DK-RICAM Workshop on PDE-Constrained Optimization

March 6 – March 7, 2014
held at RICAM, S2 416,
Johannes Kepler University Linz

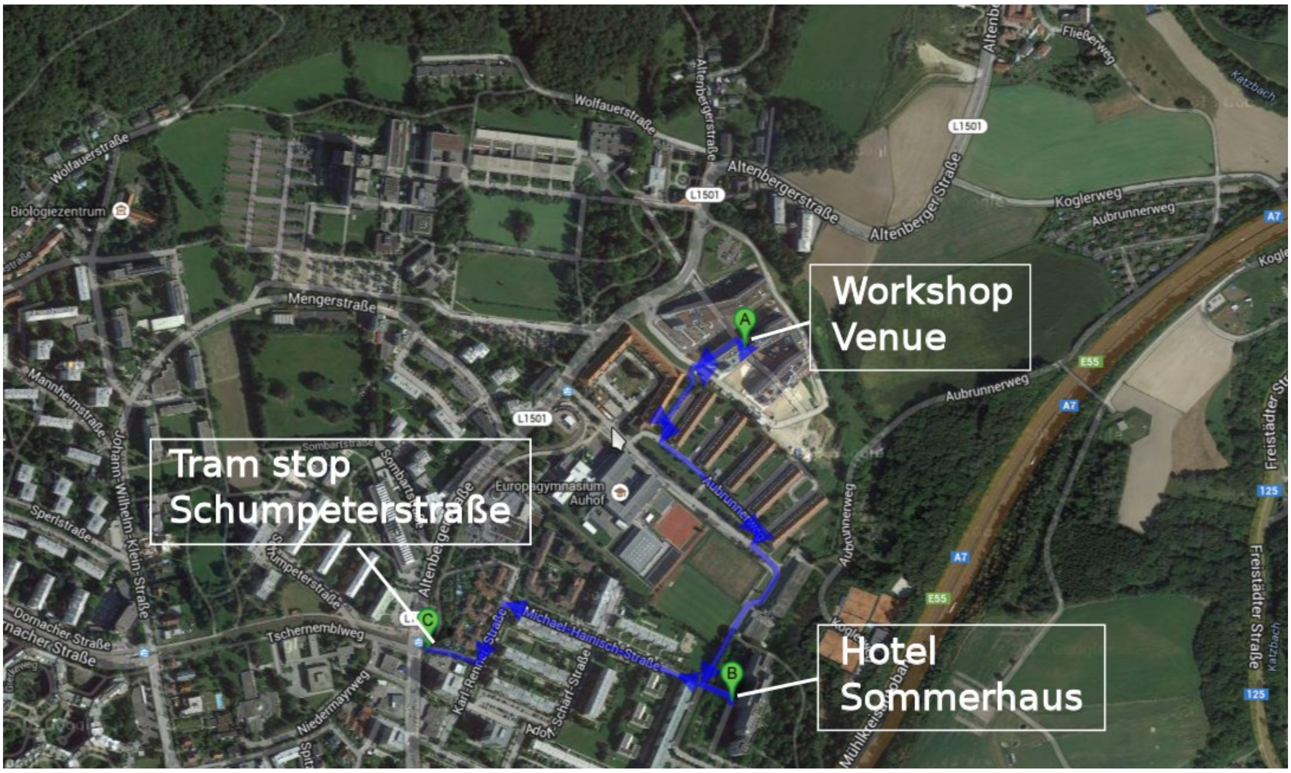
Timetable Thursday, March 6, 2014

Slot	Speaker
09:00 – 09:05	**Welcome**
09:05 – 09:35	**Esther Klann:** A Mumford-Shah type approach for tomography data
09:40 – 10:10	**Houcine Meftahi:** Uniqueness and stable determination in the inverse Robin transmission problem with one measurement
10:15 – 10:45	**Kevin Sturm:** A new approach to the differentiability of a minimax function
10:50 – 11:20	**Coffee Break**
11:20 – 11:50	**Samuel Amstutz:** Topological asymptotic analysis for a class of quasilinear elliptic equations
11:55 – 12:25	**Antoine Laurain:** Controlling the footprint of droplets
12:30 – 14:00	**Lunch**
14:00 – 14:30	**Valeria Simoncini:** On preconditioning PDE-constrained optimization problems with control constraints
14:35 – 15:05	**Roland Herzog:** Old and New Convergence Results for Krylov Subspace Methods in Hilbert Space
	Coffee Break
15:45 – 16:15	**John Pearson:** Fast Iterative Solvers for Reaction-Diffusion Control Problems
16:20 – 16:50	**Monika Wolfmayr:** Functional a posteriori error estimates for time-periodic parabolic optimal control problems
18:30	**Workshop Dinner at “Wia z'haus Lehner”**

Timetable Friday, March 7, 2014

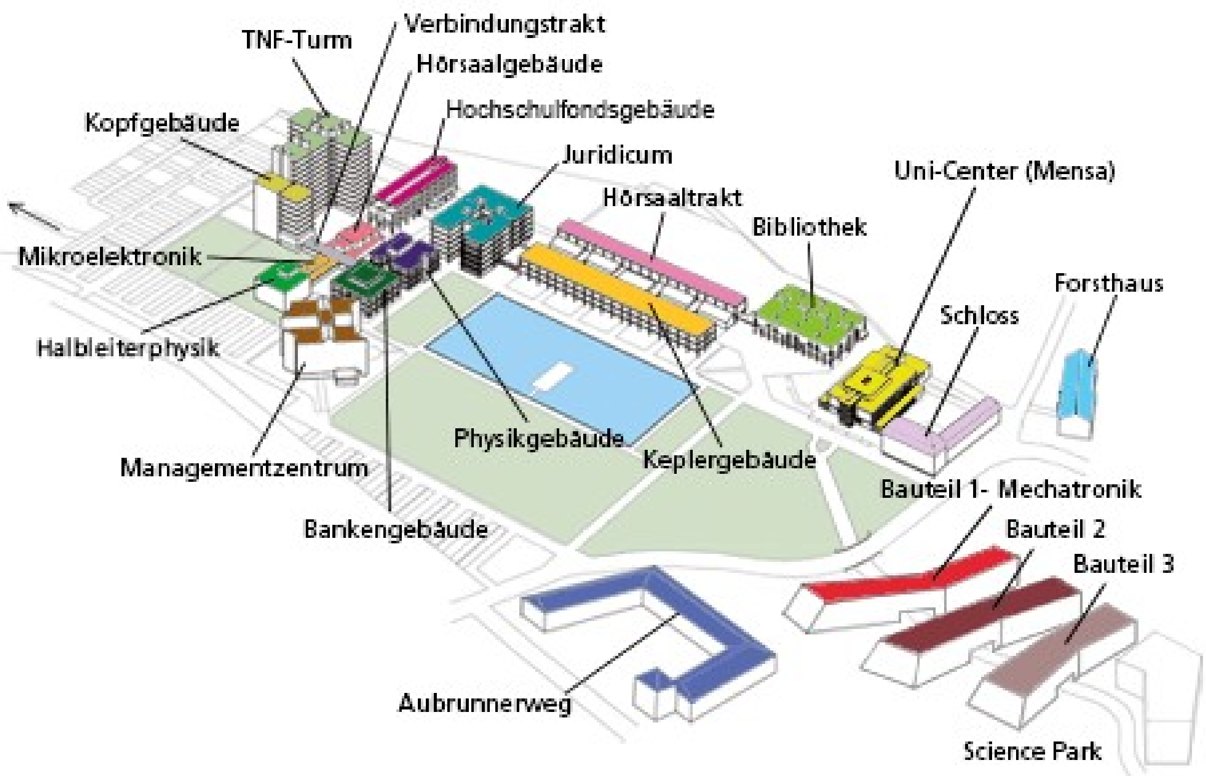
Slot	Speaker
09:00 – 09:30	**Chamakuri Nagaiah:** Large scale PDE constrained optimization of cardiac debrillation
09:35 – 10:05	**Peter Gangl:** Design Optimization of Electric Machines Using Shape Optimization and Sensitivity-Based Topology Optimization
10:10 – 10:40	**Wolfgang Krendl** The Herrmann Johnson Method for the first biharmonic boundary value problem on general polygonal domains: Mapping properties and preconditioning strategy
10:40 – 11:00	**Coffee Break**
11:00 – 12:30	**Time for discussion/colaboration**
12:30 – 14:00	**Lunch**
14:00 – 17:00	**Time for discussion/colaboration**

Venue



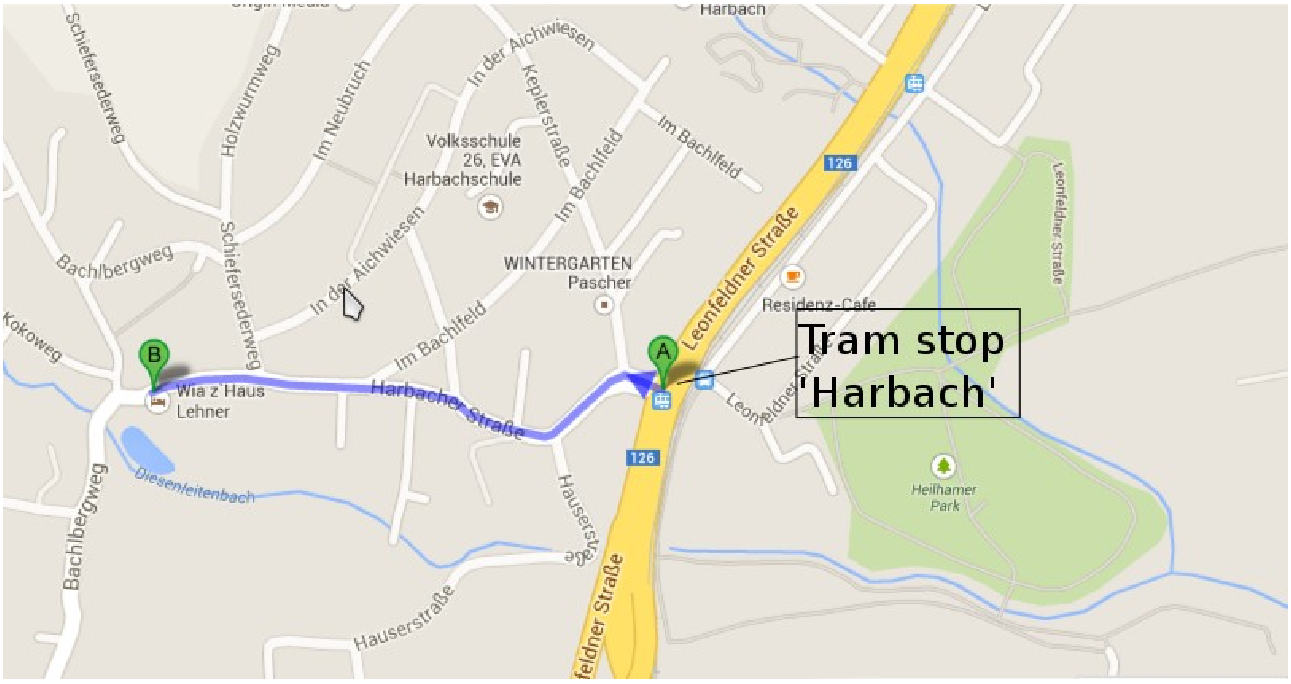
Campus Map

The workshop is held in building "Science Park, Bauteil 2" on the 4th floor (RICAM). The dining hall for lunch is in Uni-Center (Mensa).



Workshop Dinner on Thursday, March 6 in “Wia z'haus Lehner”

Arrival: Take tram number 1 or 2 to Harbach – cross underneath the street towards “Oberbank” - walk along Harbacher Straße for about 8 minutes until you arrive at Wia z'haus Lehner



List of abstracts

Samuel Amstutz:

Topological asymptotic analysis for a class of quasilinear elliptic equations

Topological asymptotic expansions for quasilinear elliptic equations have not been studied yet. Such questions arise from the need to apply topological asymptotic methods in shape optimization to nonlinear elasticity equations as in imaging to detect sets with codimensions ≥ 2 (e.g. points in 2D or segments in 3D). In this work we provide topological asymptotic expansions for a class of quasilinear elliptic equations perturbed in non-empty subdomains. The obtained topological gradient can be split into a classical linear term and a new term which accounts for the non linearity of the equation.
Co-author: A. Bonnafé

Nagaiah Chamakuri:

Large scale PDE constrained optimization of cardiac defibrillation

The bidomain model consist of a system of elliptic partial differential equations coupled with a non-linear parabolic equation of reaction-diffusion type, where the reaction term, modeling ionic transport is described by a set of ordinary differential equations. An extra elliptic equation for the solution of an extracellular potential needs to be solved on the torso domain. Anatomically realistic such multiscale models of torso embedded whole heart electrical activity are computationally expensive endeavor on its own right and solving optimal control of such models in an optimal manner is the most challenging issue.

The optimal control approach is based on minimizing a properly chosen cost functional depending on the extracellular current as input at the boundary of torso domain, which must be determined in such a way that wavefronts of transmembrane voltage in cardiac tissue are smoothed in an optimal manner. In parallel computations, the domain decomposition of such realistic geometry consists of heart surrounded by torso is not a trivial task. First, we partition the heart domain into p-subdomains and similarly partition the torso domain into p-subdomains and then we solve the PDEs as a decoupled system by expense of one additional communication at each time step. The derivation of the optimality system and the description of its discretization is given. A primal-dual active set strategy is employed for treating inequality control constraints. In this talk, a parallel fnite element based algorithm is devised to solve an optimal control problem on such complex geometries and its effciency is demonstrated not only for the direct problem but also for the optimal control problem. The computations realize a model confguration corresponding to optimal boundary defbrillation of a reentry phenomenon by applying current density stimuli.
Co-authors: Karl Kunisch, Gernot Plank

Peter Gangl:
Design Optimization of Electric Machines Using Shape Optimization and Sensitivity-Based Topology Optimization
Topological sensitivities are a very useful tool for determining optimal designs. The topological derivative of a domain-dependent functional represents the sensitivity with respect to the insertion of an infinitesimally small hole. In the gradient-based ON/OFF method, proposed by M. Ohtake, Y. Okamoto and N. Takahashi in 2005, sensitivities of the functional with respect to a local variation of the material coefficient are considered. We show that, in the case of a linear state equation, these two kinds of sensitivities coincide. For the sensitivities computed in the ON/OFF method the generalization to the case of a nonlinear state equation is straightforward, whereas the computation of topological derivatives in the nonlinear case is more involved. We will show numerical results obtained by applying the ON/OFF method in the nonlinear case to the optimization of an electric motor.

Moreover, we will address the same problem by means of shape optimization where the geometry is modified by moving a material interface along a velocity field which guarantees a decrease in the objective functional.

Roland Herzog: *Old and New Convergence Results for Krylov Subspace Methods in Hilbert Space*
Krylov subspace methods represent a widely used class of iterative solution techniques for large-scale linear systems. They naturally also extend to linear systems in Hilbert spaces, and considering the methods in this infinite dimensional setting provides new insight.

In this presentation, we focus on Krylov subspace methods for definite and indefinite self-adjoint linear systems, namely the conjugate gradient (CG) and minimum residual (MINRES) methods. We review convergence results available in the literature, focusing mainly on Q-superlinear and R-superlinear convergence. New results of this type for MINRES will also be presented, which apply to a broad range of examples. The examples to be presented include the solution of the Stokes system as well as optimal control problems with partial differential equations.
Co-Author: Ekkehard Sachs

Esther Klann:
A Mumford-Shah type approach for tomography data
We present a Mumford–Shah-type approach for the simultaneous reconstruction and segmentation of a function from its tomography data (Radon transform). The sought-after function is modeled as a piecewise constant function. Hence, it consists of n sets Ω_i and the corresponding values c_i. The sets and values together with their number are found as minimizers of a Mumford–Shah-type functional. We present a minimization algorithm based on shape sensitivity analysis, as well as some numerical examples.

Wolfgang Krendl:

The Herrmann Johnson Method for the first biharmonic boundary value problem on general polygonal domains: Mapping properties and preconditioning strategy

The first order boundary value problem of the biharmonic operator is a simple model problem in elasticity for the bending of a clamped plate. For this model problem, a mixed order formulation is considered which is equivalent to the original fourth order formulation without additional assumptions on the polygonal domain such as convexity. Based on the mapping properties of the involved operators and their discrete counterparts resulting from the Herrmann-Johnson's scheme, a strategy for an efficient preconditioner will be presented.

Antoine Laurain:

Controlling the footprint of droplets

The development of engineered substrates has progressed to a very advanced level, which allows for control of the shape of sessile droplets on these substrates. Controlling local droplet shape via substrate surface tensions may be useful for directing the growth of bio-films and cell cultures because it can affect the distribution of nutrients as well as the gross shape of the film. In addition, depositing a film of material onto a substrate in a particular pattern could be affected by the droplet shape. Also, droplets can act as lenses, with focal properties controlled by locally modifying substrate tensions. In this talk, we present an optimal control for the shape of droplets on substrates. Specifically, we wish to direct the shape of the droplet-substrate interface (i.e. the liquid-solid interface) by controlling the substrate surface tension. We refer to this as droplet footprint control.

Houcine Meftahi:

Uniqueness and stable determination in the inverse Robin transmission problem with one measurement

In this talk, we consider the inverse Robin transmission problem with one electrostatic measurement. We prove a uniqueness result for simultaneous determination of the Robin parameter p, the conductivity k and the subdomain D, when D is a ball. When D and k are fixed, we prove a uniqueness result and a directional Lipschitz stability estimate for the Robin parameter p. When p and k are fixed, we give an upper bound to the subdomain D. For the reconstruction purposes, we set the inverse problem under an optimization form for a Kohn-Vogelius cost functional. We prove the existence and the stability of the optimization problem. Finally, we show some numerical experiments.

John Pearson:

Fast Iterative Solvers for Reaction-Diffusion Control Problems

In this talk, we consider the development of preconditioned iterative methods for the matrix systems arising from finite element discretizations of PDE-constrained optimization problems. We construct the relevant preconditioners by using the saddle point structure of the matrices involved to derive effective approximations of the (1,1)-block and Schur complement.

We commence by explaining how this strategy can be applied to the fundamental Poisson control problem, as well as a heat equation control problem. We then explain how to adapt these techniques to precondition the Newton systems obtained when solving reaction-diffusion control problems. We consider such problems from two main application areas: the modelling of chemical reactions, and the identification of parameters in pattern formation processes. For each problem considered we motivate and derive our preconditioners, and present numerical results to demonstrate the practical performance of our methods.

Valeria Simoncini:

On preconditioning PDE-constrained optimization problems with control constraints

Co-Authors: Margherita Porcelli, Mattia Tani

Kevin Sturm:

A new approach to the differentiability of a minimax function

In this talk, we discuss a new approach to the differentiability of a minimax of a function G. Its originality is to replace the usual adjoint state equation by an *averaged adjoint state equation*. The function G is a Lagrangian, that is a utility function plus a linear penalization of the state equation. Former results required a saddle point assumption or had other differentiability requirements. We consider the case, where the state and adjoint state are unique solutions and illustrate the result at hand of a semi-linear shape optimization problem.

Monika Wolfmayr:

Functional a posteriori error estimates for time-periodic parabolic optimal control problems

We present functional a posteriori error estimates for time-periodic parabolic optimal control problems in a new variational framework. Since we consider time-periodic problems, the multiharmonic finite element method is a very natural approach to discretize this type of parabolic problems. More precisely, we expand all - given and unknown - functions into Fourier series in time, truncate them, and then approximate the Fourier coeffcients by the finite element method. Due to the linearity and the orthogonality of the cosine and sine functions, the whole optimality system decouples into smaller systems depending only on the Fourier coeffcients with respect to a single mode. We establish inf-sup and sup-sup conditions in the new variational setting from which we deduce existence and uniqueness results by applying the theorem of Babuska and Aziz. The inf-sup condition is also very helpful for the functional a posteriori error analysis of the optimal control problem, which is based on the method presented in Repin [3] but contains proper changes regarding the new variational setting and the special features of the multiharmonic finite element method.

References

[1] U. Langer, S. Repin and M. Wolfmayr, Functional a posteriori error estimates for time-periodic parabolic optimal control problems, in preparation, 2014.
[2] U. Langer and M. Wolfmayr, Multiharmonic finite element analysis of a time-periodic parabolic optimal control problem, J. Numer. Math., 21(4):265-300, 2013.
[3] S. Repin, Estimates of deviation from exact solutions of initial-boundary value problems for the heat equation, Rend. Mat. Acc. Lincei, 13(2):121-133,

2002.
[4] M. Wolfmayr, Multiharmonic Finite Element Analysis of Parabolic Time-Periodic Simulation and Optimal Control Problems, PhD thesis, Johannes Kepler University, Linz, 2014.