methods. Test cases are taken from the class of convection diffusion and semilinear singular problems on 2D and 3D domains.

Bounded Suboptimal Controls for Systems with Distributed Parameters

Felix L. Chernousko
Russian Academy of Sciences, Moscow

Linear systems described by PDEs of the 1st or 2nd order w.r.t. time and any even order w.r.t. space are considered (for example, heat, wave, and elastic beam equations). The system is subjected to a distributed bounded control. The problem is to bring the system to the prescribed terminal state in a finite (desirably, the shortest) time. The method of solution combines (1) a purely linear decomposition technique of Fourier series and (2) the nonlinear feedback time optimal control applied to each mode. As a result, the feedback control for the original PDE system is obtained in an explicit form. This control brings the system to the prescribed terminal state in time estimated from above. Sufficient controllability conditions are obtained which are reduced to the convergence of certain series. Examples are presented.

Affine Invariant Adaptive Newton Codes for Discretized PDEs

Peter Deuflhard
Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)
(joint work with Ulrich Nowak and Martin Weiser (both ZIB))

The paper compares three different types of Newton algorithms that have recently been worked out in the general frame of affine invariance. Of particular interest is their performance in the numerical solution of discretized boundary value problems (BVPs) for nonlinear partial differential equations (PDEs). Exact Newton methods, where the arising linear systems are solved by direct elimination, and inexact Newton methods, where an inner iteration is used instead, are synoptically presented, both in affine invariant convergence theory and in numerical experiments. The three types of algorithms are: (a) affine covariant (formerly just called affine invariant) Newton algorithms, oriented toward the iterative errors, (b) affine contravariant Newton algorithms, based on iterative residual norms, and (c) affine conjugate Newton algorithms for convex optimization problems and discrete nonlinear elliptic PDEs. The latter approach is carried over to the infinite dimensional case, which means to a function space oriented affine conjugate Newton method, realized as an adaptive multilevel finite element method for nonlinear elliptic PDEs. Numerical comparisons are included.

First and Second Order Shape Optimization Algorithms Using Wavelet-Based BEM

Karsten Eppler
Technische Universität Berlin
(joint work with Helmut Harbrecht (Technische Universität Chemnitz))

The talk deals with the numerical solution of 2D-elliptic shape optimization problems. Additional equality and inequality constraints are assumed to be given in terms of shape-differentiable domain or boundary integrals. First, the realizability of the Gradient and Quasi-Newton algorithm for a boundary variational approach is discussed with respect to the minimization of the penalty- or augmented Lagrangian functional. To compute the objective and the shape gradient, a wavelet-Galerkin BEM is used for solving the state equation. To proceed in a similar way for second order optimization methods, a complete boundary integral representation of the shape Hessian is required. The related second spatial derivatives of the solution and other quantities can be obtained by BIE-methods as well. Numerical results are presented for the problem of minimizing the volume of an elastic cylindrical bar (homogeneous and isotropic material) under given inequality constraints on the bending and torsional rigidity. Furthermore, related "dual" problems (maximize torsional rigidity subject to constraints on the volume and the bending stiffness, maximize bending rigidity ..) can be treated as well.

Aerodynamic Shape Optimization Based on Adjoint Formulations of the Compressible Euler/Navier-Stokes Equations for Complex Applications

Nicolas R. Gauger
German Aerospace Center (DLR), Braunschweig
(joint work with Norbert Kroll and Joel Brezillon (both DLR))

Aerospace industry is increasingly relying on advanced numerical flow simulation tools in the early aircraft design phase. Today's flow solvers, based on the solution of the Euler and Navier-Stokes equations, are able to predict aerodynamic behavior of aircraft components under different flow conditions quite well. Within the next few years numerical shape optimization will play a strategic role for future aircraft design. It offers the possibility of designing or improving aircraft components with respect to a pre-specified figure of merit subject to geometrical and physical constraints. The presentation will focus on both algorithmic developments as well as realistic applications. One key activity is the derivation and implementation of a continuous adjoint approach for the DLR flow simulation software MEGAFLOW based on the solution of the Euler and Navier-Stokes equations. Its potential for efficient aerodynamic shape design in compressible flow will be demonstrated.

Toward Inverse Earthquake Modeling

Omar Ghattas
Carnegie Mellon University, Pittsburgh
(joint work with V. Akcelik, J. Bielak (both Carnegie Mellon University) and G. Biros (New York University))

Toward our goal of modeling strong earthquakes in seismic regions, we are interested in determining mechanical properties of sedimentary basins (such as the greater Los Angeles Basin) and descriptions of earthquake sources from seismograms of past earthquakes. This gives rise to very large inverse problems of recovering the coefficients and source of the elastic wave equation from boundary observations of the response. Our current forward simulations involve 100 million finite elements; over the next several years the desired increase in resolution and growth in basin size will require an order of magnitude increase in number of unknowns. Inversion of such forward models provides a major challenge for inverse methods. It is imperative that these methods be able to scale algorithmically to $O(10^9)$ grid points, to highly-resolved (e.g. grid-based) elastic material models of large seismic basins, and to parallel architectures with thousands of processors.

I will discuss prototype parallel algorithms for the earthquake material and source inversion problem. Tikhonov and total variation regularization treat ill-posedness associated with rough components of the model, while multiscale grid/frequency continuation addresses multiple minima associated with smooth components. Parallel inexact Gauss-Newton-Krylov methods are used to solve the optimality conditions. CG matrix-vector products are computed via checkpointed adjoints, which involve forward and adjoint wave equation solutions at each iteration. Preconditioning is via limited memory BFGS updates, initialized with approximate inverses of an approximation to the Gauss-Newton Hessian. Experience on problems with up to several million grid points suggests near mesh-independence of Newton and CG iterations, good parallel efficiency, and distinct speedups over a quasi-Newton method. However, significant difficulties remain, and I will conclude with a discussion of these, along with possible avenues for addressing them.

This work is joint with V. Akcelik and J. Bielak at Carnegie Mellon, G. Biros at Courant, and other members of the Quake Project (www.cs.cmu.edu/∼quake).

Jacobian-Free Constrained Optimization

Andreas Griewank
Technische Universität Dresden

Classical algorithms for nonlinear optimization in n variables are based on evaluating the $m \times n$ Jacobian matrix formed by the $m \leq n$ active constraint gradients. The resulting nullspace matrix is obtained at a computational cost of $O(n^3)$, unless the Jacobian has a convenient sparsity pattern.

We consider two approaches to avoid the cubic cost in the general case. Firstly, the KKT system describing local stationarity can be solved by a matrix-free iterative solver of the MINRES type. Secondly, the Jacobian as well as the Hessian of the Lagrangian can be approximated be secant updates, which are invariant with respect to linear transformations of variables and constraints. The resulting total quasi-Newton method for (equality) constrained optimization has a cost of $O(n^2)$ arithmetic operations per step and exhibits local superlinear convergence. A limited memory variant is possible and may serve as a preconditioner for an inner iteration.

Simultaneous Pseudo-Timestepping for Aerodynamic Shape Optimization

Subhendu Bikash Hazra
Universität Trier
(joint work with Volker Schulz (Universität Trier))

In this talk I present a method for solving optimization problems with PDE constraints. It is based on simultaneous pseudo-timestepping for evolution equations. The new method can be viewed as a continuous reduced SQP method in the sense that it uses a preconditioner in the form of a reduced SQP method. The Hessian is approximated by corresponding operator of its symbol. The method is applied to an boundary control problem (Neumann to Dirichlet map). The new method needs approximately 4-times more overall effort than that of the analysis problem.

Efficient Numerical Methods for MPECs in Function Spaces

Michael Hintermüller
Karl-Franzens-Universität, Graz

Mathematical Programs with Equilibrium Constraints (MPECs) frequently arise in practical applications, e.g., in the form of bilevel optimization problems. In this case one has to deal with a minimization problem with one of its constraints being a constrained minimization problem again. Typically one of the optimization variables of the upper level problems occurs as a parameter in the lower level problem. We concentrate on MPECs arising from output least squares formulations of parameter identification in variational inequalities.

The literature on numerically amenable first order optimality characterizations in a function space setting is rather scarce. Moreover, many characterizations available are merely theoretical and cannot be utilized for numerical realization. Thus, our aim is twofold:

(1) Existence of multipliers in function spaces is proved. The corresponding first order optimality system is immediately amenable to numerics.

(2) A Newton-type method with an implicit programming flavor is derived.

The existence proof for (1) utilizes rather classical tools. Since the key steps of the proof are constructive in the sense that one may derive a numerical scheme by following the proof ideas, these key steps are highlighted. They essentially consist of a penalization step which together with a smoothing step and the combination with NCP-functions allows to apply classical results. Finally passing to the limit for the regularization parameter gives our first order system.

A report on results obtained by the new algorithm shall emphasize the feasibility and efficiency of our approach. The problems include the challenging situations where the lower level problem suffers from lack of strict complementarity.

Error Estimates for Discrete Controls of Time Dependent Navier-Stokes Systems

Michael Hinze
Technische Universität Dresden

In the first part of the talk a new discretization concept for abstract control problems with control constraints is introduced. Discretization only is applied to the state variables, which in turn implicitly introduce 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 semi-smooth Newton methods are discussed.

Regularization by Discretization and Multigrid Methods for Ill-posed Problems

Barbara Kaltenbacher
Universität Erlangen

Inverse problems, such as the determination of parameters in PDEs, are typically ill-posed in the sense of unstable dependence of a solution on the data and therefore have to be regularized. This talk deals with the principles of regularization by discretization for linear and nonlinear problems, gives some convergence results and discusses computational aspects especially in the context of parameter identification in differential equations. To speed up convergence, we propose special multigrid methods that are appropriate for such unstable problems. In an application from nonlinear magnetics, namely the determination of B-H curves, we have used some of the proposed methods and show obtained numerical results.

Design of Groundwater Remediation Systems with Implicit Filtering

C. Tim Kelley
North Carolina State University, Raleigh

In this talk I discuss a model problem in optimal design of groundwater remediation/supply systems. The objective function and constraints are built with PDE solves for the flow and transport equations. The objective function and constrains are nonsmooth, nonconvex, and possibly discontinuous functions of the design variables. We show how sampling methods, implicit filtering in particular, can solve such problems.

Semi-Smooth Newton Methods for Control and State Constrained Optimal Control Problems

Karl Kunisch
Karl-Franzens-Universität Graz
(joint work with Michael Hintermüller (Karl-Franzens-Universität Graz) and Kazufumi Ito (North Carolina State University))

Open loop optimal control problems with control and state constraints lead to optimization problems with pointwise constraints in function space. Control, respectively state constraints, differ with respect to the regularity of the associated Lagrange multiplier. For the former they are L^2, for the latter Borel measures. This difference significantly effects the analysis and numerical behavior of algorithms. For efficient solution of the above problems the primal-dual active set strategy is proposed. Its equivalence to semi-smooth Newton methods is shown. Global convergence and local superlinear convergence are analyzed. To cope with the lack of regularity in the case of state constraints a continuation method is proposed.

Adaptive Wavelet Methods for Linear–Quadratic Elliptic Control Problems

Angela Kunoth
Universität Bonn
(joint work with Wolfgang Dahmen (Technische Hochschule Aachen))

We propose an adaptive algorithm based on wavelets for the fast numerical solution of control problems governed by elliptic boundary value problems with distributed or Neumann boundary control. A quadratic cost functional that may involve fractional Sobolev norms of the state and the control is to be minimized subject to linear constraints in weak form. Placing the problem into the framework of (biorthogonal) wavelets allows to formulate the functional and the constraints equivalently in terms of ℓ_2-norms of wavelet expansion coefficients and constraints in form of an ℓ_2 automorphism. The resulting first order necessary conditions are then derived as a (still infinite) system in ℓ_2. Applying the machinery developed by Cohen, Dahmen and DeVore, we propose an adaptive method which can be interpreted as an inexact gradient method, where in each iteration step the primal and the adjoint system needs to be solved up to a prescribed accuracy. In particular, we show that the adaptive algorithm is asymptotically optimal, that is, the convergence rate achieved for computing the solution up to a desired target tolerance is asymptotically the same as the wavelet-best N-term approximation of the solution, and the total computational work is proportional to the number of computational unknowns.

Reduced Order Controller Design by Solving Nonlinear Semidefinite Programs

Friedemann Leibfritz
Universität Trier

The problems of designing static or reduced order output feedback compensators that meet desired performance and/or robustness specifications are important examples of difficult and in general non convex, nonlinear control problems. Such control problems can be reformulated as nonlinear and non convex matrix optimization problems including nonlinear matrix inequalities. In this talk, we discuss some aspects of such nonlinear SDP's and present a fully iterative algorithm for finding local minimizers. Finally, we consider several reduced order output feedback design examples and demonstrate the applicability of the proposed numerical procedure.

Optimal Control Of Partial Differential Equations On Networked Domains: Domain Decomposition

Günter Leugering
Technische Universität Darmstadt

We consider the problem of optimal control of hyperbolic linear and nonlinear partial differential equations on networked domains. Examples are networks of gas-pipelines, networks of open and closed canals, networks of roads and flexible structures. We mainly focus in this talk on iterative domain decomposition techniques with respect to space and time. Convergence analysis, a posteriori error estimates and numerical evidence are provided.

In particular, in the context of optimal control of networked gas-pipelines, one has to consider the flow of gas, modeled by the Euler gas equations in each individual pipe, which undergoes a drop of pressure due to friction in the pipes. Therefore, in order to maintain the pressure within the entire system of coupled pipelines, and in order to supply the customers with gas of a certain quality and within certain pressure bounds at given boundary nodes of the network, compressors are introduced into the network as well as valves. The action of a compressor is an expensive task, and the action of the valves, in order to steer the flux of gas into the desired regions of the network (or to modify the the overall topology under certain operation scenarios), has to be taken with care in order to not produce shock waves and other unwanted dynamics within the network. The cost function involves the operational costs of the system (e.g. the consumption of gas by the compressors) and quality requirements. Obviously, this optimal control problem is a very challenging enterprise, and it is fair to say that the research on this level modeling is only in its infancy.

It is clear that the problem just described is exemplary in its nature. The scenario is directly transferable to the control of flow of sewer- and irrigation systems, traffic flow and much more. Domain decomposition methods in space and time are just one tool in the analysis of this class of problems. By those methods the problem can be dramatically reduced in its complexity and can be handled, on a local level, in parallel.

Methods Based on Multiple Grids for the Optimization of Systems Governed by PDEs

Robert Michael Lewis
College of William and Mary, Williamsburg

In the first part of this talk, we present a nonlinear programming approach to using multiple levels of discretization when the number of optimization (design) variables is fixed. The approach is based on correcting objective and constraint values computed on using a coarse mesh so they agree to first order with fine mesh values. The corrected low fidelity objective and constraint values are then used a non-linear but non-quadratic approximations in existing optimization algorithms. Global convergence (first order) is guaranteed through the use of trust-regions. In the second part of the talk, we present an argument, based on the conjugation of terms in the reduced Hessian by the solution operators of hyperbolic PDE, for why multigrid may broadly applicable to systems governed by hyperbolic equations. This idea is illustrated by an explicit example.

Recursive Global Minimization by Solution of Boundary Value Problems: Applications to Aerodynamic Shape Optimization and State Control

Bijan Mohammadi
Université de Montpellier II

We show how to reformulate some well-known minimization algorithms in term of dynamic systems. Global minimization is then presented through the solution of over-determined boundary value problem. The problem is solved using a shooting method. Hence, we see why classical descent methods are unable to perform global minimization. The complexity of the approach is negligible compared to evolutionary algorithms. But, the approach requires the knowledge of the infimum of the functional.

The approach is validated through the minimization of several strongly non-convex functionals.

The second part of the talk concerns industrial shape optimization problems. We present some new aerodynamic applications as well as a new application for the design of microfluidic devices. In each case, the multi-model PDE solver used for state evaluation is shortly presented and shape design, state control and parameter identification problems encountered in these applications are analyzed.

Preconditioning for Heterogeneous Problems

Sergey Nepomnyaschikh
Siberian Division of the Russian Academy of Sciences, Novosibirsk

Preconditioning for heterogeneous elliptic problems is considered. The basis for the construction of preconditioning operators in this talk is domain decomposition methods. Suggested domain decomposition technique involves the construction of local preconditioning operators and interface preconditioning operators. For the latter preconditioners we need to investigate Schur complements or trace theorems in the corresponding Sobolev spaces.

Simulation of Molten Carbonate Fuel Cells and their Controllability Devices

Hans Josef Pesch
Universität Bayreuth
(joint work with Kurt Chudej, Verena Petzet, Sabine Scherdel, and Klaus Schittkowski
(all Universität Bayreuth))

Molten carbonate fuel cells (MCFC) are environmentally friendly energy sources with high efficiency. Without combustion, MCFC convert chemical energy contained in fuel and oxidizer to electric energy via electro-chemical reactions. Performance, availability and service life of MCFC stacks are greatly dependent on their operating temperature. Higher operation temperatures accelerate material corrosion, which shortens the life span of the stacks. So, control of the operation temperature within a specified range and reducing temperature fluctuations and gradients are are highly desirable. By means of a hierarchy of spatial 1D models of increasing complexity, which are due to K. Sundmacher and P. Heidebrecht (Lehrstuhl für Systemverfahrenstechnik, Otto-von-Guericke-Universität Magdeburg, and Max-Planck-Institut für Dynamik komplexer technischer Systeme) the cell's dynamical behaviour is simulated, in particular the temperature distribution in the solid, and the transport of the various chemical species that are involved in the reforming reaction as well as in the anode and cathode reactions. This model consists of up to 24 partial differential equations of mixed parabolic-hyperbolic type. In addition, some of the equations are algebraic or contain an integral part. The system can be characterized as a semilinear system of partial diffential-algebraic equations. First, the temporal and spatial differentiation indices are analyzed. Since the simulation is carried through via the method of lines (MOL) by using central differences for the parabolic equation and upwind differences for the transport equations, the temporal and spatial MOL differentiation indices are additionally investigated. Because the semidiscretized ordinary diffential-algebraic system is semi-explicit, the differentiation indices equal the perturbation indices. Parameter identification and optimal control can then be performed using the software package EASYFIT of K. Schittkowski. Here the time integration is done by the RADAU5 method. Numerical results are presented which correspond to the physical behaviour as far as it is known.

(Shortly after the Oberwolfach meeting also a spatial 2D model has been simulated successfully.)

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Sensitivity Analysis and Optimization for Large-Scale Differential-Algebraic Equation Systems

Linda R. Petzold
University of California Santa Barbara

Sensitivity analysis generates essential information for design optimization, optimal control, model reduction, process sensitivity and experimental design. Recent work on methods and software for sensitivity analysis of differential-algebraic equation (DAE) systems has demonstrated that forward sensitivities can be computed reliably and efficiently. However, for problems which require the sensitivities with respect to a large number of parameters, the forward sensitivity approach is intractable, and the adjoint (reverse) method is advantageous. In this talk we give the adjoint system for general DAEs, and investigate some of its fundamental analytical and numerical properties. Then we show how the adjoint method may be employed to advantage in design optimization and optimal control.

Optimal Error Estimates for Abstract Linear-Quadratic Optimal Control Problems

Arnd Rösch
Technische Universität Berlin

Linear-qudratic problems are important subproblems in nonlinear optimization. The control has to be discretized for numerical computing. We discuss here the case of a control discretization by piecewise linear functions. For optimal controls which are lipschitz and piecewise C^2 can be proved that the convergence order of this approximation is $\sigma^{3/2}$. These strong assumptions do often not fit with optimal control problems for PDEs. For the heat equation it is shown that nonuniform grids can ensure the optimal convergence order $\sigma^{3/2}$. Numerical examples confirm the theoretical results.

Topology Optimization for Wave-Propagation Problems

Ole Sigmund
Technical University of Denmark, Lyngby

The lecture starts with a short introduction to the topology optimization method and a review of the state of the art in the field. Then the application of the method to wave-propagation problems is motivated by examples of band gap materials and structures. Band gap materials are composite materials that inhibit wave-propagation in certain frequency ranges. For the material problem a max-min formulation allows for maximization of the relative band gap size. For the structural problem various formulations of the optimization problem allows for the systematic design of wave-guiding structures, focusing lenses and resonant devices.

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A Smooth Domain Method for Crack Problems

Jan Sokołowski
Université Henri Poincaré Nancy I

Equilibrium problems for elastic bodies in domain with cracks are considered [1]. Inequality type boundary conditions are imposed at the crack describing a mutual nonpenetration between the crack faces. A new formulation for such problems is proposed [2] in smooth geometrical domains for two dimensional elasticity.

The resulting mathematical model allows us to solve numerically the crack problem in a smooth domain. The error estimates for the finite element approximation are obtained and the results of computations for a scalar model problem are given [3]. The elasticity case is considered in [4].

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Error Estimates for Elliptic Optimal Control Problems

Fredi Tröltzsch
Technische Universität Berlin

The talk surveys error estimates for optimal control problems of elliptic equations that are discretized by numerical approximation of the state equation and/or of the control functions. First, we report on the case of a semilinear equation with homogeneous Dirichlet boundary condition, nonlinear integral functional and distributed control subject to box constraints. Here, the equation is discretized by a finite element method and the control function is taken piecewise constant. L^2- and L^∞-estimates are stated for the difference between a continuous reference control and its discrete counterpart. A test example confirms the predicted error estimate of order h, the mesh size of the grid. The main part of the talk is focussed on linear-quadratic elliptic problems with boundary observation and box-constrained control acting in a Robin boundary condition. We concentrate on the discretization of controls while keeping the equation undiscretized. The error analysis is presented for piecewise constant and piecewise linear controls on uniform grids. Again, the error is of the order of the mesh size.

Mesh Independence of Semismooth Newton Methods for Variational Inequalities

Michael Ulbrich
Universität Hamburg
(joint work with Michael Hintermüller (Karl-Franzens-Universität Graz))

We consider a class of variational inequalities that can be reformulated as an equivalent semismooth operator equation. For the solution of this problem, a q-superlinearly convergent Newton-type method is presented. We show that for appropriate numerical discretizations this Newton iteration is mesh independent. The results are applied to a control constrained optimal control problem for semilinear elliptic equations. Numerical results are presented that confirm the mesh independence and efficiency of the method.

Primal-Dual Interior Point Methods for PDE-Constrained Optimization

Stefan Ulbrich
Technische Universität München

We propose and analyze primal-dual interior point Newton methods for control-constrained optimization problems for PDEs. The algorithm is based on following the central path by applying Newton's method to the optimality system with perturbed complementarity condition. We consider the general framework, where the reduced Hessian is the sum of a multiplication operator and an operator that is bounded from L^p to L^q for some $q > p$.

In the case $q = \infty$ we prove quadratic local convergence of the corrector and global linear convergence of the primal-dual path following algorithm. For $q \leq \infty$ we use a smoothing step together with a projection on a neighborhood of the central path to obtain global linear and locally superlinear convergence of the algorithm. We briefly discuss sufficient conditions for regularity and the choice of smoothing steps.

Finally, we present numerical results for a control-constrained elliptic control problem by using the primal-dual algorithm with nested iteration on refined grids. Moreover, we show that the proposed algorithm is also efficient for state-constrained problems.

Numerical Optimization of Laser Surface Hardening of Steel

Stefan Volkwein
Karl-Franzens-Universität, Graz

Laser surface hardening of steel is formulated in terms of an optimal control problem with bilateral control constraints, where the state equations are a semilinear heat equation and an ordinary differential equation, which describes the evolution of the high temperature phase. To avoid the melting of the steel we have to impose pointwise state constraints for the temperature. Utilizing a penalty approach these constraints are treated numerically. In this talk we present an error analysis for the model equations utilizing a POD (Proper Orthogonal Decomposition) Galerkin semi- implicit Euler approximation. Features of the obtained error estimate are discussed for a numerical example of the laser hardening. To solve the optimal control problem, a nonlinear primal-dual active set strategy is applied. Within this algorithm the optimal control problems with equality constraints are solved by a variant of the non-linear conjugate gradient method, which is globally convergent. Finally, also an three-dimensional example is presented.

An Adaptive Multilevel Central Path Method for Optimal Control

Martin Weiser
Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)
(joint work with Peter Deuflhard (ZIB))

A novel approach to the numerical solution of optimal control problems for ODEs with control and state constraints is presented. The method is directly based on interior point concepts in function space - realized via an adaptive multilevel scheme applied to the complementarity function and numerical continuation along the central path. Existence and convergence results for the central path are presented. An adaptive continuation stepsize control is worked out in the framework of inexact affine invariant Newton methods. Finally, the effectiveness of the method is documented by the successful treatment of the windshear problem.

Edited by Matthias Heinkenschloss

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