TECHNISCHE UNIVERSITÄT CHEMNITZ

Fakultät für Mathematik

# Chemnitz FEM-Symposium 2009

Chemnitz FEM Symposium

*Programme*

*Collection of abstracts*

*List of participants*

Chemnitz, September 28 - 30, 2009

# Scientific topics:

The symposium is devoted to all aspects of finite elements and wavelet methods in partial differential equations.

The topics include (but are not limited to)

- adaptive methods,
- parallel implementation,
- high order methods.

This year we particularly encourage talks on

- Solver and Domain Decomposition
- Sensitivity Analysis and Algorithmic Differentiation for FEM
- FEM for Maxwell Equations

# Invited Speakers:

**Axel Klawonn** (Universität Duisburg-Essen)

**Andrea Walther** (Universität Paderborn)

**Martin Costabel** (Université de Rennes, France)

### Scientific Committee:

Th. Apel (München), R. Herzog (Chemnitz), G. Haase (Graz), H. Harbrecht (Bonn),
B. Heinrich (Chemnitz), M. Jung (Dresden), U. Langer (Linz),
A. Meyer (Chemnitz), A. Rösch (Duisburg), O. Steinbach (Graz)

WWW: `http://www.tu-chemnitz.de/mathematik/fem-symposium/`

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Chemnitz, September 28 - 30, 2009

# Programme for Monday, September 28, 2009

| Time | Solver and Domain Decomposition | Flow Problems I |
|---|---|---|
| 9:00 | **Opening**<br>A. Meyer<br>*Room*: "Berlin" | |
| | **Solver and Domain Decomposition**<br>*Chairman*: A. Meyer<br>*Room*: "Berlin" | |
| 9:05 | A. Klawonn ... 7<br>Highly scalable parallel domain decomposition methods with an application to arterial wall modeling | |
| 9:55 | R. Herzog ... 8<br>Preconditioned conjugate gradient method for optimal control problems with control and state constraints | |
| 10:20 | S. Beuchler ... 9<br>Quasioptimal multilevel based solvers for hp-FEM discretizations in 3D | |
| 10:45 | *Tea and coffee break* | |
| | **Solver and Domain Decomposition**<br>*Chairman*: A. Klawonn<br>*Room*: "Berlin" | **Flow Problems I**<br>*Chairman*: T. Linß<br>*Room*: "Schwarzenberg" |
| 11:10 | S. Rhebergen ... 10<br>Multigrid optimization for space-time discontinuous Galerkin discretizations | C. Suciu ... 14<br>Finite element LES and VMS methods on tetahedral meshes |
| 11:35 | C. Köstler ... 11<br>Iterative Stokes solvers in geodynamic modeling | J. Prokopova ... 15<br>Numerical simulation of compressible flow in time-dependent domain with the motivation by the airflow in human vocal folds |
| 12:00 | O. Fortmeier ... 12<br>Comparing different graph models for partitioning tetrahedral grids on distributed-memory computers | D. Nikolaenko ... 16<br>Adaptive algorithms for combustion problems |
| 12:25 | J. Březina ... 13<br>Parallel Schur complements for solution of fracture flow problem using PETSc library | E. Özkaya ... 17<br>Automatic Differentiation Techniques for Aerodynamic Shape Optimization |
| 12:50 | *Lunch* | |

| | **Optimal Control**<br>*Chairman*: R. Herzog<br>*Room*: "Berlin" | **Flow Problems II**<br>*Chairman*: T. Mitkova<br>*Room*: "Schwarzenberg" |
|---|---|---|
| 14:30 | G. Wachsmuth ... 18<br>Regularization results and error estimates for optimal control problems with sparsity functional | C. Waluga ... 22<br>A hybrid mortar method for Stokes problems on non-matching meshes |
| 14:55 | J. Pfefferer ... 19<br>Finite element error estimates for Neumann boundary control problems on graded meshes | G. Matthies ... 23<br>Local projection stabilisation on layer-adapted meshes for convection-diffusion problems with characteristic layers |
| 15:20 | K. Eppler ... 20<br>The two-norm discrepancy in second order shape optimization methods | M. Bause ... 24<br>Stabilized finite element methods for nonstationary and nonlinear convection-diffusion-reaction equations |
| 15:45 | K. Chrysafinos ... 21<br>Convergence of space-time approximations for optimal control problems related to parabolic PDE's | J. Löwe ... 25<br>Numerical results for the simulation of natural convection in a square cavity with stabilized finite elements |
| 16:10 | *Tea and coffee break* | |
| | **Non-standard Discretisations**<br>*Chairman*: G. Matthies<br>*Room*: "Berlin" | **BEM and FEM-BEM**<br>*Chairman*: K. Eppler<br>*Room*: "Schwarzenberg" |
| 16:30 | T. Vejchodský ... 26<br>Discrete maximum principles for linear and higher-order finite elements | M. Windisch ... 30<br>Robust BE domain decomposition methods in acoustics |
| 16:55 | V. Rukavishnikov ... 27<br>The finite element method for a boundary value problem with double singularity | S. Weißer ... 31<br>Adaptive FEM with local Trefftz trial functions for elliptic equations |
| 17:20 | U. Hetmaniuk ... 28<br>Special finite element shape functions based on component mode synthesis | O. Steinbach ... 32<br>Stable coupling of finite and boundary element methods |
| 17:45 | H. Egger ... 29<br>Solution strategies for systems arising from discontinuous Galerkin discretizations | A. Radcliffe ... 33<br>FEM-BEM coupling for the exterior Stokes problem with conforming and non-conforming finite elements |
| 19:00 | *Meeting of the Scientific Committee* | |

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| | | |
|---|---|---|
| | **FEM for Maxwell Equations**<br>*Chairman*: O. Steinbach<br>*Room*: "Berlin" | |
| 9:00 | M. Costabel . . . 34<br>Recent progress in the analysis of the convergence of FEM for Maxwell eigenvalue problems | |
| 9:50 | S. Zaglmayr . . . 35<br>Gauging strategies for high order finite element discretizations of Maxwell's equations | |
| 10:15 | T. Mitkova . . . 36<br>Explicit local time stepping for Maxwell's equations | |
| 10:40 | *Tea and coffee break* | |
| | **FEM for Maxwell Equations**<br>*Chairman*: M. Costabel<br>*Room*: "Berlin" | **Adaptive Methods**<br>*Chairman*: A. Rösch<br>*Room*: "Schwarzenberg" |
| 11:00 | G. Lube . . . 37<br>A MHD problem on unbounded domains - coupling of FEM and BEM | P. Steinhorst . . . 41<br>Adaptive FEM for rotational symmetric piezoelectric problems |
| 11:25 | J. Li . . . 38<br>Convergence analysis of finite element methods for $H(curl)$-elliptic interface problems | A. Miedlar . . . 42<br>Adaptive solutions of eigenvalue problems for PDEs |
| 11:50 | M. Fleck . . . 39<br>BEM-based FEM for eddy current problems | T. Linß . . . 43<br>Robust pointwise a posteriori error estimates for time-dependent singularly perturbed problems |
| 12:15 | S. Engleder . . . 40<br>Boundary element methods for the eddy current model | T. Apel . . . 44<br>A posteriori error estimates for anisotropic discretizations of singularly perturbed model problems |
| 12:40 | *Lunch* | |
| 14:00 | *Excursion* | |
| 18:00 | *Conference Dinner (in* **"Fichtelberghaus"***)* | |

# Programme for Wednesday, September 30, 2009

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|---|---|
| | **Sensitivity Analysis and Algorithmic Differentiation for FEM**<br>*Chairman*: T. Apel<br>*Room*: "Berlin" |
| 9:00 | A. Walther ... 45<br>Algorithmic differentiation for FEM: Sensitivity analysis and the computation of adjoints |
| 9:50 | T. Neckel ... 46<br>FEM simulations of incompressible flow using automatic differentiation in the PDE framework Peano |
| 10:15 | U. Naumann ... 47<br>Challenges for adjoint compiler technology |
| 10:40 | *Tea and coffee break* |

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|---|---|---|
| | **Sensitivity Analysis and AD**<br>*Chairman*: A. Walther<br>*Room*: "Berlin" | **Modelling**<br>*Chairman*: M. Bause<br>*Room*: "Schwarzenberg" |
| 11:00 | P. Stumm ... 48<br>Structure exploiting adjoints | J. Paul ... 52<br>A decoupling strategy for a system of Stefan problem and Navier-Stokes equations with a free capillary surface |
| 11:25 | R. Schneider ... 49<br>On the evaluation of finite element sensitivities to nodal coordinates | M. Müller ... 53<br>Numerical challenges in modeling Stokes for planetary mantle convection |
| 11:50 | D. Holfeld ... 50<br>On the efficient adjoint computation for flow control problems | M. Kuhn ... 54<br>Optical modeling based on locally adapted simulation techniques |
| 12:15 | J. Hild ... 51<br>Real-time control of hydrodynamic models on networks | E. Azadravesh ... 55<br>Generating a 3D model for evaluation of dowel bars misalignment and their effects on horizontal movements of concrete pavements, using Abaqus/Standard and Abaqus/Explicit FE simulation |

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|---|---|
| 12:45 | **Closing**<br>A. Meyer<br>*Room*: "Berlin" |
| 13:00 | *Lunch* |

# Highly scalable parallel domain decomposition methods with an application to arterial wall modeling

Axel Klawonn[1]

Highly scalable parallel domain decomposition methods for elliptic partial differential equations are considered with a special emphasis on problems arising in elasticity. The focus of this talk is on Finite Element Tearing and Interconnecting (FETI) methods, a family of nonoverlapping domain decomposition methods where the continuity between the subdomains, in principle, is enforced by the use of Lagrange multipliers. Algorithmic variants are described and theoretical convergence estimates are presented together with numerical results confirming the parallel scalability properties of these methods. Parallel and numerical scalability of the methods for more than 65 000 processor cores of the JUGENE supercomputer at the Forschungszentrum Jülich is shown. An application of a dual-primal FETI method to a nontrivial biomechanical problem from nonlinear elasticity modeling arterial wall stress is given, showing the robustness of our domain decomposition methods for such problems.

The work presented here is based on different joint projects with Oliver Rheinbach, Dept. of Mathematics, Essen and Olof Widlund, Courant Institute, New York, as well as on a joint cooperation with Jörg Schröder and Dominik Brands, Institute of Mechanics, Essen.

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# Preconditioned conjugate gradient method for optimal control problems with control and state constraints

Roland Herzog[1] Ekkehard Sachs[2]

We consider saddle point problems arising as (linearized) optimality conditions in elliptic optimal control problems. In the spirit of Bramble and Pasciak, it turns out that the preconditioned systems are symmetric positive definite with respect to a suitable scalar product. We extend previous work of Schöberl and Zulehner by considering problems with control and state constraints. It stands out as a particular feature of this approach that only those matrices which represent the inner products need to be preconditioned, e.g., by multigrid cycles. Thus the preconditioner becomes independent of the underlying forward and adjoint differential equations. Numerical examples in 2D and 3D are given which illustrate the performance of the method.

References:

[1] J. Schöberl, W. Zulehner, Symmetric Indefinite Preconditioners for Saddle Point Problems with Applications to PDE-Constrained Optimization, SIAM Journal of Matrix Analysis and Applications 29(3), p.752–773, 2007

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# Quasioptimal multilevel based solvers for hp-FEM discretizations in 3D

Sven Beuchler[1]

In this talk we investigate the discretization of an elliptic boundary value problem in 3D by means of the hp-version of the finite element method using a mesh of hexahedrons. The corresponding linear system is solved by a preconditioned conjugate gradient method. The construction of the preconditioner is based on an inexact additive overlapping Schwarz method which was suggested by Pavarino, [1]. The remaining subproblems are treated by a tensor product based preconditioner. This preconditioner uses a basis transformation into a basis which is stable in $L_2$ and $H^1$. The construction is based on interpretations of the p-FEM mass and stiffness matrix as weighted h-FEM matrices and a simultaneous diagonalization of these matrices using wavelets.

The preconditioner is implemented into the finite element program `SpCAdHp` for *hp*-discretizations of scalar elliptic and linear elasticity problems using hexahedral elements with hanging nodes. In the main part of the talk, we illustrate the efficiency of the presented quasioptimal *hp*-solver on several numerical examples.

References:

[1] L. F. Pavarino, Additive schwarz methods for the *p*-version finite element method, *Numer. Math.*, 66(4):493–515, 1994.

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# Multigrid optimization for space-time discontinuous Galerkin discretizations

Sander Rhebergen[1] Jaap van der Vegt[2]

Space-time discontinuous Galerkin discretizations of partial differential equations result in large systems of algebraic equations that need to be solved at each time-step. To efficiently solve these algebraic equations, we combine a pseudo-time integration method with new $h$-multigrid techniques using explicit Runge-Kutta type time integrators as smoother. A two- and three-level Fourier analysis is used to investigate and optimize the multigrid algorithm for second, third and fourth order space-time discontinuous Galerkin discretizations of the two-dimensional linearized Euler equations. We will compare our optimized schemes with current pseudo-time Runge-Kutta time integrators.

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# Iterative Stokes solvers in geodynamic modeling

Christoph Köstler[1]

The conservation equations of momentum, mass, and energy for a fluid with infinite Prandtl number are solved in a 2-D Cartesian domain as well as in a 3-D spherical shell. In every time step a stationary Stokes system is solved. Viscosity varies by several (5 to 10) orders of magnitude, according to the conditions in the Earth's mantle, providing challenges for both, multigrid and Krylov subspace solvers. Finite-element discretization and solution methods are parallelized with MPI and domain decomposition.

We make a comparison between a preconditioned MINRES method and a CG method to the Schur complement equation and analyze the convergence behavior. Validity of the preconditioner-induced MINRES norm for the original Stokes system and the necessity to scale the preconditioner for the Schur complement will be discussed and appropriate stopping criteria for the iteration process will be derived.

Even more important for handling high viscosity variations is a multigrid solver for evaluating the inverse of the momentum operator. We use a geometric multigrid with matrix-dependent and grid-dependent transfer operators. A possible further improvement of the coarsening strategy is also discussed in Markus Müller's talk.

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# Comparing different graph models for partitioning tetrahedral grids on distributed-memory computers

Oliver Fortmeier[1] Timo Henrich[2] H. Martin Bücker[3]

At RWTH Aachen University the finite element solver DROPS is being developed within the SFB 540 "Model-based experimental analysis of kinetic phenomena in fluid multi-phase reactive systems." This parallel software package is designed to simulate two-phase flow problems arising from studying the behavior of droplets or falling films with a free surface. Typically, the analysis of such three-dimensional phenomena that are close to reality involves a high demand of both memory resources and computing time. To cope with these problems, we pursue two strategies: adaptive mesh-refinement and parallel computing. First, the refinement algorithm aims for locally refining the tetrahedral mesh in domains of interest. The output of this algorithm is a hierarchy of tetrahedral grids representing the computational domain. While evolving in time during the course of the simulation, the domains of interest may change, and thus, the hierarchy of tetrahedral grids may change as well. Second, the tetrahedra of the finest grid are distributed among several processes. In this domain decomposition setting, each process is responsible for a subdomain, which is represented by a subset of tetrahedra. Finding an appropriate distribution of the tetrahedra among the processes is generally done by graph partitioning techniques that decompose a graph into "equally-sized" subgraphs while minimizing edges connecting vertices in different subgraphs.

In this work, we present and compare graph models representing the tetrahedra hierarchy in DROPS. These models allow to distinguish between "computationally expensive" and "computationally inexpensive" tetrahedra. Therefore, algorithms for graph partitioning may find a distribution offering a good balance of the computational work while minimizing communication among processes. To augment the graph with information about computational effort, we utilize the degrees of freedom to weight each tetrahedron. This is of particular importance in the context of two-phase flow problems where the computational cost of tetrahedra may vary dramatically.

We conclude by giving detailed results when using different graph models. The numerical results are obtained by investigating several problems occurring in two-phase flow simulations performed by DROPS.

References:

[1] S. Groß, V. Reichelt, and A. Reusken. A finite element based level set method for two-phase incompressible flows. Comput. Vis. Sci., 9(4):239?257, 2006.
[2] S. Groß and A. Reusken. Parallel multilevel tetrahedral grid refinement. SIAM J. Sci. Comput., 26(4):1261?1288, 2005.

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# Parallel Schur complements for solution of fracture flow problem using PETSc library

Jan Březina[1]

A mixed-hybrid formulation of the water flow problem in a saturated porous medium with fractures results in a linear system with a symmetric indefinite matrix. Particular pattern of the matrix allows two successive constructions of a Schur complement, which leads to a positive-definite matrix with significantly reduced size and condition number. We present how to use the PETSc library to compute the Schur complements and to solve the resulting system in parallel.

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# Finite element LES and VMS methods on tetahedral meshes

Carina Suciu[1] Volker John[2] Adela Kindl[3]

Finite element methods for problems given in complex domains are often based on tetrahedral meshes. This talk demonstrates that the so-called rational Large Eddy Simulation model and a projection-based Variational Multiscale method can be extended in a straightforward way to tetrahedral meshes. Numerical studies are performed with an inf-sup stable second order pair of finite elements with discontinuous pressure approximation.

The talk contains several turbulence models on tetrahedral meshes. In particular, it was shown that a FEVMS method with an adaptive large scale space can be extended in a straightforward way to such meshes. Computations were performed with the $P_2^{bubble}/P_1^{disc}$ pair of finite element spaces. One could not distinguish one method to be better than all other ones. Only the adaptive VMS method gave improved results in comparison with the VMS method with uniform static large scale space. In addition, it will be shown at a flow through a reactor that the indicator of the adaptive VMS method predicts the distribution of the turbulence intensities correctly.

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# Numerical simulation of compressible flow in time-dependent domain with the motivation by the airflow in human vocal folds

Jaroslava Prokopova[1]

The contribution is concerned with compressible flow in a time-dependent domain with applications to the airflow in human vocal folds. The mathematical model of this problem is represented by the compressible Navier-Stokes equations or the compressible Euler equations. For the treatment of the time-dependent domain the Arbitrary Lagrangian-Eulerian (ALE) method is used. The governing equations are written in the ALE formulation and discretized in space by the discontinuous Galerkin finite element method. The time discretization is carried out by a linearized semi-implicit unconditionally stable method. Some results of our computations in a domain with the shape of human vocal folds will be presented.

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# Adaptive algorithms for combustion problems

Dmitry Nikolaenko[1] Gundolf Haase[2] Helfried Steiner[3]

In jet flames, convection, diffusion and chemical reactions take place. Combustion problems are characterized by turbulence and multiscaleness in space and time. A laminar non-premixed counterflow configuration (as a 1D problem) is considered. Here, fuel and oxidizer are fed separately into the combustor and, therefore, have to get mixed before reaction. There can be distinguished advective, diffusive and chemical time scales, which relate to the corresponding terms of the underlying differential equations. In this work, temporal adaptive algorithm based on the error estimate of Runge-Kutta-Fehlberg (RKF45) method has been implemented. Thereby the whole computational interval is divided into subintervals where different timesteps for RKF45 are applied. Also it is determined in which subintervals we can neglect chemistry in the calculations and a spatial adaptive strategy is developed. Due to that, a speed-up of calculation has been reached. The results obtained are presented and discussed.

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# Automatic Differentiation Techniques for Aerodynamic Shape Optimization

Emre Özkaya[1] Nicolas R. Gauger[2]

We focus on how to efficiently conpute gradient vectors for aerodynamic shape optimization problems by the use of the reverse mode of automatic differentiation (AD). The state equations are the Euler as well as Navier-Stokes equations, either laminar or turbulent. Both methods of AD, operator overloading and source transformation, are applied to aerodynamic shape optimization problems. Here, the computed gradient vectors are relatively large in size and the memory problems of AD are solved by applying two innovative techniques for steady state problems. The first technique is the reverse propagation technique and the other one is the one-shot optimization approach. Furthermore, we present techniques for the MPI parallelization of AD-generated adjoint routines in this context.

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# Regularization results and error estimates for optimal control problems with sparsity functional

Gerd Wachsmuth[1] Daniel Wachsmuth[2]

A recent research area in optimization are nonsmooth problems which lead to sparse solutions. For example, this approach is successfully used in image processing and signal compression. The talk deals with optimal control problems featuring a nonsmooth term in the objective function which causes sparse solutions, i.e., solutions which vanish on parts of the domain. The problems are regularized to permit the use of the semi-smooth Newton method and read as

$$\text{Minimize} \quad J(y,u) = \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)} + \beta\|u\|_{L^1(\Omega)}$$

$$\text{s.t.} \quad \begin{cases} Ay = u & \text{in } \Omega \\ y = 0 & \text{on } \partial\Omega \\ u_a \le u \le u_b & \text{in } \Omega. \end{cases}$$

Error estimates with respect to the regularization parameter $\alpha$ are provided and convergence as $\alpha \to 0$ is obtained. Moreover, finite element approximations are studied. A-priori as well as a-posteriori error estimates are developed and an adaptive method is used to discretize the problem. The theory is confirmed by numerical results which will be presented.

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# Finite element error estimates for Neumann boundary control problems on graded meshes

Johannes Pfefferer[1] Thomas Apel[2] Arnd Rösch[3]

In this talk we will discuss a priori error estimates for a specific elliptic linear-quadratic optimal control problem in 2D with Neumann boundary control and inequality constraints on the control variable. The domain is assumed to be polygonal and maybe non-convex. The approximations of the optimal solution are constructed in a postprocessing step by a projection of the discrete adjoint state. Although the quality of these approximations is in general affected by the appearance of corner singularities, we will show that the order of convergence can be improved provided the mesh is sufficiently graded. The quality of the approximations of the optimal control problem is demonstrated by numerical examples.

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# The two-norm discrepancy in second order shape optimization methods

Karsten Eppler[1]

For second order sufficient optimality conditions, the two-norm discrepancy is essantial: shape differentiability is ensured in a certain space, but the shape Hessian of integral objectives cannot be coercive in this strong norm. However, the second order remainder allows a refined estimate in a weaker space. Hence, a strict local minima of second order is provided by strict coercivity in the weak norm. Ill-posedness of a shape problem takes place, if the shape Hessian at stationary domains defines a compact, degenerate operator. We will present illustrational examples for both cases.

Finally, we will comment on some algorithmic aspects of the abovementioned considerations. In particular, we recommend a modified viewpoint for the use of the Hadamard shape gradient representation in descent algorithms.

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# Convergence of space-time approximations for optimal control problems related to parabolic PDE's

Konstantinos Chrysafinos[1]

We discuss discontinuous Galerkin finite element methods for optimal control problems related to semi-linear parabolic PDE's. The main objective is the minimization of the energy functional, using controls of distributed and Robin type. The approximation schemes under consideration are discontinuous in time but conforming in space. We present results regarding the convergence of discrete schemes of arbitrary order. The proposed technique is based on stability estimates at arbitrary time points under minimal regularity assumptions on the given data, and a discrete compactness argument for discontinuous Galerkin schemes.

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# A hybrid mortar method for Stokes problems on non-matching meshes

Christian Waluga[1] Herbert Egger[2]

Interface problems typically arise from coupling of non-matching meshes or different physical models. A flexible way to treat interface conditions of different character are Mortar methods, which enforce jump conditions across the interface by Lagrange multipliers. Those methods however involve certain difficulties, as the Lagrange multiplier space in the resulting saddle point problem has to be chosen carefully to obtain inf-sup-stability.

Methods, that satisfy interface conditions only approximately (e.g. Nitsche-type methods) can be formulated without Lagrange multipliers. This makes it possible to circumvent difficulties, as no inf-sup condition has to be satisfied for the interface functions. Unfortunately, most methods introduce a lot of coupling across the interface, which reduces the practicability for parallel computations. We investigate a method, that is related to such methods. It introduces additional (hybrid) variables to reduce the coupling to a minimum. This hybridization yields a Schur complement system for the interface variables only.

We summarize the analysis and numerical results in case of Poisson's problem. We also discuss the extension of the proposed method to the Stokes problem, using a nonconforming $P_1 - P_0$ mixed finite element (lowest order Crouzeix-Raviart element). Numerical results for incompressible flow problems are given and their agreement with the derived a-priori estimates of the error in the energy- and $L^2$-norm is examined.

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# Local projection stabilisation on layer-adapted meshes for convection-diffusion problems with characteristic layers

Gunar Matthies[1] Sebastian Franz[2]

We consider singularly perturbed convection-diffusion problems on the unit square where the solution $u$ exhibits exponential and characteristic layers. In order to stabilise the discretisation, layer-adapted meshes and the local projection method are applied.

Using bilinears, the error between the solution $u$ and the finite element solution $u^N$ converges with first order while the error between $u^N$ and the bilinear interpolant $I^N u$ of the solution $u$ shows second order convergence.

For enriched $\mathcal{Q}_p$ elements which already contain the space $\mathcal{P}_{p+1}$, the error between the solution $u$ and the finite element solution $u^N$ shows the convergence order $p+1$ in the $\varepsilon$-weighted energy norm. Furthermore, the error between $u^N$ and a special interpolant $I^N u$ provides the convergence order $p+1$ in the local projection norm.

The theoretical results are confirmed by numerical results. The influence of the chosen enrichment will be discussed.

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# Stabilized finite element methods for nonstationary and nonlinear convection-diffusion-reaction equations

Markus Bause[1]

Fluid flow problems with simultaneous reactive multicomponent transport of chemical species arise in many technical and environmental applications. The numerical solution of nonstationary convection-diffusion-reaction models is a challenge when convection is dominant and small layers of the concentrations arise. Here, the numerical approximation of such systems with SUPG stabilized higher order finite element methods and additional shock-capturing stabilization is studied theoretically and numerically. An anisotropic nonlinear variant of the shock-capturing methods is used.

As a model problem of our analysis we consider solving the scalar quasilinear convection-diffusion-reaction equation

$$\alpha u + \vec{b} \cdot \nabla u - \nabla \cdot (a \nabla u) + r(u) = f \text{ in } \Omega\,, \qquad u = 0 \text{ on } \partial\Omega\,.$$

Rigorous error estimates are given for the numerical approximation scheme within a $hp$ finite element framework and discussed in detail. In particular the design of the stabilization parameter is studied carefully.

Numerical results for transport systems of different complexities are presented. The results illustrate that shock-capturing in combination with a higher order finite element method is efficient to further reduce spurious oscillations in crosswind directions and avoid negative concentrations. This is of importance for coupled systems of equations in which inaccuracies in one concentration affect all other ones.

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# Numerical results for the simulation of natural convection in a square cavity with stabilized finite elements

Johannes Löwe[1]

The non-isothermal incompressible Navier-Stokes equations with Boussinesq approximation for buoyancy effects are solved by a numerical method based on a stabilized finite element discretization and implicit-explicit Runge-Kutta methods. The computed solutions for a square cavity with differentially heated side walls and Rayleigh numbers up to $Ra = 10^8$ are compared to reference data and the influence of stabilization is studied on coarse and fine meshes. Especially we want to test some proposals for the stabilization parameters based on a-priori error analysis for the linearized subproblems and evaluate their performance for time-dependent problems.

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# Discrete maximum principles for linear and higher-order finite elements

Tomáš Vejchodský[1]

This talk surveys the general theory for the discrete maximum principles (DMP) for the linear second order elliptic problems discretized by the finite element method. We concentrate on the definition of the discrete Green's function (DGF) and its properties. We show that the validity of the DMP is equivalent to the nonnegativity of the DGF. Special emphasis will be given to the case of nonhomogeneous Dirichlet and Robin boundary conditions.

This general theory can be applied to the case of linear finite elements yielding the well-known maximal angle condition for the corresponding mesh. The theory can be equally well applied to higher-order finite elements, but the analysis of the nonnegativity of the DGF is more complicated. However, for triangular elements, we present numerical experiments, where we test the nodal values of the higher-order DGF. The results indicate that the higher-order approximations allow for weaker angle conditions then the linear approximations. In addition, the maximal angle condition for the linear elements seems to reshape into the minimal angles condition for the higher-order case.

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# The finite element method for a boundary value problem with double singularity

Victor Rukavishnikov[1]

We present a new approach for numerical solution of the boundary value problem with double singularity. The specificity of solving these problems is generated by discontinuous input data (the coefficients of the equations, the right hand sides of the equation and of the boundary conditions) in combination with the presence of salient points on the boundary of the domain.

The diffraction problem with discontinuity of coefficients on the domain with a slot and a boundary contained $2\pi$ angles has been considered. For this problem we introduce a definition of $R_\nu$-generalized solution and two weak matching conditions on the slot, construct the approximation using the singular mortar finite element method, and suggest the new method of numerical analysis on computer that permits to parallelize the process of computations.

We have carried out a series of calculations of model boundary value problems with double singularity. We have made the comparison of errors for the found approximate generalized (weak) solution and approximate $R_\nu$-generalized solution in the norm of the space $C$ in the mesh points.

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# Special finite element shape functions based on component mode synthesis

Ulrich Hetmaniuk[1] R. Lehoucq[2]

The finite element solution of

$$\begin{cases} \text{find } u \in H_0^1(\Omega) \text{ such that} \\ \int_\Omega \nabla v(x) \cdot (c(x)\nabla u(x))dx = \int_\Omega f(x)v(x), \quad \forall v \in H_0^1(\Omega) \end{cases} \tag{1}$$

has been the subject of much research. Difficulties arise when the coefficient $c$ associated with the second order linear elliptic operator is rough or highly oscillating so that a naive application of the finite element method necessitates a highly refined mesh.

We will present a new finite element discretization for problem (1). Our discretization is based upon the classic idea of component mode synthesis and exploits a decomposition of $H_0^1(\Omega)$ into subspaces orthogonal for the inner product defined by

$$a(u, v) = \int_\Omega \nabla v(x) \cdot (c(x)\nabla u(x))dx. \tag{2}$$

This decomposition is a well-known result, at the heart of the analysis and development of domain decomposition methods for elliptic partial differential equations and modern component mode synthesis methods for the numerical solution of the global eigenvalue problem.

Combining this space decomposition with local eigendecompositions results in our new special finite element method. Numerical experiments illustrate the effectiveness of the proposed shape functions.

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# Solution strategies for systems arising from discontinuous Galerkin discretizations

Herbert Egger[1]

We investigate the discretization of elliptic and hyperbolic pdes by discontinuous Galerkin methods, and consider hybridization as a tool for obtaining efficient implementations as well as for designing efficient solvers for the arising linear systems. In particular, we investigate the use of multilevel and domain decomposition techniques for the efficient solution.

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# Robust BE domain decomposition methods in acoustics

Markus Windisch[1] Olaf Steinbach[2]

In this talk we will present a boundary element tearing and interconnecting approach for the Helmholtz equation. In contrary to the Laplace equation it is in general not known if local Dirichlet or Neumann problems admit a unique solution. So one has to stabilize the standard approach to get rid of artificial eigenfrequencies of the local problems. In this talk we will present a stabilized approach which leads to a uniquely solvable discrete system. This will be done in two steps: First Robin boundary conditions are introduced to ensure the solvability of the local problem. But the Steklov-Poincare operator, which is used in the formulation may not well defined if the local Dirichlet problem is not uniquely solvable. So we introduce an alternative formulation for the local problem which leads to an always well defined and uniquely solvable formulation. Additionally, one can prove that also the discrete local and the discrete global problem have a unique solution.

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# Adaptive FEM with local Trefftz trial functions for elliptic equations

Steffen Weißer[1]

We discuss a special finite element method that solves the stationary isotropic heat equation with Dirichlet boundary conditions on arbitrary polygonal and polyhedral meshes. The method uses a space of locally harmonic trial functions to approximate the solution of the boundary value problem. According to this choice, we obtain a variational formulation on the skeleton of the domain. This formulation contains one Steklov-Poincaré-Operator for each element. These operators are constructed by means of boundary integral formulation. Therefore, the proposed finite element method can be used on general polygonal non-conform meshes. Hanging nodes are treated quite naturally. The material properties are assumed to be constant on each element. We also discuss adaptive mesh refinement to handle cases, when the material properties are given as a continuous function.

In a second step we have a look at a posteriori error estimates which can be used for further mesh refinement. Standard methods are based on triangular or quadrilateral meshes. The challenging part is to handle the arbitrary polygonal and polyhedral meshes. Therefore, we make use of functional analytic estimates to overcome these problems.

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# Stable coupling of finite and boundary element methods

Olaf Steinbach[1]

We prove in the case of a Lipschitz interface the stability of the coupling of finite and boundary element methods when the direct boundary integral equation with single and double layer potentials is used only. In particular we prove an ellipticity estimate of the coupled bilinear form. Hence we can use standard arguments to derive stability and error estimates for the Galerkin discretization for all pairs of finite and boundary element trial spaces.

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# FEM-BEM coupling for the exterior Stokes problem with conforming and non-conforming finite elements

Alastair Radcliffe[1]

Galerkin finite element - boundary integral equation formulations are presented for the coupling of a finite element modelled interior region to a boundary integral supported exterior region for the two-dimensional steady state exterior Stokes problem.

The solutions in the exterior are represented using both single- and double-layer hydrodynamic potentials which allows a well conditioned symmetric structure for the entire system-matrix when using (stabilized linear) conforming finite elements, for which results will be presented.

Similar formulations and results will also be indicated for **preliminary work** extending the FEM-BEM coupling to use non-conforming Crouzeix-Raviart finite elements for the velocity, where stabilization is not required but overall system-matrix symmetry is lost.

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# Recent progress in the analysis of the convergence of FEM for Maxwell eigenvalue problems

Martin Costabel[1]

Finite element approximation of the Maxwell eigenvalue problem can notoriously go wrong, even if the standard “stability plus consistency” conditions are satisfied. The reason is that - depending on the choice of the variational formulation - one has to deal with a problem with a non-compact resolvent, or with a non-standard eigenvalue problem for a mixed formulation.

Recently, D.N. Arnold, R. Falk and R. Winther have shown a general framework in which the spectrally correct approximation of the Maxwell eigenvalue problem is a reward for the obedience of the finite element spaces to some algebraic structure, in the presence of uniform estimates of compatible interpolation operators in the appropriate norms (keywords “discrete subcomplexes of the de Rham complex” and “uniformly bounded cochain projectors”). These arguments cover the spectrally correct convergence for the $h$ version FEM using edge elements of arbitrary order on simplicial meshes.

For the $p$ and $hp$ versions of the edge element method, the available known interpolants do not quite fit into this scheme. In particular, it is hard to prove $L^2$ interpolation error estimates uniformly in p. A recently found tool, the regularized Poincaré integral operator, can help here. This tool answers a variety of questions in the regularity theory of vector analysis on Lipschitz domains. In the analysis of computational electromagnetics, it can be used to complete the proof of the discrete compactness property of the $p$ version edge element methods on various 2 and 3 dimensional meshes, thereby showing spectrally correct convergence of these methods. These results have been obtained in joint work with D. Boffi (Pavia), M. Dauge (Rennes), L. Demkowicz (Austin), R. Hiptmair (Zürich), A. McIntosh (Canberra).

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# Gauging strategies for high order finite element discretizations of Maxwell's equations

Sabine Zaglmayr[1]

In order to guarantee unique solvability for magnetostatic Maxwell's equations additional constraints, so called gauging conditions, have to be imposed. In particular, we consider Coulomb gauge which enforces orthogonality to gradient fields and discuss several realizations, e.g. via Lagrange multipliers.

By a careful construction of high order Nedelec-type finite elements the Coulomb gauge can be realized by a two step strategy: First, uniqueness of the discrete magnetostatic problem can be ensured by eliminating part of the high order basis functions (and appropriate handling of the low order space). In a second step the orthogonality to gradients is restored by postprocessing.

Both subproblems use reduced bases and are better conditioned than the original problem, so the overall performance can be improved considerably. The efficiency of our approach is illustrated by numerical examples.

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# Explicit local time stepping for Maxwell's equations

Teodora Mitkova[1] Marcus Grote[2]

The accurate and reliable simulation of electromagnetic wave phenomena is of fundamental importance in a wide range of engineering applications, such as wireless communication, photonic crystals, radar technology, and near field scanning optical microscopy. In the presence of complex geometry, adaptivity and mesh refinement are certainly key for the efficient numerical solution of Maxwell's equations. Hence to address the wide range of difficulties involved in the numerical simulation of time-dependent electromagnetic waves, we consider symmetric interior penalty (IP) discontinuous Galerkin (DG) methods for the spatial discretization, which yield a block-diagonal mass matrix with fixed block size determined by the number of degrees of freedom per element only. Hence, when combined with explicit time integration, the resulting time-marching schemes are truly explicit. Locally refined meshes, however, impose severe stability constraints on explicit time-stepping schemes, where the maximal time-step allowed by a CFL condition is dictated by the smallest elements in the mesh. When mesh refinement is restricted to a small region, the use of implicit methods, or a very small time step in the entire computational domain, are very high a price to pay. To overcome the stability restriction, we consider local time-stepping schemes, which allow for arbitrarily small time-steps precisely where small elements in the mesh are located. Numerical experiments validate the theoretical results and illustrate the efficiency of the proposed time integration schemes, which are fully explicit and energy conserving.

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# A MHD problem on unbounded domains - coupling of FEM and BEM

Gert Lube[1] Wiebke Lemster[2]

The Maxwell equations describe processes in the elektromagnetic context. From this one can derive the following magnetohydrodynamic (MHD) problem

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E} \qquad \text{in } \Omega_c$$
$$\nabla \times \frac{1}{\mu}\mathbf{B} = \begin{cases} \sigma\left(\mathbf{E} + \mathbf{u} \times \mathbf{B} + j^c\right) & \text{in } \Omega_c \\ 0 & \text{in } \Omega_v \end{cases}$$
$$\nabla \cdot \mathbf{B} = 0 \qquad \text{in } \Omega.$$

In the so-called direct problem, the magnetic induction $\mathbf{B}$ and the electric field $\mathbf{E}$ are unknown and $\mathbf{u}$ is a given incompressible flow field. The domain $\Omega$ consists of conducting regions $\Omega_c$ (e.g. the Earth core) and insulating regions $\Omega_v$ (e.g. vacuum). After semidiscretization in time with the implicit Euler-scheme, a Lagrange finite element approach is used in the bounded region $\Omega_c$ and bounded regions of $\Omega_v$. A boundary element approach is used in the unbounded insulating region of $\Omega_v$ following ideas of Kuhn/Steinbach (Math. Meths. Appl. Sc. 25 (2002), 357-371). We present results on the well-posedness of the continuous problem and for the semidiscrete coupled problem arising within each time step. Then we discuss algorithmic aspects for the solution of the coupled problem. Finally we present first results of the numerical analysis based on previous results in Chan er.al. (SINUM 44 (2006) 5, 1877-1902) and Guermond et al. (JCP 221 (2007) 1, 349-369).

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# Convergence analysis of finite element methods for $H(curl)$-elliptic interface problems

Jingzhi Li[1] Ralf Hiptmair[2] Jun Zou[3]

In this talk we analyse a finite element method for solving $H(curl)$-elliptic interface problems in general three-dimensional polyhedral domains with smooth material interfaces. The continuous problems are discretized by means of the first family of lowest order Nédélec $H(curl)$-conforming finite elements on a family of tetrahedral meshes which resolve the smooth interface in the sense of sufficient approximation in terms of a parameter $\delta$ that quantifies the mismatch between the smooth interface and the triangulation. Optimal error estimates in the $H(curl)$-norm are obtained for the first time. The analysis is based on a so-called $\delta$-strip argument, a new extension theorem for $H^1(curl)$-functions across smooth interfaces, a novel non-standard interface-aware interpolation operator, and a perturbation argument for degrees of freedom for $H(curl)$-conforming finite elements. Numerical tests are presented to verify the theoretical predictions and confirm the optimal order convergence of the numerical solution.

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# BEM-based FEM for eddy current problems

Marvin Fleck[1]

We analyse a method related to Domain Decomposition Methods and Trefftz-FEM. A Boundary Element Method is used to construct trial functions for Finite Element Methods on arbitrary polyhedral meshes. The functions are determined by their Dirichlet values on the boundaries of mesh elements.
While the choice of Dirichlet data for trial functions of polynomial degree is natural in the case of 2-dimensional scalar-valued problems, treatment of 3D vector-valued equations is more complicated. We give a short introduction to the boundary element formulation of eddy current problems and discuss strategies for constructing suited trial functions.

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# Boundary element methods for the eddy current model

Sarah Engleder[1]

Magnetic Induction Tomography is a contactless imaging modality, which aims to obtain the conductivity distribution of the human body. The method is based on exciting the body by magnetic induction using an array of transmitting coils to induce eddy currents. A change of the conductivity distribution in the body results in a perturbed magnetic field, which can be measured as a voltage change in the receiving coils. Based on these measurements, the conductivity distribution can be reconstructed by solving an inverse problem.
The forward problem of this method can be described by the eddy current model. In this talk a boundary element method for this eddy current problem will be presented. The use of suitable preconditioners and fast boundary element methods will be discussed.

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# Adaptive FEM for rotational symmetric piezoelectric problems

Peter Steinhorst[1]

A special class are threedimensional problems are such with rotational symmetry, which can be characterized by a twodimensional generating profile. For linear piezoelectric material behaviour, an extension of twodimensional FEM to rotational symmetric problems will be shown. Reminding the transversal isotropic material characteristics, the cases of axial and radial poling directions have to be considered. For the aim of adaptive mesh refinement, also the used error estimator has to be adapted. Some numerical examples demonstrate, that a sufficient accuracy can be obtained with substantial lower effort on computing time and memory requirement in comparison to true threedimensional FEM. The topic of the talk is written down as a part of [1].

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# Adaptive solutions of eigenvalue problems for PDEs

Agnieszka Miedlar[1] Volker Mehrmann[2]

We introduce a new adaptive algorithm (AFEMLA) for elliptic PDE-eigenvalue problems. In contrast to other approaches the algebraic eigenvalue problem does not have to be solved to full accuracy. It incorporates the iterative solution of the resulting finite dimensional algebraic eigenvalue problem in the adaptation process in order to balance the cost with the costs for the iterative eigenvalue method.

In order to determine the error estimates, we only solve the algebraic eigenvalue problem on the current coarse grid and use classical perturbation results from finite dimensional eigenvalue problems to determine the errors on the fine mesh. The accuracy of the method is guaranteed by using a posteriori error estimators that incorporate the discretization errors, approximation errors in the eigenvalue solver and roundoff errors.

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# Robust pointwise a posteriori error estimates for time-dependent singularly perturbed problems

Torsten Linß[1] Natalia Kopteva[2]

A singularly perturbed reaction-diffusion problem with a small parameter is considered. The efficiency of standard numerical methods deteriorates as the parameter approaches zero. Bounds for the Green's function are derived that allow the design of robust, with respect to the perturbation parameter, a posteriori error estimators. These in turn enable adaptive grid refinement in both space and time.

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# A posteriori error estimates for anisotropic discretizations of singularly perturbed model problems

Thomas Apel[1] Serge Nicaise[2]

Anisotropic meshes are characterized by elements with large or even asymptotically unbounded aspect ratio. Such meshes are known to be particularly effective for the resolution of directional features of the solution, like edge singularities and boundary layers.

In the talk we present a posteriori error estimates for discretizations with anisotropic meshes. We focus on results obtained in joint work with Serge Nicaise and Sergey Grosman for singularly perturbed model problems: an anisotropic diffusion model equation and a simplyfied shell model.

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# Algorithmic differentiation for FEM: Sensitivity analysis and the computation of adjoints

Andrea Walther[1]

The provision of exact and consistent derivative information is important for numerous applications arising from optimization purposes as for example optimal control problems. However, even the pure simulation of complex systems may require the computation of derivative information. Implicit integration methods are prominent examples for this case.

The talk will present the technique of algorithmic (or automatic) differentiation (AD) to compute exact derivative information for function evaluations given as computer programs. This includes a short overview of the history of AD and a description of the main variants of AD, namely the forward mode to compute sensitivities and the reverse mode for the provision of adjoints. A discussion of complexity estimates follows yielding the important cheap gradient result. Subsequently, I will sketch briefly a rounding error analysis and different implementation strategies. Then several aspects closely connected with the computation of sensitivity and adjoint information for finite element discretizations and related techniques are emphasized. This covers also the structure exploitation in time and space. Some examples stemming optimal flow control problems illustrate the presented aspects.

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# FEM simulations of incompressible flow using automatic differentiation in the PDE framework Peano

Tobias Neckel[1] Hans-Joachim Bungartz[2]

Modern CSE applications such as multi-physics or fluid-structure interaction simulations need more and more efficient methods. Partitioned approaches have proven to be suitable for such simulations but heavily depend on the efficiency of the individual solvers. Therefore, the C++ PDE framework *Peano* [1] has been developed. *Peano*'s flow solver supports incompressible fluid flow on regularly or adaptively refined Cartesian grids using low-order finite elements in combination with space-filling curves and a very cache-efficient stack data concept. The steady-state or time-implicit discretisation of the Navier-Stokes equations result in a non-linear system of equations $B(\mathbf{u}, p) = 0$ with velocities $\mathbf{u}$ and pressure $p$. In *Peano*, this nonlinear system is solved with Newton's method within the PETSc toolkit [2] by explicitly assembling the Jacobian.

We use the well-known benchmark flow around a cylinder to compare three different approaches to compute the Jacobian: A tuned finite difference approximation, the computation of the exact Jacobian via the automatic differentiation (AD) tools ADOL-C [3] and cppAD [4], and finally the analytical differentiation of contributions to the nonlinear function $B$. All three versions are implemented using a strictly cell-wise operator evaluation. The analytical approach results in the lowest assembly times needing 0.4–2.6% of the total non-linear iteration durations (decreasing with increasing mesh resolution). The implementations via finite differences, ADOL-C and ccpAD show an overhead of a factor of about 5.5, 2.7, and 18, respectively. While different implementations using ADOL-C have been tested, including also tapeless variants, an efficient one-touch strategy for the tape has been used to obtain these runtimes with ADOL-C, recording data only in the very first call on the first cell and evaluating this record on all cells with the corresponding data.

Thus, we removed the bottleneck for steady-state or time-implicit non-linear solutions concerning the computation of the Jacobian. All three approaches may easily be extended to other ansatz functions or other applications within our *Peano* framework for regular or adaptive Cartesian grids. The AD variants possess the advantage that no changes in the code regarding the Jacobian are necessary for such extensions. The efficient one-touch strategy for ADOL-C is usable for any other (finite element) discretisation using a direct, cell-wise assembly.

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# Challenges for adjoint compiler technology

Uwe Naumann[1]

Given a program for evaluating a multivariate vector function $y = F(x)$, where $F : R^n \rightarrow R^m$, an adjoint compiler transforms the source code into a program that computes $\bar{x} += F'(x)^T \cdot \bar{y}$ at a computational complexity of $O(m)$ and where $F'(x)$ denotes the Jacobian of $F$ at $x$. Adjoint compilers for both C/C++ and Fortran are developed by our group. A number of successful applications, including various finite element codes, have been reported on. Users include the Max-Planck-Institute for Meteorology in Hamburg (adjoint error correction), QinetiQ Group plc in the UK (shape optimization), and oceanographers at MIT in the US (data assimilation).

We have been collaborating with colleagues at Argonne National Laboratory, US, and INRIA, France, to tackle some of the many open challenges for developers of adjoint compilers. Various hard combinatorial and static program analysis problems need to be faced. They range from approximate solutions for the NP-hard DATA-FLOW REVERSAL problem to the definition of adjoint communication patterns for programs using MPI. Re-applicability of the compilers to their own outputs with the aim to generate higher derivative codes is highly desirable.

The talk aims to set the stage for further off-line discussions with potential users of adjoint compiler technology. A large fraction of the audience is expected to belong to this category. We plan to give a survey of our activities in this area giving people an impression of why adjoint compilers are useful tools for computational science and engineering and what makes their development theoretically and practically challenging.

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# Structure exploiting adjoints

Philipp Stumm[1] Andrea Walther[2]

In this presentation, we consider the numerical solution of PDE constrained optimal control problems of the form

$$J(u,q) = j(u(T)) + R(q) \to \min!$$

$$\begin{aligned} s.t.\ \partial_t u + \nabla \cdot f(u) &= S(q) \qquad in\ \Omega \\ f(u) \cdot n &= f^b(u) \qquad on\ \Gamma \\ u(0,x) &= u_0(x) \end{aligned}$$

with the nonlinear flux $f : \mathbb{R} \to \mathbb{R}$ and the state $u : [0,T] \times \Omega \subset [0,T] \times \mathbb{R}^d \to \mathbb{R}$. The normal direction vector is denoted by $n$. The distributed control is given by $q : [0,T] \to \mathbb{R}$. Regularization terms are represented by $R(q)$. The boundary of $\Omega$ is denoted by $\Gamma$. We apply a discontinuous Galerkin method to transform the PDE into an ODE. Furthermore, the integrals in the ODE are replaced by quadrature rules and the time stepping procedure is performed by an explicit Runge-Kutta method. To compute the gradient required for a calculus-based optimization one may use Algorithmic Differentiation (AD). We present the integration schemes that are automatically generated when differentiating the discretized state equation by AD. We analyze the convergence behavior of AD generated adjoints and show that the AD adjoints yield a discretized version of the adjoint of the discretize-then-optimize approach.

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# On the evaluation of finite element sensitivities to nodal coordinates

Rene Schneider[1] Andrea Walther[2] Peter K. Jimack[3]

We present a derivation of the derivative of general systems of finite element equations with respect to the coordinates of the nodes in the underlying finite element mesh. The resulting expressions allow the systematic evaluation of such derivatives without the need to resort to algorithmic differentiation or the expense associated with finite difference approximations. The principal motivation for this work comes from problems in optimal design, however other potential applications are also described. The results obtained are validated through numerical examples and compared with algorithmic differentiation.

References:

[1] Schneider R, Jimack P, On the evaluation of finite element sensitivities to nodal coordinates, Electronic Transactions on Numerical Analysis, 32:134-144, Special Volume: Selected Papers from the 20th Chemnitz Finite Element Symposium, 2008.

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# On the efficient adjoint computation for flow control problems

Denise Holfeld[1] Andrea Walther[2]

The efficient provision of adjoint information is indispensable for numerous applications in flow control. The complex physical background necessitate a very fine mesh. Thus a corresponding high number of timesteps is required to simulate flows accurately. We want to combine advanced methods of numerical models and methods of mathematical control to improve the flow qualities. For that purpose we modify the common flow simulation software SEMTEX based on a spectral element method. We present a new approach for the exploitation of structure in time and space. For this purpose, recent results for the algorithmic differentiation of finite element discretization and implicit time stepping procedures are combined with appropriate checkpointing strategies.

Adapted to the given structure different techniques for the adjoint calculation are applied to minimize the effort. For flexible parts, like the target function, we use algorithmic differentiation. On the other hand, the timestepping loop of the simulation code is hand adjoint, because this part will remain constant for the considered applications.

Numerical results for a flow control problem illustrate the resulting numerical effort for the computation of the required adjoint information.

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# Real-time control of hydrodynamic models on networks

Johannes Hild[1]

We present the development and implementation of a software framework, which is suited to compute the optimal weir control for an urban drainage system in real-time. The framework aims to generate an infinite sequence of optimal control parameters in a moving horizon setting in real-time. The objective of the real-time control is as follows: Moveable weir structures are driven to channel flows with major and minor pollution distributions through the network into their corresponding destination.

This problem is not only of practical relevance for hydraulic engineering but also related to continuous matching and transport problems, like traffic problems on networks. To solve the problem, the urban drainage system is represented by an hydrodynamic model based on the nonlinear shallow water equations and other hydrological conservation laws.

This model is best suited for a finite volume discretization on networks, therefore the state variables - water level, flow rate and pollution density - are computed by an explicit Godunov scheme to guarantee fast and robust evaluations.

The optimization process is executed by the external optimization tool IPOPT, which is based on a set of quasi-Newton methods. It is therefore necessary to provide not only objective information of the network flow but also gradient information. The successful interfacing of the automatic differentiation tool ADOL-C with a C++-template technique fulfills this task and provides fast and robust gradient information.

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# A decoupling strategy for a system of Stefan problem and Navier-Stokes equations with a free capillary surface

Jordi Paul[1] E. Baensch[2] A. Schmidt[3]

We consider an FEM approximation of a coupled system consisting of a Stefan problem and the Navier-Stokes equations with free capillary boundary. To use existing solvers and data structures, the Navier-Stokes equations have to be decoupled from the Stefan problem, with special attention paid to the phase boundary.

Inspired by coordinate transformation techniques we develop a decoupling that works well with the existing formulation for the free surface problem, which decouples the geometry and the flow field. Since the solver uses a finite element formulation on an unstructured tetrahedral mesh, the grid is transformed according to the movement of the phase boundary. This keeps elements from changing the phase but makes occasional remeshing necessary.

This problem arises from the mathematical modelling of a melting process, in which a thin wire is heated by a laser, and is currently under research in the SFB 747.

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# Numerical challenges in modeling Stokes for planetary mantle convection

Markus Müller[1]

Mantle convection simulation is challenging because it needs huge parallel computers and adaptivity to control the strongly varying parameters. In the case of planetary core simulations also the Maxwell equations are involved. In this talk planetary convection is investigated from a numerical point of view, theoretical analysis as well as practical tests are performed. The stability criteria for the numerical formulation of the physical model will be made clear using the well known simulation code TERRA as an example. For the incompressible case and the TERRA specific treatment of the an-elastic approximation, two inf-sup stable grid modifications can be found, which are both compatible with hanging nodes. For the $Q_{1_h}Q_{1_{2h}}$ element pair a simple numeric test is introduced to prove the stability for any given (TERRA-)grid. For the $Q_{1_h}P_{1_{2h}}^{disc}$ element pair and 1-regular refinements with hanging nodes an existing general proof can be adopted. The influence of the slip boundary condition is known to be destabilizing. For the incompressible case a cure can be adopted from the literature. but the general case is still not clear. The necessary conditions for the expansion of the stability results to the an-elastic approximation will be pointed out.
Additionally a small numerical framework is presented in order to measure the effect of different numerical approaches to improve the handling of strongly varying viscosity. The framework is applied to investigate how block smoothers with different block sizes, combination of different block smoothers, different prolongation schemes and semi coarsening influence the multi-grid performance.
The talk is intended to raise interest of the mathematical experts for the numerical challenges of this physical model.

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# Optical modeling based on locally adapted simulation techniques

Michael Kuhn[1] Frank Wyrowski[2] Joachim Schöberl[3]

Advanced photonic systems combine optical elements of different length scales and different optical properties. These properties have a large impact on the efficiency and accuracy of modeling techniques that can be applied for the simulation of such systems. So, geometrical optics methods are well suited for lens modeling whereas rigorous methods as Finite Element methods are required for systems with scales close to the wavelength of light.

In this talk we present the concept of Unified Optical Modeling that is strongly based on domain decomposition ideas. It includes several aspects of optical simulation, one of them being the combination of different simulation techniques. We discuss how optical systems have to be decomposed into sub-problems that allow an efficient solution or make a solution feasible at all. In particular, the talk will adress how Finite Element methods can be integrated into this concept. Results using the optical simulation software VirtualLab(TM) (www.lighttrans.com) are presented.

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# Generating a 3D model for evaluation of dowel bars misalignment and their effects on horizontal movements of concrete pavements, using Abaqus/Standard and Abaqus/Explicit FE simulation

Ehsan Azadravesh[1] Ali Mansourkhaki[2]

A 3D FE model is generated to evaluate dowel bars misalignment and their effects on horizontal movements of concrete pavements, using Abaqus/Standard and Abaqus/Explicit. The modeling method details are presented as well. For dowel and concrete modeling, 8-node solid-brick elements are used. The concrete damage plasticity model is used for concrete plastic behavior. The interaction between dowel and surrounding concrete is simulated by surface to surface hard contact model without separation after contact. Various degrees of dowel bars misalignment is evaluated. The analysis is implemented with Abaqus/Standard and Abaqus/Explicit and the results are compared. The obtained results show that the Explicit and Standard Abaqus solvers have similar results. However, Explicit solver is more efficient than Standard solver.

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# Application of Beltrami equations to generation of spatial adaptive grids

Vladimir D. Liseikin[1] A.M. Kharitonchik A.V. Kofanov

The paper presents recent results related to the development of algorithms and codes for generating both structured and unstructured adaptive spatial grids with the use of the inverted Beltrami equations. An original description of the method was given in the monograph: V.D. Liseikin "A Computational Differential Geometry Approach to Grid Generation", 2004, Berlin, Springer.

Control of grid properties is performed by metrics introduced in the physical geometry under consideration. Applications of the algorithms developed to some applied problems are demonstrated.

The work over the paper was supported by the Russian Foundation for Basic Research (RFBR), Award 07-01-00336 and the Integrated Grant of the Siberian Branch of the Russian Academy of Sciences 2009-2001, Award N94.

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**Notes:**

## Internet access:

A laptop with internet connection is available in the coffee room on the first basement floor. (Look for the FEM logo.)

| | |
|---|---|
| username: | "fem09" |
| password: | "chemnitz" |

Wireless network is also available in most of the hotel, please contact reception regarding prices and further information.

## Food:

The conference fee includes:

- Lunch on all three days of the symposium, (restaurant opposite reception)
  **Drinks are on your own expense.**
- The conference dinner on Tuesday ("Fichtelberghaus").
- Tea, coffee, soft drinks and snacks during breaks.

Dinner on the other days is not included. There is a range of restaurants in the town center of Oberwiesenthal if you prefer to leave the hotel.

## Recreation:

The hotel offers for free (15:00–22:00, contact reception):

- sauna,
- gymm.

Services available for a fee:

- solarium,
- massages.