# 3rd Chinese-German Workshop on Computational and Applied Mathematics, Sept. 28 - Oct. 2, 2009, Heidelberg, Germany

**Titles and abstracts**

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## (I) German participants

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### 1. Eberhard Bänsch (U Erlangen)

*Titel:* Free surface flows in engineering applications

*Abstract:* multiphase flows including strong interface effects like surface tension have a wide range of applications. In this talk we present some concrete problems from engineering.

We show how to address this type of free boundary problems for the Navier-Stokes equations by a finite element method. The key ingredients for the method are a variational formulation of the curvature terms and a stable, semi-implicit time discretization, decoupling the computation of the flow field and the geometry.

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### 2. Peter Bastian (U Heidelberg)

*Titel:* Generic software components for finite elements

*Abstract:* In this talk we describe PDELab, an extensible C++ template library for finite element methods based on the Dune software framework. PDELab considerably simplifies the implementation of discretization schemes for systems of partial differential equations by setting up global functions and operators from a simple element-local description. A general concept for incorporation of constraints eases the implementation of essential boundary conditions, hanging nodes and varying polynomial degree. The underlying Dune software framework provides parallelization and dimension-independence as well as a large variety of different types of meshes.

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### 3. Hans Georg Bock (U Heidelberg)

*Titel:* Parameter estimation and optimum experimental design revisited

*Abstract:* The development and quantitative validation of complex nonlinear differential equation models is a difficult task that requires the support by numerical methods for sensitivity analysis, parameter estimation, and the optimal design of experiments.

The talk first presents particularly efficient "simultaneous" boundary value problems methods for parameter estimation in nonlinear differential equations, which are based on the generalized Gauss-Newton method and a time domain decomposition by multiple shooting or collocation. Local and global convergence properties of optimization methods are critically discussed and some commonly made claims are classified as urban legends. A numerical analysis of the well-posedness of the problem by means of a generalized inverse is given which leads to an assessment of the error of the resulting parameter estimates. Based on these approaches, efficient optimal control methods for the determination of one, or several complementary, optimal experiments are developed, which maximize the information gain subject to constraints such as experimental costs and feasibility, the range of model validity, or further technical constraints.

Several applications will be discussed that arise in chemical reaction kinetics, enzyme kinetics and systems biology, and transport and degradation processes in soil. They indicate a wide scope of applicability of the methods, and an huge potential for reducing the experimental effort and accelerating the modeling process. (Joint work with A. Altmann-Dieses, S. Bandara, S. Körkel, E. A. Kostina, and J. P. Schlöder)

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**4. Malte Braack (U Kiel)**

*Titel:* Dual-based a posteriori error estimation for quasi-periodic problems

*Abstract:* For stationary problems the dual-weighted-residual method (DWR) yields reliable a posteriori error bounds for output functionals. Transferring this theory to non-stationary problems is not easy from the practical point of view, because an additional non-stationary adjoint problem has to be solved containing the primary solution as coefficient. This implies storage of the primal solution and the locally refined meshes at each time step.

As alternative, we will present an a posteriori error estimation technique for the computation of functionals depending on averages of the solution for nonlinear time dependent problems based on duality techniques, where the exact solution is assumed to be (quasi) periodic. So we are interested in accurate determination of linear functional output for the time average of the primary solution.

This leads to an a posteriori error estimator which consists of an averaged residual weighted by sensitivity factors coming from a stationary dual problem. It is no longer necessary to solve a non-stationary adjoint problem or to store the locally refined meshes due to the fact that mesh adaption is accomplished after every period of the primal solution. The resulting adaptive algorithm is applied to a linear test problem with known exact solution and to the non-steady Navier-Stokes equations in order to verify the model assumptions. (Joint work with E. Burman and N. Taschenberger)

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**5. Carsten Carstensen (HU Berlin)**

*Titel:* Computational challenges in the calculus of variations

*Abstract:* The computational nonlinear PDEs involve minimisation problems with various striking challenges such as measure-valued solution concepts or ghost solutions. The presentation starts with a class of degenerate convex minimisation problems and convergent adaptive finite element methods. The motivation for those comes from computational microstructures in case of a sufficient convexification. Finte plasticity is one example where the quasiconvexification is not known in closed for and hence numerical relaxation is required. Polyconvex minimisation problems and their finite element analysis is discussed as well as some $L^1$ penalty finite element method. The Mania example for the Lavrentiev phenomena for singular minimisers with convergence towards the wrong solution studied as well as its remedy via the penalty finite element method.

## References


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[2] C and Georg Dolzmann: An a priori error estimate for finite element discretisations in nonlinear elasticity for polyconvex materials under small loads. *Numer. Math.* 2004.

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**7. Vincent Heuveline (U Karlsruhe)**

*Titel:* Emerging hardware and numerical simulation: a walk of seven bridges over the gap


*Abstract:* Emerging hardware solutions currently rely on a plethora of different underlying concepts and offer a huge computational potential. In turn however they reveal diverging technologies and many uncertainties. Broad scalability is hitting Amdahl's law and the memory wall. Heterogeneity on system and on chip level is growing and for many platforms, taking advantage of their intrinsic features remain an even more challenging task. Missing standards, different processing models and incomplete tool chains impede unified approaches and programmer's productivity. Solutions in numerical simulation make particular demands on performance, accuracy and reliability of computations.

This talk discusses perspectives and efforts in hardware-aware numerics on multi-/manycore processors and accelerators. The focus is on the link between contemporary numerical methods, candidate approaches in high performance computing and hardware-related constraints.


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**8. Michael Hinze (U Hamburg)**

*Titel:* Numerical analysis of parabolic control problems with state constraints


*Abstract:* In this talk we discuss parabolic optimal control problems with pointwise state constraints. The optimization problem is approximated using variational discretization [3] combined with linear finite elements in space and a discontinuous Galerkin scheme in time for the discretization of the state equation. Error bounds for control and state are obtained both in two and three space dimensions. To achieve these bounds uniform estimates for the discretization error of the state are proven which use natural regularity requirements on the optimal state [2]. For the numerical analysis of the optimal control problem we use an approach which avoids error estimates for the adjoint state and which was developed in [1] for the analysis of elliptic optimal control problems with gradient constraints.
(Joint work with Klaus Deckelnick, Magdeburg)

## References

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[2] Deckelnick, K., Hinze, M.: *Variational Discretization of Parabolic Control Problems in the Presence of Pointwise State Constraints*, Priority Programme 1253, Preprint-Nr.: SPP1253-08-08, 2009.

[3] Hinze, M.: *A variational discretization concept in control constrained optimization: the linear-quadratic case*, J. Computational Optimization and Applications 30:45-63, 2005.

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**9. Dietmar Kröner (U Freiburg)**

*Titel:* Modelling and numerical simulations for shallow water flows

*Abstract:* Geophysical flows in the oceans and in the atmosphere are described by the compressible or incompressible Navier-Stokes-equations in 3D with free boundaries. Because of the different scales of the vertical and horizontal characteristic values of this flow the full 3D-system can be reduced to so-called shallow water flow models. In particular these are 1D, 2D and 3D models with one layer or multi-layer or a combination of these models. They can be also used as a model hierarchy in an adaptive modelling concept. In this contribution we will present different models within this hierarchy and present some numerical results. (Joint work with S. Brdar, A. Dedner, C. Gersbacher, and N. Shokina)

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**9. Andreas Prohl (U Tübingen)**

*Titel:* Modeling, analysis, and numerics of electroosmotic flow

*Abstract:* The coupled Navier-Stokes-Nernst-Planck-Poisson system e.g. describes electrokinetically driven mass transport in microfabricated chip devices. The model combines the classical semi-conductor equations and the incompressible Navier-Stokes equations, where the Lorentz force attributes to charge distributions in the fluid.
In the talk, we discuss solvability of the problem, and characterize weak solutions (energy, entropy laws, nonnegativity of charges,...). A fully practical finite element based space-time discretization is proposed, where corresponding solutions exist, are stable, satisfy above properties, and converge to weak solutions once a compatibility assumption (next to LBB) regarding choices of FE-spaces for pressure, and charge densities is satisfied.
In a complementatory scenario, we introduce a splitting-/projection scheme where solutions approximate locally existing strong solutions at optimal rates. (Joint work with M. Schmuck (MIT Boston))

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**10. Rolf Rannacher (U Heidelberg**

*Titel:* On the adaptive Newmark scheme for the wave equation

*Abstract:* We discuss residual-based a posteriori error estimation and time-step adaptation

in the classical Newmark scheme for solving the acoustic or elastic wave equation. The analysis exploits the equivalence of the Newmark scheme to the Crank-Nicolson scheme and thereby its close relationship to the continuous Galerkin cG(1) method. (Joint work with M. Geiger and H. K. Hesse)

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**11. Hans-G. Roos (TU Dresden**

*Titel:* Finite element methods for singularly perturbed problems: some recent results

*Abstract:* We first consider the two-dimensional convection-diffusion-problem

$$-\epsilon\Delta u + b_1 u_x + b_2 u_y + cu = f \text{ in } \Omega = (1,2)^2,$$

with, for simplicity, homogeneous Dirichlet boundary conditions in the convection-dominating regime. Let us discretize the problem with a stabilized finite element method on layer adapted meshes, see [2] and the recent survey [1]. In that survey we discussed several stabilization methods, including SDFEM, CIP and dG. Recently, a new variant of local projection stabilization (LPS) was proposed and analyzed. It turns out that especially LPS is more stable than its coercivity suggest and that the new variant of LPS eliminates the disadvantages of the older version. In the second part we introduce mortaring techniques for layer-adapted meshes. The approach allows to use non-matching meshes and simplifies, consequently, the construction of "optimal" layer-adapted meshes. Finally, we discuss parabolic initial-boundary value problems and its discretization in space on Shishkin meshes. For the - scheme and dG in time we present some robust error estimates.

## References


[1] Hans-G. Roos: Stabilized FEM for convection-diffusion problems on layer-adapted meshes, *Journal Comput. Math.*, (2009), 266-279.

[2] H.-G. Roos, M. Stynes and L. Tobiska: Robust Numerical Methods for Singularly Perturbed Differential Equations, second edn., Springer Series in Computational Mathematics, 2008.


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**12. Ekkehard Sachs (U Trier)**

*Titel:* Numerical solution of algebraic Riccati equations

*Abstract:* Algebraic Riccati equations play an important role in systems control and are solved routinely. However, for applications in control of partial differential equations, these equations grow tremendously in size and classical Riccati solvers are no longer applicable.

In this talk we consider iterative solvers based on Newton's method where the linear solvers used are also iterative schemes themselves. This approach leads to an inexact Newton's method and classical convergence theorems are available. One the other hand, it is well known, that for exact Newton's method applied to algebraic Riccati equations, also called Kleinman-Newton method, not only local, but also nonlocal convergence statements can be shown by using monotonicity arguments. We address the question if these monotone convergence results can be carried over to an inexact version of the Kleinman-Newton method. We show two approaches where this goal can be achieved successfully. Furthermore, we indicate how this scenario can be generalized for other problems and we support this by numerical results.

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### 13. Reinhold Schneider (U Kiel)

*Titel:* A posteriori error estimators for finite element sparse grid discretization

*Abstract:* We consider residual a posteriori error estimators for a tensor product of elliptic operators. The sparse grid approximation is based on an $H^{-1}$ frame of nodal finite element functions over all levels of discretization. (No wavelelet nor hierarchical bases are required.) The sparse grid or hyperbolic cross approximation renders the curse of dimnsionality. The difficulty is that the sparse grid or hyperbolic cross approximation is not dealing with a single grid, but a collection of several anisotropic grids on the tensor product domain. On a sequence of combination of grids, the error estimator consists of contributions local estimators. The overall eror is estimated by summing over alll combinations. We consider reliability, efficiency of this estimators and convergence of the adaptive scheme. (Joint work with H. Harbrecht (U Bonn)).

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### 14. Volker Schulz (U Trier)

*Titel:* Efficient shape optimization for certain and uncertain aerodynamic design

*Abstract:* Aerodynamic design is a big challenge for the efficiency of numerical algorithms. It is within the class of PDE constrained optimization problems but reveals structural properties that are nevertheless unique. In this talk, algorithmic concepts based on the shape calculus and one-shot ideas are discussed for application test cases close to reality. Numerical results and novel shapes for optimal wings are presented, as well. Furthermore, as is typical in practical applications, the issue of uncertainty of input parameters and geometries arises. This requires the development of optimization techniques related to non-intrusive polynomial chaos. Results from a collaborative effort with the DLR in Braunschweig will be presented.

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### 15. Ernst P. Stephan (U Hannover)

*Titel:* Efficient solution strategy for two-body elasto-dynamic contact problem with Coulomb friction

*Abstract:* For the development of a simulation tool for medical applications, e.g. impairments of a patient's knee caused by metabolic diseases, a fast and accurate solution strategy for two-body elasto-dynamic contact problems with Coulomb friction is of central importance as it is the core problem in biotribology. To model this contact problem two linear elastic bodies $\Omega_1$ and $\Omega_2$ are considered whose boundaries $\Gamma_l = \partial\Omega_l$ can be decomposed into the disjoint Dirichlet, Neumann and contact segments $\Gamma_{lD}$, $\Gamma_{lN}$ and $\Gamma_{lC}$. In the first step of developing a solution strategy a contact to Neumann technique is applied to split the problem into a one-body contact problem where the Coulomb friction is reduced to Tresca friction and into a Neumann problem. As in [1] we use a continuous transfer operator $T: H^{1/2}(\Gamma_{2C}) \to H^{1/2}(\Gamma_{1C}^*)$ to transfer the information in the CtN-algorithm. Here $\Gamma_{1C}^*$ is an extension of $\Gamma_{1C}$ such that the efficient hp-Mortar technique can later be applied to discretize $T$. In the second step of the solution strategy we introduce a mixed formulation for the one-body contact problem which reduces the non-differentiable friction functional to a bilinear form and eliminates the $\frac{d}{dt}u$ part in the test function. In the last step we use the Newmark time integration method to reduce the dynamic problem to a sequence of static problems and finally introduce a hp-FEM discretization in space where the non-penetration condition is only enforced in the Gauss-Lobatto points, [2]. Concluding we present numerical experiments to emphasize the algorithm's efficiency. (Joint work with Lothar Banz)

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**16. Lutz Tobiska (U Magdeburg)**

*Titel:* Supercloseness and superconvergence of stabilized low order finite element discretizations of the Stokes Problem


*Abstract:* The supercloseness and superconvergence property of stabilized finite element methods applied to the Stokes problem are studied. We consider both consistent residual based stabilization methods as well as nonconsistent local projection type stabilizations. Moreover, we are able to show the supercloseness of the linear part of the MINI-element solution which has been previously observed in practical computations. The results on supercloseness hold on three-directional triangular, axiparallel rectangular, and brick type meshes, respectively, but certain extensions to more general meshes are also discussed. Applying an appropriate postprocess to the computed solution, we establish superconvergence results. Numerical examples illustrate the theoretical predictions. (Joint work with Hagen Eichel and Hehu Xie)


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**17. Stefan Turek (TU Dortmund)**

Titel: FEM multigrid techniques for viscoelastic flow


Abstract: Similar to high Re number flows which require special discretization and solution techniques to treat the multiscale behaviour, viscoelastic fluids are very difficult to simulate for high Weissenberg (We) numbers ("elastic turbulence"). While many researchers believe that the key tools are appropriate stabilization techniques for the tensor-valued

convection-reaction equation for the extra stress, we explain the concept of log conformation representation (LCR) which exploits the fact that the conformation tensor is positive definite and shows exponential behaviour. Together with appropriate FEM techniques and monolithic Newton-multigrid solvers for the resulting fully implicit approaches, significantly higher We numbers seem to be reachable than compared with the standard formulation. We demonstrate this behaviour for several flow configurations with benchmarking character.

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**18. Boris Vexler (TU München)**

*Titel:* A priori error estimates for nite element discretization of state constrained optimal control problems governed by parabolic equations

*Abstract:* In this talk we present a space-time nite element discretization of an optimal control problem, which is governed by a linear parabolic equation and is subject to pointwise state constraints in time. For the temporal discretization of the state equation we employ discontinuous Galerkin method (dG(0)) and for the spatial discretization we use usual conforming nite elements. The main di culty for the numerical analysis of this problem is the lack of temporal regularity of the optimal solution. We propose a technique which overcomes this di culty and present a priori error estimates for both temporal and spatial discretization errors. (Joint work with Rolf Rannacher and Dominik Meidner)

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**19. Christian Wieners (U Karlsruhe)**

*Titel:* Duality methods in incremental infinitesimal plasticity

*Abstract:* The time-discrete problem in infinitesimal plasticity for every increment can be formulated as a minimization problem in the displacement variable and the plastic strain. Equivalently, the increment can be characterized by minimizing the free energy of the (generalized) stress subject to kinematic and admissibility constraints.
For the fully discrete problem it turns out that it is advantageous to approximate simultaneously both, the primal and the dual problem, with leads to a corresponding mixed formulation. Moreover, this allows to estimate the error of the discrete dual solution by the interpolation error of the primal solution.
We define corresponding primal minimization problems (for displacement and plastic strain) and constraint dual minimization problems (for the stress) also for extended plasticity models including (infinitesimal) Cosserat rotations or nonlocal plastic terms, and we show equivalence of both minimization problems.
Finally, we show that a suitable nonlinear Schur complement reduction of the discrete dual-primal problem leads to efficient solution algorithms for the extended plasticity models. This is illustrated by several numerical experiments.

## References

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[2] P. Neff, K. Chelminski, W. Mller, C. Wieners: A numerical solution method for an infinitesimal elasto-plastic Cosserat model. *Mathematical Models and Methods in Applied Sciences (M3AS)* 17 (2007) 1211-1240

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## German PhD students

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### 1. Adrian Hirn (U Heidelberg)

*Titel:* Finite element approximation of the p-Stokes equation with pressure-gradient stabilization based on local projections

*Abstract:* There is a large class of incompressible fluids that cannot be adequately described using the Navier-Stokes theory and which are generally referred to as non-Newtonian fluids. In this talk a finite element method with pressure-gradient stabilization based on local projections will be presented for a fluid with shear-dependent viscosity.

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### 2. Joscha Gedicke (HU Berlin)

*Titel:* Adaptive computation of eigenvalue problems

*Abstract:* This talk summarises some recent results on a posteriori error estimators, convergence and quasi-optimal complexity for elliptic eigenvalue problems. For a simple symmetric eigenvalue model problem a refined a posteriori error analysis and the convergence of the first-order adaptive finite element method (AFEM) is presented. The $H^1$ stability of the $L^2$ projection provides reliability and efficiency of the edge-contribution of standard residual-based error estimators for $P_1$ finite element methods. In fact, the volume contributions and even oscillations can be omitted for Courant finite elements. This allows for a refined averaging error estimator. A quasi-optimal convergence analysis leads to a combined adaptive finite element method with an iterative algebraic eigenvalue solver for the Laplace eigenvalue problem of quasi-optimal computational complexity. The analysis is based on a direct approach for eigenvalue problems and allows the use of higher order conforming finite element spaces with fixed polynomial degree $k > 0$. The optimal adaptive finite element eigenvalue solver (AFEMES) involves a proper termination criterion for the algebraic eigenvalue solver and does not need any coarsening. Numerical evidence illustrates the optimal computational complexity. A posteriori error estimators for a non-symmetric eigenvalue model problem based on standard residual and averaging techniques are revised. Moreover, several postprocessing techniques attached to the dual weighted residual (DWR) paradigm plus two new dual-weighted error estimators are compared in numerical experiments. The first new estimator utilises an auxiliary Raviart-Thomas mixed finite element method and the second exploits an averaging technique in combination with ideas of DWR. (Joint work with Carsten Carstensen)

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### 3. Kathrin Hatz (U Heidelberg)

*Titel:* Estimating parameters in optimal control problems

*Abstract:* The discipline of mathematical optimization has grown to an indispensable tool for science an technology. But not only scientists optimize processes. There is evidence to assume that many processes in nature have been optimized in the course of evolution, as, for example, human motion. Our goal is to develop models of human motion that capture this optimality aspect. In particular, we want to model processes as the solution of an optimal control problem. This new type of model is expected to lead to new and highly interesting insights into human motion in many elds of research. In order to identify an optimal control model for a concrete process, one has to determine the optimization criterion and system parameters of the optimized process. This requires the solution of a parameter estimation problem that is constrained by an optimal control problem. We provide and discuss two numerical approaches for solving such a bilevel problem (based on the direct and the indirect method for solving optimal control problems), both based on multiple shooting and the generalized Gau -Newton method. Applications for optimal control models in various elds are described. We focus on the eld of orthopedy and show that modelling the underlying system dynamics already poses a serious challenge. Finally, our method is illustrated by means of numerical results for a benchmark problem.

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**4. Jevgenin Vihharev (U Heidelberg)**

*Titel:* Optimal control problems in digital image processing

*Abstract:* We consider different techniques for motion estimation in digital image processing. The emphasis is on the variational control approach. We present different examples such as optical Stokes flow estimation, 3D motion estimation of atmospheric layers and modeling of the atmospheric transport of chemicals.

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**5. Leonard Wirsching (U Heidelberg)**

*Titel:* Multi-level iteration schemes for nonlinear model predictive control

*Abstract:* Nonlinear model predictive control (NMPC) has become a well-established control approach, both theoretically and computationally. Efficient numerical methods based on direct multiple shooting have been developed by Diehl et al. However, its application to time-critical systems requiring fast feedback is still a major computational challenge.

In this talk, we investigate the new concept of multi-level iteration schemes. This approach extends the concept of real-time iterations by distributing the computations occurring in SQP iterations among up to four independent levels. It operates with ultra-fast feedback on the lowest level, where small QPs are solved very quickly using an online active set strategy. On the second level the nonlinear constraints are evaluated to improve feasibility, on the third level the Lagrange gradient is evaluated by means of adjoint sensitivities to improve nonlinear optimality, and on the topmost level the complete derivative information is generated.

We apply multi-level iteration schemes to a test problem from chemical engineering. We give details on the implementation and discuss the computational performance of the scheme.

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**6. Winnifried Wollner (U Heidelberg)**

*Titel:* Adaptive FEM for PDE constrained optimization with pointwise state constraints

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

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

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

$$u \leq \psi \ \text{ on } \overline{\Omega}.$$

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.

## (II) Chinese participants

### 1. Aihui Zhou (Chinese Academy of Sciences, Beijing)

*Titel:* Adaptive hexahedral finite element methods for electronic structure calculations

*Abstract:* In this presentation, we will introduce some adaptive hexahedral finite element discretizations for the first-principles electronic structure calculations. We will also talk about a parallel implementation of the component mode synthesis on the locally refined hexahedral mesh. And we will report several numerical experiments in quantum chemistry and materials science. This talk is based on some joint work with X. Dai, X. Gao, X. Gong, L. Shen, Z. Yang, and D. Zhang.

### 2. Chunxiong Zheng (Tsinghua University, Beijing)

*Titel:* Gaussian beam summation method for the boundary value problem of high frequency Helmholtz equation

*Abstract:* We propose an asymptotic numerical method for the boundary value problem of high frequency Helmholtz equation. The basis idea is to approximate the propagating waves with a summation of Gaussian beams by the least squares algorithm. Gaussian beams are asymptotic solutions of linear wave equations in the high frequency regime. The key ingredient of the proposed method is the construction of a finite-dimensional Gaussian beam space which has good approximating property. When the exact solution of boundary value problem contains some strongly evanescent wave modes, the direct implementing of least squares algorithm would fail. To remedy this problem, we resort to the domain decomposition technique to separate the definition domain into a boundary layer region and its complementary interior region. The former is handled by a domain-based discretization method, and the latter by the least squares algorithm. Schwarz iterations should be performed based on suitable transmission boundary condition at the interfaces of these regions. Numerical tests demonstrate that the proposed method is very competitive.

### 3. Danping Yang (East China Normal University, Shanghai)

*Titel:* Finite element approximation for optimal control problems with some global state constraints

*Abstract:* There have been extensive researches for finite element approximations of optimal control problems in the literatures, most of which focused upon control-constrained problems. In recent years, many researches started to examine the finite element approximations of optimal control problems with the state constraints. One typical example of optimal control problems of state constraint reads:

$$\begin{cases} \min_{y\in K} \mathcal{J}(u,y) = \frac{1}{2}\int_\Omega (y-y_d)^2 + \frac{\alpha}{2}\int_\Omega u^2, \\ \text{s.t.} \quad Ay = u+f \ \text{ in } \Omega, \quad y=0 \ \text{ on } \partial\Omega, \end{cases}$$

where $A$ is an elliptic partial differential operator of the second order and $K$ is a convex constraint set. The state-constrained control problems are frequently met in applications but much more difficult to handle. The specific case of point-wise state constraints have been studied. In applications of engineering, there exist many state-constrained optimal control problems of global types. For example, one may care more about how to control the integral value, $K = \{y : \gamma \leq \int_\Omega y \leq \beta\}$, $L^2$-norm constraint: $K = \{y : \int_\Omega y^2 \leq \beta$, energy-norm constraint: $K = \{y : \int_\Omega |\nabla y|^2 \leq \beta\}$ and etc.. In this talk, we will discuss finite element approximations for optimal control problems with some global state-constraints. We will analyze the optimality conditions of the exact and discrete optimal control systems. Then derive and prove a priori error estimates and a posteriori error estimators. Some numerical examples are performed to confirm theoretical results.

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**4. Dehao Yu (Chinese Academy of Sciences, Beijing)**

*Titel:* Hypersingular integral equations and related numerical methods

*Abstract:* In many scientific and engineering problems, such as acoustics, electromagnetic scattering and fracture mechanics, one encounters integral equations with hypersingular kernels. The hypersingular integrals have some quite different properties from regular and weak singular integrals. The standard numerical integration is not effective for hypersingular integrals, and some special numerical integration should be developed. One of the major problems arising from the numerical methods, such as the boundary element method, for solving such integral equations, is how to evaluate the following hypersingular integrals on the interval and on the circle eciently:

$$\begin{aligned} I_1(a,b,s,f) &:= \int\!\!\!\!\!\!=_a^b \frac{f(t)}{(t-s)^{p+1}}\,dt, \quad s \in (a,b),\ p = 1,2, \\ I_2(c,s,f) &:= \int\!\!\!\!\!\!=_a^b \frac{f(t)}{\sin^2 \frac{t-s}{2}}\,dt, \quad s \in (c, c+2\pi), \end{aligned}$$

which should be understand in the Hadamard sense.

In 1983 the method using series expansion of the integral kernel was first suggested by D.H. Yu. He solved the harmonic and biharmonic natural boundary integral equations on circle successfully. Then numerous works have been devoted to this area. The method of subtracting the singularity, the method of regularization, the approximate integration formulas for finite-part integrals, and the indirect method are also developed. In this talk we will mainly discuss the Newton-Cotes methods on the interval and on the circle. The related superconvergence results and the generalized extrapolation for computation of hypersingular integrals have also been presented. Some numerical examples are given to illustrate the theoretical analysis and the validity of the method.

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**5. Jun Hu (Peking University)**

*Titel:* Adaptive nonconforming methods for high-order partial differential equations

*Abstract:* In this talk, we present some recent results on adaptive finite element methods for a class of nonconforming elements for both the second and the fourth order elliptic problems. We give a posteriori error analysis and prove the convergence and optimality of their adaptive versions for these methods. This is a joint work with Professor Zhongci Shi from Chinese Academy of Sciences, China, and Professor Jinchao Xu from Penn State University, USA.

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**6. Ningning Yan (Chinese Academy of Sciences, Beijing)**

*Titel:* Some finite element schemes for state-constrained optimal control problems

*Abstract:* In this talk, we discuss the numerical methods for the optimal control problems with pointwise state constraints. The traditional approaches often need to deal with the delta-singularity in the dual equation, which causes many diculties in its theoretical analysis and numerical approximation. In our new approaches we reformulate the state-constrained optimal control as a constrained minimization problems only involving the state, whose optimality condition is characterized by a fourth order elliptic variational inequality. Moreover, the fourth order elliptic variational inequality can be rewritten to a system of variational inequalities with mixed form involving the state and control (but without costate). Based on above results, the direct numerical algorithms (nonconforming finite element approximation and mixed finite element approximation) are proposed for the inequalities. The error estimates of the finite element approximation and mixed nite element approximation are derived. The adaptive finite element mesh refinement is discussed based on a posteriori error estimates. Numerical experiments are presented to illustrate the effectiveness of the new approaches.

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**7. Pingbing Ming (Chinese Academy of Sciences, Beijing)**

*Titel:* Economical heterogeneous multiscale method for homogenization problems

*Abstract:* In this talk, I will report some recent work for the heterogeneous multi- scale method (HMM for short) with finite element method as a macroscopic solver for the homogenization problems. Firstly, we shall introduce HMM with some novel numerical integration schemes, which are dierent from the standard schemes used in the standard finite element method, while are proven quite ecient in HMM; Next, some new full discretization HMM for the parabolic homogenization method are reported. Finally, we shall present some recent theoretical progress for FE-HMM. The efficient of the methods are confirmed by the numerical results in both two-dimensional problems and three-dimensional problems. This is a joint work of R. Du in Institute of Computational Mathematics and Scientific/Engineering Computing, AMSS, Chinese Academy of Sciences.

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**8. Pingwen Zhang (Peking University)**

*Titel:* Numerical method of the self-consistent field theory

*Abstract:* The self-consistent field theory (SCFT) has provided a particularly successful framework for the study of the phase behavior of block copolymers and other soft materials. In this talk, an ecient spectral method is developed to solve the self-consistent field theory of diblock copolymer melt. A prior symmetric information of basis function is not required, and the periodic structure can be adjusted automatically during the iteration as well. In view of the multiply solutions of high nonlinear the self-consistent field equations, an efficient approach of estimating initial values for specific phases is given, which is efficient both for real space and Fourier space. The method could be easily used to reproduce all known diblock copolymers stable phases, and discover some new meta-stable phases.

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**9. Shao-Chun Chen (Zhengzhou University)**

*Titel:* Anisotropic Lagrange and Hermite interpolation of any order

*Abstract:* Interpolation theory is the foundation of finite element methods. Anisotropic interpolation is the foundation of the anisotropic finite element methods. In this talk after reviewing some ex- isted anisotropic interpolation theorems, we present a new way to analyze the anisotropic interpolation error whose idea is using Newton's formula of the interpolation polynomials. The special properties of divided differences are presented, with them the anisotropic interpolation error for any order Lagrange interpolation on triangle, rectangle, tetrahedron and cube, as well as a kind of Hermite interpolation on rectangle and cube are obtained.

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**10. Weiying Zheng (Chinese Academy of Sciences)**

*Titel:* Uniaxial perfectly matched layer for Helmholtz equations in layered media

*Abstract:* In this talk, we propose a uniaxial perfectly matched layer (UPML) technique for solving the time-harmonic scattering problems in two-layer media. The exterior region of the scatterer is divided into two half spaces by an infinite plane, on two sides of which the wave number takes different values. We surround the computational domain where the scattering field is desired by a layer of fictitious medium such that the wave of any frequency entering this medium decays exponentially. By imposing homogenous boundary condition on the outer boundary of the PML layer, we have proved that the solution of the PML problem converges exponentially to the solution of the original scattering problem in the computational domain as the thickness of the layer tends to infinity. Some numerical experiments will also be presented in this talk. (Joint work with Zhiming Chen)

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**12. Xuejun Xu (Chinese Academy of Sciences, Beijing)**

*Titel:* Local multilevel methods for adaptive finite element methods

*Abstract:* In this talk, I will present some local multilevel algorithms for solving the linear algebraic systems arising from the adaptive conforming and nonconforming finite element methods. The abstract Schwarz theory is applied to analyze the multilevel methods with Jacobi or Gauss-Seidel smoother performed on local nodes on each level. It is shown that the local multilevel methods are optimal, which means that the convergence rates are independent of the mesh sizes and mesh levels. Numerical experiments are given to confirm our theoretical results. This talk is based on joint works with Huangxin Chen and R.H.W. Hoppe.

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**13. Yang Xiang (Hong Kong University of Science and Technology)**

*Titel:* A continuum model for dislocation dynamics in a slip plane

*Abstract:* We derive a continuum model for the Peach-Koehler force on dislocations in a slip plane. To represent the dislocations, we use the disregistry across the slip plane, whose gradient gives the density and direction of the dislocations. The continuum model is derived rigorously from the Peach-Koehler force on dislocations in a region that contains many dislocations. The resulting continuum model can be written as the variation of an elastic energy that consists of the contribution from the long-range elastic interaction of dislocations and a correction due to the line tension effect. We validate our model by performing linear stability analysis and numerical simulation and comparing the results with those of discrete dislocation dynamics model.

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**14. Zhong-Ci Shi (Chinese Academy of Sciences, Beijing)**

*Titel:* Recent progress on Wilson nonconforming finite element

*Abstract:* Wilson nonconforming finite element (1973) is a very useful rectangular element in practice. It is shown in many engineering computations that the convergence behavior of this element is better than that of the commonly used bilinear element. However, mathematical studies carried out so far cannot justify it. I have spent many years on this problem. The results obtained by use of standard finite element analysis are not satisfied. Recently (2007–) we tackle this problem from a different view point, i.e. from Mechanics, where the Wilson element was originated. We have succeeded in proving both mathematically and numerically that the Wilson element is free of shear locking for a wide class of bending dominated plane elasticity problems, while the bilinear element suffers from shear locking. Therefore, we elucidate a long-standing folklore: why Wilson element does a better job in many practical applications than the bilinear element.

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**15. Ziqing Xie (Hunan Normal University, Changsha)**

*Titel:* The computational methods of finding multiple solutions of semilinear elliptic equations and their related topics

*Abstract:* In this talk, we first recall the history of the computational methods for finding the multiple solutions of nonlinear PDEs. Then we briefly introduce the search-extension method pro- posed by Chen and Xie and provide its theoretical foundation. Based on it, a so-called accelerated search extension method is proposed for the multiple solutions of semilinear elliptic equations moti- vated by the two-grid method proposed by Xu. To improve the eciency of the cascadic multigrid method for semilinear elliptic equations further, a new extrapolation cascadic multigrid method is suggested. The numerical experiments verify the eciency of our approaches.

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## Chinese PhD students

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**1. Huangxin Chen (Chinese Academy of Sciences, Beijing)**

*Titel:* Convergence and optimality of adaptive nonconforming finite element methods for nonsymmetric and indefinite Problems

*Abstract:* Recently an adaptive nonconforming finite element method (ANFEM) has been developed by Carstensen and Hoppe. In this talk, we will extend their result to nonsymmetric and indefinite problems. The main tools in our analysis are a posteriori error estimators and a quasi-orthogonality property. In this case, we need to overcome two main difficulties: one stems from the nonconformity of the finite element space, the other is how to handle the eect of a nonsymmetric and indefinite bilinear form. Two ANFEM algorithms (ANFEM I, ANFEM II) are proposed for the lowest order Crouzeix-Raviart element. It is shown that both ANFEM algorithms are a contraction for the sum of the energy error and a scaled volume term between two consecutive adaptive loops. Moreover, optimality in the sense of optimal algorithmic complexity can be shown for ANFEM II. Numerical experiments confirmed the theoretical findings will be reported. This talk is based on a joint work with R.H.W. Hoppe and Xuejun Xu.

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**2. Wei Jiang (Beijing University)**

*Titel:* A numerical study of wrinkling evolution of an elastic film on a viscous layer

*Abstract:* The wrinkling phenomenon at the nanoscale has been simultaneously observed in various thin film systems by many research groups, and has attracted ever more attention because of its many important applications. In the talk, the wrinkling phenomenon of a compressed elastic thin film bonded to a viscous layer is studied. It is believed that it has important potential applications for designing stress relaxation strategies in semiconductor industries. We generalize Huang-Suo model to a 1+2-dimensional mathematical model for anisotropic elastic thin films with cubic crystalline symmetry, and apply both the linear stability analysis (LSA) and long time numerical simulations to studying the two-dimensional wrinkles evolution. LSA shows that, for materials with cubic crystalline symmetry, the sign of the degree of elastic anisotropy $\zeta = \frac{C_{12}+2C_{44}}{C_{11}} - 1$ plays an important role in the anisotropy of the buckling instability of the thin film system. More precisely, the growth rate of the fastest growing wave number, taking as a function of directions, reaches a peak in the $< 100 >$ directions for $\zeta > 0$ and in the $< 110 >$ directions for $\zeta < 0$. A highly efficient semi-implicit spectral method is established. The numerical experiments of long time wrinkling evolution processes of a 1+2-dimensional system verified the LSA results, successfully simulated anisotropic wrinkling pattern formation and coarsening, produced a power law scaling and reproduced certain featured phenomena observed in physical experiments.

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**3. Jianzhen Qian (Peking Universit)**

*Titel:* Well-posedness in critical spaces for viscoelastic fluid systems

*Abstract:* This report is concerning the mathematical study of viscoelastic fluid systems of Oldroyd type models. The background with also existing well-posedness results for such macroscopic models will be presented. The report will mainly describe our recent work on studying the well-posedness in critical spaces for both the incompressible and the compressible fluid model systems. Specifically, existence and uniqueness of local solutions are proved with initial data in Besov spaces of low regularity and they are also shown to exist globally in time provided the initial data are small under certain norms.

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**4. Xuying Zhao (Chinese Academy of Sciences, Beijing)**

*Titel:* Convergence analysis of the adaptive finite element method with the red-green refinement

*Abstract:* In this paper, we analyze the convergence of the adaptive conforming P1 element method with the red-green refinement. Since the mesh after refining is not nested into the one before, the Galerkin-orthogonality does not hold for this case. To overcome such a difficulty, we prove some quasi-orthogonality instead under some mild condition on the initial mesh (Condition A). Consequently, we show convergence of the adaptive method by establishing the reduction of some total error. To weaken the condition on the initial mesh, we propose a modified red-green refinement and prove the convergence of the associated adaptive method under a much weaker condition on the initial mesh (Condition B).

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**5. Tao Zhou (Chinese Academy of Sciences, Beijing)**

*Titel:* Convergence analysis for stochastic collocation methods to scalar hyperbolic equations with a random wave speed

*Abstract:* For a simple model of a scalar wave equation with a random wave speed, Gottlieb and Xiu (Commun. Comput. Phys., 3 (2008), pp. 505-518) employed the generalized polynomial chaos (gPC) method and demonstrated that when uncertainty causes the change of characteristic directions, the resulting deterministic system of equations is a symmetric

hyperbolic system with both positive and negative eigenvalues. Consequently, a consistent method of imposing the boundary conditions is proposed and its convergence is established under the assumption that the expansion coecients decay fast asymptotically. In this work, we investigate stochastic collocation meth- ods for the same type of scalar wave equation with random wave speed. It will be demonstrated that the rate of convergence depends on the regularity of the solu- tions; and the regularity is determined by the random wave speed and the initial and boundary data. Numerical examples are presented to support the analysis and also to show the sharpness of the assumptions on the relationship between the random wave speed and the initial and boundary data. An accuracy enhancement technique is investigated following the multi-element collocation method proposed by Foo, Wan and Karniadakis (J. Comput. Phys., 227 (2008), pp. 9572-9595).