



Workshop within the GAMM activity group 'Optimization with Partial Differential Equations'

PDE Constrained Optimization - recent challenges and future developments



March 27-29, 2008
in Hamburg



last update:
March 26, 2008

Speakers

	Invited talks	50 Min + 10 Min
A	Walter Zulehner	Multigrid Methods for Mixed Variational Problems and their Convergence Analysis
B	Karl Kunisch	Some Considerations for Numerical Realization of Closed Loop Optimal Control
C	Ekkehard Sachs	Optimization Methods in Finance
D	Ralf Kornhuber	Constrained Minimization and Multigrid
	Contributed talks	25 Min + 5 Min
01	Thomas Slawig	CO_2 -Uptake of the Ocean - Parameter Optimization in Biogeochemical Models
02	Michael Köster	Efficiently Solving Optimal Control Problems in CFD Using Space-Time Multigrid Techniques
03	Martin Engel	A Newton-Multigrid Method for One-Shot PDE-Constrained Optimization
04	Jens Saak	Efficient numerical solution of large scale matrix equations arising in LQR/LQG design for parabolic PDEs
05	Dieter Sirch	L^∞ -error estimates in non-convex domains with application to optimal control
06	Timo Tonn	A-Posteriori Error Estimators for RBM Applied to Quadratic Non-Linear PPDEs (Involving Non-affine Coefficient Functions)
07	Peter Benner	Some Approximation Results for Differential Operator-Riccati Equations in PDE Control
08	Anton Schiela	State Constrained Optimal Control with Discontinuous States
09	Hanne Tiesler	Identification of Material Parameters for Thermal Ablation
10	Winnifried Wollner	Adaptive FEM for PDE Constrained Optimization with Pointwise State Constraints
11	Martin Pach	Shape Optimization Under Uncertainty – A Stochastic Programming Perspective
12	Adel Hamdi	Alternating approach for solving design optimization problem
13	Stephan Schmidt	Analytic and Discrete Shape Hessian Approximations
14	Caslav Ilic	Ingredients for Practical Large-Scale Aerodynamic Optimization
15	Ralf Leidenberger	Automatic Differentiation for the Optimization of a Ship Propulsion and Steering System
16	Marcus Wagner	Edge detection within optical flow by multidimensional control
17	Morten Vierling	A semismooth Newton algorithm for the semi-discretization of pde constrained optimization problems with control constraints

Schedule

Thu, 27/03

13:30 - 14:30 Invited talk A
14:30 - 15:00 Coffee break
15:00 - 17:00 Contributed talks 01-04
17:00 - 17:30 Coffee break
17:30 - 18:30 Contributed talks 05-06
18:30 - Meeting of the GAMM activity group

Fri, 28/03

09:00 - 10:00 Invited talk B
10:00 - 10:30 Coffee break
10:30 - 12:30 Contributed talks 07-10
12:30 - 14:00 Lunch
14:00 - 16:00 Contributed talks 11-14
16:00 - 16:30 Coffee break
16:30 - 17:30 Invited talk C

Sat, 29/03

09:00 - 10:00 Invited talk D
10:00 - 10:30 Coffee break
10:30 - 12:00 Contributed talks 15-17

All talks are going to take place in H5 at the ground floor of the Geomatikum.

Abstracts

A

Multigrid Methods for Mixed Variational Problems and their Convergence Analysis

Walter Zulehner

Johannes Kepler University Linz

We consider two different approaches for mixed problems, such as KKT systems for PDE-constrained optimization problems, to take advantage of the multigrid idea.

One way is to use an outer iteration, typically a block-preconditioned Richardson method, applied to the (discretized) mixed problem. Multigrid techniques (as an inner iteration or approximation) can be used for setting up the blocks of the block-preconditioner.

The other way is to use multigrid methods directly applied to the (discretized) mixed problem as an outer iteration based on appropriate smoothers (as a sort of inner iteration). This approach is also known as one-shot multigrid strategy. One of the most important ingredients of such a multigrid method is an appropriate smoother.

In this talk we consider typical examples for these two approaches applied to an elliptic control problem and discuss the convergence analysis of these methods.

B

Some Considerations for Numerical Realization of Closed Loop Optimal Control

Karl Kunisch

University of Graz

Open loop optimal control solutions are not stable with respect to system perturbations. This suggests considering alternatives based closed loop concepts. We discuss the possibility of obtaining suboptimal solutions of the Hamilton Jacobi Bellman equation by means of POD-based model reduction. Further we address receding horizon ideas in conjunction with control Ljapunov functions.

Ljapunov-function concepts can also be used advantageously to suggest feedback control strategies: We illustrate this point by optimal control of the potential term in the Schrödinger equation.

C

Optimization Methods in Finance

Ekkehard Sachs

University of Trier, Virginia Tech - Blacksburg

There is a widespread use of mathematical tools in finance, whose importance has grown over the last two decades. We give an overview over some of the applications of optimization in finance, in particular the pricing of derivative products.

As an example we take an in-depth look at the problem of hedging barrier options. We review approaches from the literature and illustrate advantages and shortcomings. Then we

rephrase the problem as an optimization problem and point out that it leads to a semi-infinite programming problem. We give numerical results and put them in relation to known results from other approaches.

As an extension we consider the robustness of this approach. We show how the optimality is lost, if the market data change. To avoid this effect, one can formulate a robust version of the hedging problem and solve it numerically. The results illustrate the robustness of this approach and its advantages.

We conclude with an outlook on other optimization problems in finance, in particular calibration problems and their challenges.

D

Constrained Minimization and Multigrid
Carsten Gräser, **Ralf Kornhuber**, Oliver Sander
Freie Universität Berlin

Starting from a reinterpretation of classical multigrid methods in terms of successive minimization, we present a hierarchy of generalizations to elliptic obstacle problems which finally lead to novel active set methods. A novel minimization approach is proposed for a class of optimal control problems with control constraints. In this case, straightforward application of nonsmooth Newton techniques to the Lipschitz-continuous Schur complement leads to novel preconditioned Uzawa-type algorithms which can be regarded as generalizations of well-known primal-dual active set methods.

01

*CO*₂-Uptake of the Ocean - Parameter Optimization in Biogeochemical Models

Thomas Slawig

University of Kiel

A lot of atmospherical *CO*₂ is dissolved in the water of the ocean. For the prediction of global climate scenarios the capability of the oceans to dissolve and store *CO*₂ and the sensitivities of these effects to climate change itself are crucial. The numerical investigation of the *CO*₂ uptake of the oceans is based on coupled fluid mechanical and nonlinear biogeochemical transport models. The latter are undergoing current research, and thus the problem of model and parameter choice and optimization is important. A characteristic point is that the models have to be run into periodic states to evaluate their quality. We show the model structures and present the techniques for parameter optimization based on efficient calculation of periodic solutions. Here we propose variants of Newton's method that can be used to compute the periodic state and a cost derivative simultaneously.

02

Efficiently Solving Optimal Control Problems in CFD Using Space-Time Multigrid Techniques

Michael Hinze, **Michael Köster**, Stefan Turek

TU Dortmund

In this talk, we deal with the optimal control of the nonstationary Navier–Stokes problem over a fixed time interval $[0, T]$. The usual way to solve is to deal with the primal and dual equation in a separate fashion, e.g. first solving for the primal, then for the dual, then repeating this process.

Although this is the most common and natural way, in some sense it contradicts the nature of the problem. The analysis shows that the full KKT system for optimal control of the nonstationary Navier–Stokes equations over a fixed time cylinder is of elliptic type when treating space and time in a coupled manner. Then, the most natural solver for an elliptic problem – at least of linear type – is multigrid. This algorithm promises excellent convergence rates, being independent of the global mesh size of the space-time cylinder. Embedded as preconditioner for the linear subproblems in a nonlinear Newton iteration, this approach leads to fast convergence of the whole iteration.

Based on the One-Shot approach, we discretise the distributed optimal control KKT system on unstructured meshes with \tilde{Q}_1/Q_0 finite elements in space and standard implicit and semi-explicit timestepping schemes in time. For solving the discrete problem, we present a space-time multigrid solver that is able to simultaneously solve for primal and dual variables. Numerical analysis shows the high potential of this type of preconditioner, allowing the outer Newton iteration to converge in only very few nonlinear steps.

03

A Newton-Multigrid Method for One-Shot PDE-Constrained Optimization

Martin Engel

University of Bonn

We present a Newton-Multigrid method for the fast solution of PDE-constrained optimization problems. Applying an (inexact) Newton method to the first-order optimality conditions yields a sequence of quadratic optimization problems. Since these QPs are indefinite and notoriously ill-conditioned, efficient preconditioning is mandatory when solving the coupled system with iterative solution methods. We propose a multigrid solver with a relaxation method that is based on constraint preconditioning. In order to solve control-constrained problems, our multigrid method is employed within a primal-dual active-set approach.

04

Efficient numerical solution of large scale matrix equations arising in LQR/LQG design for parabolic PDEs

Jens Saak

TU Chemnitz

Feedback control of systems governed by partial differential equations has been an engineers desire for many decades now. Linear Quadratic Regulator (LQR) design and Linear Quadratic Gaussian (LQG) design have been investigated in the literature since the pathbreaking work of Lions, showing that these methods are valuable tools in achieving this task.

The solution of large scale Lyapunov and Riccati equations is a major task in applying the above techniques to semi-discretized partial differential equations constraint control problems. The software package LyaPack has shown to be a valuable tool in the task of solving these equations since its introduction in 2000.

Here we want to discuss recent improvements and extensions of the underlying algorithms and their implementation.

05

L^∞ -error estimates in non-convex domains with application to optimal control

Thomas Apel, Arnd Rösch, **Dieter Sirch**

Universität der Bundeswehr München

In this talk pointwise error estimates for an optimal control problem for a two-dimensional elliptic equation with pointwise control constraints are derived. The domain is assumed to be non-convex. A priori mesh grading is used to treat the corner singularities. For discretizing the state linear finite elements are used, the control is approximated by using piecewise constant ansatz functions. First it is proven that the L^∞ -error of the finite element approximation of the state equation with Dirichlet boundary conditions is of order $h^2 |\ln h|$. In contrast to previous publications the norm of the function, that has to be approximated, is separated from the constants in this estimate. In order to get this optimal estimate in the case of a non-convex domain a stronger mesh grading is necessary than for the error estimates in the H^1 - and L^2 -norms. Using this estimate one can derive a pointwise error estimate for the optimal control problem. Approximations of the optimal solution of the continuous optimal control problem are constructed by a projection of the discrete adjoint state. For this approximation a convergence order of $h^2 |\ln h|$ is shown.

A-Posteriori Error Estimators for RBM Applied to Quadratic Non-Linear PPDEs (Involving Non-affine Coefficient Functions)

Timo Tonn

University of Ulm

In "A reduced-basis method for solving parameter-dependent convection-diffusion problems around rigid bodies.", K.Urban, T.Tonn, 2006, we consider a convection-diffusion problem in a box in which rigid bodies are present. The location and orientation of these bodies are subject to a set of parameters. In order to use a reduced-basis method, we perform a two-step method. In the first step, we transform the parameter-dependent geometric situation to a reference situation (also mapping the mesh). Then, we use the Empirical Interpolation Method (EIM) in order to separate the parameter from the variables of the PDE.

In this subsequent paper we present the error analysis for the quadratic non-linear convection-diffusion problem equipped with possible non-affine (w.r.t. the parameter) coefficient functions. The error analysis itself is based on "Certified real-time solution of parametrized steady incompressible Navier-Stokes equations: rigorous reduced-basis a posteriori error bounds", K.Veroy, A.T.Patera, 2005, which itself invokes the Brezzi-Rappaz-Raviart theory for the analysis of variational approximations of non-linear PDEs. In addition to some slight generalizations, the main new contribution is the incorporation of the non-affine coefficient functions for rigorous, quantitative, sharp and inexpensive a-posteriori error estimation for both the field variable and the linear-functional output.

Some Approximation Results for Differential Operator-Riccati Equations in PDE Control

Peter Benner, Hermann Mena

TU Chemnitz

The solution of linear-quadratic optimal control problems for linear parabolic PDEs on finite time horizons is known to be a feedback control where the control function is defined via the solution of a differential operator Riccati equation. The practical solution of such PDE constraint optimal control problems usually requires the discretization of the underlying PDE. Correspondingly, a matrix differential Riccati equation (DRE) yields the solution of the semi-discretized (in space) linear-quadratic optimal control problem. In this talk we will discuss the convergence of the solutions of the matrix DRE to the solution of the operator DRE. The results extend earlier work by Banks and Kunisch (and others) for algebraic Riccati equations arising in the context of linear-quadratic optimal control problems with infinite time horizon.

State Constrained Optimal Control with Discontinuous States

Anton Schiela

Zuse Institute Berlin

State constrained optimal control is well understood in the case where the control-to-state mapping yields continuity of the states. Then a Slater point asserts existence of measure

valued Lagrange multipliers. If continuity and boundedness of the states does not hold, the situation is less clear, and it is the purpose of this talk to shed some light on this situation.

We discuss a new result on optimality conditions, which exploits a Slater condition also in the case of discontinuous and possibly unbounded states. It applies, if the space of those controls that yield continuous states is dense in the space of all controls. In this case we can show existence of measure valued Lagrange multipliers, which have just enough additional regularity to make the positivity and complementarity conditions well defined.

09

Identification of Material Parameters for Thermal Ablation

Hanne Tiesler

CeVis, University of Bremen

We focus on the identification of thermal and electrical conductivities for thermal ablation, e.g. radio-frequency ablation. Radio-frequency ablation of tumors means that a probe, which is connected to an electric generator, is placed inside the malignant tissue and heated by an electric current such that the proteins coagulate and the tissue cells die.

To compute an optimal probe placement we need the thermal and the electrical conductivities which are not known exactly. From measurement data of the temperature distribution the parameters are reconstructed by formulating the inverse problem as an optimal control problem. Thus, we solve a minimization problem with the heat equation and the potential equation as constraints, and where those two equations are coupled through source terms of the heat equation. We use a finite element method to solve the constraining PDE system.

10

Adaptive FEM for PDE Constrained Optimization with Pointwise State Constraints

Winnifried Wollner

University of Heidelberg

In this talk we will consider an optimization problem of the form

$$\min J(q, u) = \frac{1}{2} \|u - u^d\|^2 + \frac{\alpha}{2} \|q\|^2,$$

subject to the control constraints $q \in Q^{\text{ad}}$ with some closed convex set $Q^{\text{ad}} \subset L^2(\Omega)$. In addition the control q and the state u are connected by a second order elliptic equation, e.g.

$$(\nabla u, \nabla \phi) = (q, \phi) \quad \forall \phi \in H_0^1(\Omega).$$

We are here especially interested in an additional constraint of the form

$$u \leq \psi \quad \text{on } \bar{\Omega}.$$

For the solution of the problem we consider an interior point method. We will derive a posteriori error estimates for the error in the value of the cost functional with respect to the interior point parameter as well as with respect to the discretization parameter. The findings will be substantiated by numerical examples.

We present an algorithm for shape-optimization under stochastic loading, and representative numerical results. Our strategy builds upon a combination of techniques from two-stage stochastic programming and level-set-based shape optimization. In particular, usage of linear elasticity and linear objective functions permits to obtain a computational cost which scales linearly in the number of *linearly independent* applied forces, which often is much smaller than the number of different realizations of the stochastic forces. Numerical computations are performed using a level-set method with composite finite elements both in two and in three spatial dimensions.

Our talk concerns a design optimization problem, where the constraint is a state equation that is solved by some given fixed point solver. To exploit the domain specific experience and expertise invested in the simulation tool we propose to augment it by a corresponding adjoint solver, and based on the resulting approximate reduced derivatives, also an optimization iteration, which actually changes the design. To coordinate the three iterative processes, we consider an augmented Lagrangian function that should be consistently reduced whatever combination of sequence of primal, dual and optimization steps one chooses. This function depends on weighting coefficients which involve the primal and dual residuals and on the Lagrangian. The key question is the choice of the weighting coefficients and the construction of a suitable preconditioner in order to get a reasonable convergence rate of the coupled iteration.

Shape derivatives allow using all surface mesh nodes as a design parameter but often suffer from high frequency noise. The impact this noise has on the performance is determined by the shape Hessian. We will first study the shape Hessian for a Stokes fluid analytically via its symbol using Fourier analysis. Next, we develop a numerical scheme to approximate the symbol very cost effective via impulse response techniques by observing wave propagations through the discrete operator. Comparisons with the analytical results show the correctness of the numerical method. Based on this information, we construct a preconditioner for the gradient turning our steepest descent method into an approximative Newton scheme. We conclude with application examples for shape optimization in both Stokes and Navier-Stokes fluid problems.

Ingredients for Practical Large-Scale Aerodynamic Optimization
Nicolas Gauger, **Caslav Ilic**, Stephan Schmidt, Volker Schulz
DLR Braunschweig

Adjoint-based optimization in industrial aerodynamic applications does not realize in practice the independence of the size of the design space implied by the adjoint approach. We show the reasons behind this by analyzing the procedures and complexities in a typical optimization setup. We follow by demonstrating on example problems several methods which may be used to remove the observed obstacles: the surface mesh node parametrization, preconditioning of the gradient descent, and shape derivatives in gradient computation. Theoretical considerations leading to these methods are stated briefly as well. Finally, we stack the methods together on a 2D Euler transonic/supersonic drag optimization example, producing runtime complexity near to independent of the number of design variables.

Automatic Differentiation for the Optimization of a Ship Propulsion and Steering System
Ralf Leidenberger, Karsten Urban
University of Ulm

In this talk, we present an approach to optimize complex nonlinear functionals arising in numerical simulations. In particular, we use gradient based optimization algorithms. The underlying numerical simulations are carried out with a finite volume method in two as well as three space dimensions. The computation of the required derivatives is realized with automatic differentiation. Finally, we apply this approach for the optimization of an industrial ship propulsion and steering system.

Automatic differentiation (AD) is well-known as a method to compute derivatives within a numerical simulation. The idea of this approach is to differentiate the source code of a computer program line by line. The main known advantages of automatic differentiation are a regularization effect compared to numerical differentiation (in particular in complex nonlinear problems), and the possibility to obtain sensitivities directly in the simulation. The regularization effect enables the application of gradient based optimization algorithms for the numerical optimization instead of gradient-free optimization algorithms. This is useful in particular in cases when the computation of derivatives with finite differences is not possible, not stable or too costly.

The Voith-Schneider-Propeller (VSP) is an industrial propulsion and steering system of a ship combined in one module constructed and manufactured by Voith Turbo Marine, Heidenheim (Germany). In order to optimize the efficiency of the VSP, we simulate the flow around the VSP and use numerical optimization. In order to compute the efficiency, we need tangential and normal forces, acting on the blades of the VSP. These forces are given by the integral of the pressure over the blade surfaces.

We apply this automatic differentiation optimization approach firstly in the two dimensional case on the code CAFFA, which is a freeware program for flow simulation written by Ferziger and Peric. In the three dimensional case, we use the commercial program Comet from CD-adapco. The talk is partly based upon joint work with CD-adapco.

Edge detection within optical flow by multidimensional control
 Christoph Brune, Helmut Maurer, **Marcus Wagner**
 BTU Cottbus

We discuss the reformulation of the optical flow problem as a multidimensional control problem of Dieudonné-Rashevsky type,

$$\begin{aligned}
 F(x, u) &= \int_{\Omega} \left(I_{s_1}(s) x_1(s) + I_{s_2}(s) x_2(s) + I_t(s) \right)^2 ds \\
 &+ \mu \cdot \int_{\Omega} r(s, u_{11}(s), u_{12}(s), u_{21}(s), u_{22}(s)) ds \longrightarrow \inf!; \quad (x, u) \in W_0^{1,p}(\Omega, \mathbf{R}^2) \times L^\infty(\Omega, \mathbf{R}^{2 \times 2}); \\
 Jx(s) &= \begin{pmatrix} u_{11}(s) & u_{12}(s) \\ u_{21}(s) & u_{22}(s) \end{pmatrix} \quad (\forall) s \in \Omega; \\
 u \in U &= \left\{ u \in L^p(\Omega, \mathbf{R}^{2 \times 2}) \mid |u_{11}(s)|^q + |u_{12}(s)|^q + |u_{21}(s)|^q + |u_{22}(s)|^q \leq R^q \quad (\forall) s \in \Omega \right\},
 \end{aligned}$$

which allows a simultaneous detection of edges within the flow via the control variables u_{ij} . Numerical solutions by direct methods will be presented.

A semismooth Newton algorithm for the semi-discretization of pde constrained optimization
 problems with control constraints
 Michael Hinze, **Morten Vierling**
 University of Hamburg

We consider the semi-discretization proposed by Hinze for control constrained optimal control problems of tracking type. Therefor the solution operator associated with the equality constraints is replaced by a finite element approximation while the control itself is not discretized and remains a function in the Hilbert space L^2 . It has been shown, that the order of convergence of the semi-discretization is essentially that of the finite element approximation. For those problems we present a semismooth Newton method, which operates in function space but is fully implementable as the approximations can be represented on refinements of the original triangulation allowing jumps along the border between active and inactive set.

This leads to an active set strategy, where computation takes place on the inactive set only, as can be expected according to a result of Hintermüller, Ito and Kunisch. If the smoothing parameter from the objective functional is sufficiently large, global convergence can be shown. Otherwise a damping strategy is proposed and numerically tested. The method has been implemented for linear elliptic and parabolic problems and quadratic convergence is observed for piecewise linear standard finite elements in space. In the parabolic case the time is discretized following a piecewise constant discontinuous galerkin approach, so convergence occurs linearly in time.

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