

Ē. Ė $= HA1$ **RESEARCH INSTITUTE** FOR MATHEMATICS

> MIP & PDE WORKSHOP

March 10.-13., 2008

HAUSDORFF

Junior Trimester Program

Schedule of the Workshop

Pia Bales

Hierarchical modelling and optimal control on gas networks

During the last years there has been intense research in the field of simulation and optimization of gas transport in networks. The equations describing the transport of gas in pipelines are based on the Euler equations, a hyperbolic system of nonlinear partial differential equations, mainly consisting of the conservation of mass, momentum and energy. The transient flow of gas may be described appropriately by equations in one space dimension. For the whole network, adequate initial and boundary values as well as coupling conditions at the junctions are needed. Although solving one-dimensional equations does not pose a challenge, the complexity increases with the size of the network. Thus, we present a hierarchy of models that describe the flow of gas in pipelines qualitatively different: The most detailed model we use consists of the isothermal Euler equations (continuity equation and momentum equation). A common simplification of the momentum equation leads to a semilinear model, which is only valid if the velocity of the gas is much less than the speed of sound ($v \ll c$). Further simplifications lead to the steady state model.

In order to estimate the model error of the simplified models, i.e. of the semilinear and the steady state model, with regard to some quantity of interest one has to solve adjoint systems on the network. For these appropriate coupling conditions are required. In this talk we present a strategy how to decide in which regions of the network which model has to be used to reduce the complexity of the whole problem whereas the accuracy of the solution is maintained. We give numerical examples of an algorithm that switches adaptively between the three models on one pipe. In addition, we use the solutions of the adjoint system to optimize control variables with respect to quantities of interest.

Debora Clever

Optimal Boundary Control for Glass Cooling Processes with Restrictions on the Temperature Gradient

One important production step in glass manufacturing is the cooling of the molten and already formed glass down to room temperature. If this cooling is done too fast the thermal stresses cause cracks inside the material. Hence the hot glass is put in a furnace and the cooling is controlled by governing the temperature inside the oven. Since this process takes place at temperatures up to 1000C radiative heat transfer plays an important role in its modeling leading to a sys-

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tem of time dependant partial differential algebraic equations. These PDAEs are considered as constraints of the optimal control problem. Since the furnace only operates in certain regions there are point wise constraints on the control as well. The minimization of internal stresses is implemented by considering the gradient of the glass temperature in the target functional. For the calculation of the optimal control a pro jected gradient method is used where the gradient of the reduced target functional is determined by solving the state system forwards and the adjoint system backwards in time.

Ismael Regis de Farias Jr.

A branch-and-cut approach to piecewise linear optimization

Any nonlinear function can be approximated, to an arbitrary degree of accuracy, as a piecewise linear function. Finding the maximum (or minimum) of a piecewise linear function therefore is an important problem with a wide variety of applications in a diverse set of fields. From a mathematical and computational point of view, it is also very interesting, given the intractability of the model and the need for solving it within a reasonable amount of time. We will discuss how branch-and-cut, the premier algorithm in mathematical programming for solving discrete optimization problems exactly, can be used to tackle piecewise linear optimization, especially separable. We will then present some of our contributions to the method. In the end, we will discuss further research, a few open questions, and some new directions.

(Joint work with Ming Zhao.)

Simone Göttlich

Supply network models - discrete and continuous approaches

Optimal utilization of production networks is an important question arising in the context of supply chain planning. Motivated by this problem we propose a network model which is suitable for the approximation of continuous material flows. Additionally, we explain reasonable extensions to adopt the model to real-world situations. The subject of optimization will be the optimal routing of goods under certain constraints determined by the equations of the network model. We comment on optimization techniques and their improvements, inclusion of discrete decisions and computational results.

Martin Gugat

I. Optimal switching control of a string

In many control application, switching between different control devices occurs. Here the problem to control a finite string to the zero state in finite time by controlling the state at the two boundary points is considered, where at each moment in time one of the boundary controls must be switched off, that is its control value must be equal to zero. The corresponding optimal control problem where the objective function is the $L²$ norm of the controls is solved explicitly in the sense that controls that are successful and minimize at the same time the objective function are determined as functions of the initial state.

II. Networks of sloped channels with friction: Existence of solutions for subcritical flow.

As a model for networks of sloped channels we consider a graph where on each edge of the graph, a quasilinear hyperbolic PDE models the flow. Due to slope and friction, in these PDEs source terms appear. The edges are coupled by algebraic node conditions, that guarantee conservation of mass. We show that locally around continuously differentiable stationary states, the corresponding initial boundary value problem has a continuously differentiable solution.

Stephan Held

Gate Sizing in VLSI-Design

Gate sizing is one of the key tasks in VLSI-design. A VLSI-chip is composed of millions of small circuits, which implement some elementary logic function, e.g. a two-bit AND, OR, XOR, etc. . The layout of each circuit can be chosen from a small finite set of different predefined layouts with varying timing characteristics. One optimization task is to assign each circuit to a layout such that all timing constraints are fulfilled and the resource consumption in terms of power and area is minimized. An accurate analysis of the timing constraints involves the solutions of nonlinear differential equations. Thus this problem combines a) a discrete optimization problem, b) PDE-constraints and c) huge instance sizes. The presentation will give an overview on the problem and its solution methods.

Oliver Kolb

Optimal control for gas and water supply networks

We are interested in simulation and optimization of flow processes in gas and water supply networks. Those networks consist of various components like compressors, pumps and valves connected by pipes. The aim is to run the network cost efficiently whereas demands of consumers have to be satisfied. This results in a complex nonlinear mixed integer problem and we want to treat continuous as well as integer variables in our problems. Therefore, we apply methods provided by discrete optimization. Additionally, we use a numerical network simulation tool to verify the computed results and a sequential quadratic programming solver for local optimization. Gradient information is obtained by an adjoint approach. The applied methods of discrete optimization require a description of the gas and water dynamics in all components by piecewise linear constraints. At first, we need a (simple) discretization of the underlying system of hyperbolic partial differential equations for all pipes. After the discretization process, the linearization of all nonlinearities in the discretized PDE as well as the other constraints, e.g. the compressor equations, is the next crucial step. Here, we introduce an adaptive approach for the linearization process to handle the complexity on the one hand and the aimed accuracy on the other. Further, we present numerical simulation and optimization results based on our model.

Dennis Michaels

Convex relaxations of nonlinear mixed-integer optimization problems

Many real-world problems give rise to nonlinear mixed-integer optimization problems (MINLPs). In chemical engineering, this includes the question of finding an optimal process design for reactive distillation processes, for instance. A variety of methods has been developed to find good feasible solutions of MINLP. But the most efficient algorithms cannot guarantee to arrive at a globally optimal solution, in general. Therefore, to prove global optimality or to evaluate known solutions with respect to their quality, strong global bounds on the optimal value of the underlying MINLP have to be computed. This is achieved by considering convex relaxations of the original problem.

If the given optimization problem involves polynomial functions only, results from real algebra are available to define hierachies of semi-definite relaxations.For the general case, such nice results are not at hand. Therefore, arbitrary nonlinearities must be replaced by convex under- and concave overestimators. In order to build strong convex relaxations providing a useful global bound, the convex and concave estimators have to be chosen best possible. This leads to the question of determining the convex and concave envelopes of a function which will be the main topic of this talk. In particular, we will present a structural result for the family of so-called (n-1) convex functions.This result will be used to derive a description for the envelopes of three important classes of bivariate functions. Moreover an outer-description for the envelopes of an arbitrary affine rational function will be also presented.

(Based on works with M. Ballerstein, J. Gangadwala, U.-U. Haus, M. Jach, A. Kienle, A. Seidel-Morgenstern and R. Weismantel)

Hausdorff Institute Bonn **Exercise 2** and post in the Workshop on MIPs and PDEs

Sebastian Sager

Optimization with binary valued control functions - theory, methods, and applications

Optimal control problems have typically a continuous nature. However, for many practical processes, also combinatorial aspects play an important role. In this talk we are especially interested in the case of control functions that may only take values from a discrete set. Typical examples are gears in transport or on-off valves in chemical engineering. We will present theoretical properties of such optimal control problems, especially of convex reformulations, and present a numerical algorithm to exploit them. This algorithm is based on a direct method for optimal control, hence on a "first discretize, then optimize" approach. We will recall basic properties of Bock's direct multiple shooting method and explain how it can be used within the novel algorithm for mixed-integer optimal control problems. Finally, we will present numerical results for several applications.

Marc Steinbach

Combinatorial Issues in Operating Incompressible Network Flows

Operative planning in large networks with nonlinear fluid dynamics leads to large-scale discrete-continuous control problems that are to date intractable in the sense of locating global optima within a prescribed tolerance. It is often possible, however, to find local optima without fixing combinatorial variables a priori. To this end, the reformulation of binary decisions by complementarity constraints (MPCC), equilibrium constraints (MPEC), or even standard nonlinear constraints (NLP) has recently gained interest in the (continuous) optimization community. The lecture reports on planning problems for incompressible network flows, with a focus on discrete decisions like pump switching. We discuss open problems as well as successful NLP reformulation techniques applied in minimum-cost operation of water supply networks.

Carsten Ziems

Adaptive Multilevel SQP–Methods for PDE–constrained Optimization

We present a class of adaptive multilevel SQP-methods for the solution of optimization problems governed by nonlinear elliptic or parabolic partial differential equations. Starting with a coarse finite element discretization of the underlying optimization problem we combine an efficient composite-step trust-region SQP-method with an implementable adaptive refinement strategy for the current discretization based on estimators such that the infinite-dimensional problem is well represented in each iteration. When working with elliptic PDEs the algorithm uses in addition implementable accuracy requirements for the inexactness in iterative linear equation solves on the current grid such as the linearized PDE and adjoint PDE. We prove global convergence to a first-order optimality point of the infinite-dimensional problem. Numerical results will be presented as well as the relevance for branch and bound algorithms in discrete--continuous nonlinear optimal control problems.

(Joint work with Stefan Ulbrich.)

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Poppelsdorf **e** Poppelsdorfer Schloß Lessingstr Botanischer \$ Garten SÜDSTADT **Kam** Reuterstr Sebastianstr Flodelingsweg \mathcal{S}_λ 500 m s_{nburgstr.} Ô POPPELSDORF © Geographisches Institut der Universität Bonn

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