DFG-Sonderforschungsbereich 393

”Parallele Numerische Simulation für Physik und Kontinuumsmechanik”

and

Fakultät für Mathematik, Technische Universität Chemnitz

Chemnitz FEM-Symposium 2005

Programme

Collection of abstracts

and

List of participants

Chemnitz, September 19 - 21, 2005

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

- variational inequalities - contact and free boundary value problems,
- partial differential equations in optimization and optimal control,
- special treatment of singularities and singularly perturbed problems,
- parabolic and time-dependent problems.

Invited Speakers:

Gert Lube (Göttingen)

Reinhold Schneider (Kiel)

Fredi Tröltzsch (Berlin)

Barbara Wohlmuth (Stuttgart)

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Programme for Monday, September 19, 2005

Start at 09:00

Chairman: A. Meyer

9:00	–	9:05	A. Meyer Welcome
9:05	–	9:50	B. Wohlmuth Hybrid discretization techniques for variational inequalities
10:00	–	10:15	R. Unger Subspace cg-techniques for innner-domain-restrictions
10:20	–	10:45	S. Geyn A Boundary Element Method for an elastoplastic contact problem

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cookie break

Chairman: B. Wohlmuth

11:10	–	11:35	S. Nepomnyaschikh Domain decomposition preconditioning for elliptic problems with jumps in coefficients
11:40	–	12:05	S. Beuchler New shape functions for triangular p-FEM using integrated Jacobi polynomials
12:10	–	12:35	M. Bebendorf Computing approximate LU decompositions of FE discretizations with almost linear complexity

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Lunch

Chairman: S. Nepomnyaschikh

14:30	–	15:15	R. Schneider Wavelets for linear scaling computation in electronic structure calculation
15:25	–	15:40	U. Kähler $\mathcal{H}^2$ matrix based Wavelet Galerkin BEM

Tea and coffee break

Chairman: M. Bebendorf

16:05 – 16:30 H. Harbrecht
Adaptive Wavelet Galerkin BEM

16:35 – 17:00 F. Leydecker
An Adaptive Finite Element / Boundary Element Coupling Method for Electromagnetic Problems

17:05 – 17:30 K. Schmidt
Mixed *hp*-adaptive FEM of the eddy current model

short break

Chairman: R. Schneider

17:45 – 18:10 S. Grosman
Convergence of adaptive FEM on anisotropic meshes for singularly perturbed reaction-diffusion equation

18:15 – 18:40 Y. Kondratyuk
Adaptive Finite Element Algorithms of Optimal Complexity for the Stokes Problem

18:45 – 19:10 W. Dörfler
A convergent adaptive hp-strategy

Dinner

20:00 Wine reception

Programme for Tuesday, September 20, 2005

Start at 09:00

Chairman: M. Jung

09:00 – 09:45	G. Lube Finite element methods for parabolic problems with emphasis on the singularly perturbed case
09:55 – 10:20	M. Bause Higher order mixed finite element methods for elliptic and parabolic equations with solutions of low regularity
10:25 – 10:50	J. Rang A comparison of time-discretization/linearization approaches for the incompressible Navier-Stokes equations

cookie break

Chairman: G. Lube

11:15 – 11:40	G. Matthies Solving the Navier-Stokes equations by multigrid methods using quasi divergence free functions
11:45 – 12:10	F. Schieweck On the reference mapping for quadrilateral and hexahedral elements on multilevel adaptive grids
12:15 – 12:40	T. Linß Anisotropic meshes and streamline-diffusion stabilization

Lunch

Chairman: G. Matthies

14:15	–	14:40	V. Liseikin New Approaches for Generating Adaptive Numerical Grids
14:45	–	15:10	F. Lippold FENFLOSS - a parallel implementation of the FEM in CFD-Engineering

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15:30 Excursion

Dinner

Programme for Wednesday, September 21, 2005

Start at 09:00

Chairman: W. Dörfler

09:00	–	09:45	F. Tröltzsch Optimal control of PDEs – from optimality conditions to numerical methods
09:55	–	10:20	A. Rösch On the numerical verification of optimality conditions for optimal control problems
10:25	–	10:50	J. Saak An LQR approach to tracking control for parabolic systems

cookie break

Chairman: T. Apel

11.15	–	11:40	C. Pester On the computation of singularity exponents
11:45	–	12:00	G. Winkler Optimal Control Problem on non-convex Domains

short break

Chairman: B. Heinrich

12:15	–	12:40	B. Jung Nitsche- and Fourier-finite-element method for the Poisson equation in axisymmetric domains with re-entrant edges
12:45	–	13:10	V. Rukavishnikov The Finite Element Method for the Boundary Value Problem with Strong Singularity of Solution
13:15	–	13:20	A. Meyer Closing

Lunch

Higher order mixed finite element methods for elliptic and parabolic equations with solutions of low regularity

Markus Bause[1]

In this talk a higher order finite element approach to the *coupled variably saturated groundwater flow and bioreactive contaminant transport model* is considered. Higher order techniques have proved advantageous in the reliable numerical simulation of biochemically reacting transport processes, due to their less inherent numerical diffusion. For the calculation of the groundwater flow field mixed finite element methods are prefered due to their inherent conservation properties and since they provide a flux approximation as part of the formulation itself. Typically, lowest order mixed Raviart–Thomas elements are used for solving the parabolic-elliptic degenerate Richards equation describing the motion of groundwater, since this model admits solutions of low regularity only.

Here, our numerical results obtained by a higher order mixed finite element approach of Brezzi-Douglas-Marini type to elliptic, parabolic and degenerate partial differential equations with solutions of low regularity are presented and carefully compared to corresponding results based on lowest order Raviart–Thomas mixed finite element calculations. The application of the mixed Brezzi-Douglas-Marini finite element technique to the nonlinear degenerate Richards equation and its implementation in the *parallel software* environment *M++* is also addressed.

References:

[1] M. Bause, P. Knabner. Computation of variably saturated subsurface flow by adaptive mixed hybrid finite element methods, Adv. Water Resour., **27**:565–581, 2004.
[2] M. Bause, P. Knabner. Numerical simulation of contaminant biodegradation by higher order methods and adaptive time stepping, Comput. Visual. Sci., **7**:61–78, 2004.

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Computing approximate LU decompositions of FE discretizations with almost linear complexity

Mario Bebendorf[1]

Although the asymptotic complexity of direct methods for the solution of large sparse finite element systems arising from second-order elliptic partial differential operators is far from being optimal, these methods are often preferred over modern iterative methods. This is mainly due to their robustness. In this article it is shown that an (approximate) *LU* decomposition can be computed in the algebra of hierarchical matrices with almost linear complexity and with the same robustness as the classical *LU* decomposition.

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New shape functions for triangular p-FEM using integrated Jacobi polynomials

Sven Beuchler[1] Joachim Schoeberl[2]

In this talk, the second order boundary value problem $-\nabla \cdot (\mathcal{A}(x,y)\nabla u) = f$ is discretized by the Finite Element Method using piecewise polynomial functions of degree p on a triangular mesh. On the reference element, we define integrated Jacobi polynomials as interior ansatz functions. If $\mathcal{A}$ is a constant function on each triangle and each triangle has straight edges, we are able to show that the element stiffness matrix has not more than $25/2p^2$ nonzero matrix entries.

The proof of this result requires several properties of Jacobi polynomials. We will present the most important relations for Jacobi polynomials which are needed.

Finally, two applications of this result are presented.

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A convergent adaptive hp-strategy

Willi Dörfler[1]

We develop a strategy that allows to decide between h- and p- refinement in the finite element solution of the Poisson problem. It can be proved that the method is convergent if the error indicators are both reliable and efficient uniformly in h and p.

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A Boundary Element Method for an elastoplastic contact problem

Sergey Geyn[1] Matthias Maischak[2] Ernst P. Stephan[3]

We consider an elastoplastic two body contact problem with friction under small strain, plain strain theories in 2D. An interaction of bodies is described by the penetration theory, J_2 flow theory with isotropic/kinematic hardening for plasticity is used. The Galerkin Boundary element method with Newton potentials is used to obtain a weak formulation of the elastoplastic contact problem. Newton potentials occur due to plastic deformations that introduce additional terms in the representation formula for displacement and stresses. Those terms are nothing more than integration of plastic part of strain tensor over domain with specific singular kernels. We obtain a discrete nonlinear system under plastic and contact constrains. These system is solved with the Newton method. The Advantage of the BE approach with respect to FE is a smaller number of unknowns that one has to manage to obtain the discrete approximation of the solution. Using boundary elements one has to overcome difficulties dealing with the boundary integrals with singular and hyper singular kernels. For polynomial functions such integrals can be easily regularized by integration by parts. Therefore recursion formulas can be used for numerical realization. All implementation was done with the scientific package maiprogs using Fortran F95. Simulation showed good agreement FEM with BEM solutions.

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Convergence of adaptive FEM on anisotropic meshes for singularly perturbed reaction-diffusion equation

Sergey Grosman[1]

Singularly perturbed reaction-diffusion problems exhibit in general solutions with anisotropic features, e.g. strong boundary and/or interior layers. This anisotropy is reflected in the discretization by using meshes with anisotropic elements. By means of a posteriori error estimation we develop an adaptive Finite Element Method, employing special anisotropic adaptive partitions. This algorithm produces well-suited meshes; we show that it converges uniformly in the energy norm.

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Adaptive Wavelet Galerkin BEM

Helmut Harbrecht[1] W. Dahmen[2] Rob Stevenson[3]

This talk is concerned with developing numerical techniques for the adaptive application of global operators of potential type in wavelet coordinates. This is a core ingredient for a new type of adaptive solvers that has so far been explored primarily for PDEs. We shall show how to realize asymptotically optimal complexity in the present context of global operators. *Asymptotically optimal* means here that any target accuracy can be achieved at a computational expense that stays proportional to the number of degrees of freedom (within the setting determined by an underlying wavelet basis) that would ideally be necessary for realizing that target accuracy if full knowledge about the unknown solution were given. The theoretical findings are supported and quantified by first numerical experiments.

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Nitsche- and Fourier-finite-element method for the Poisson equation in axisymmetric domains with re-entrant edges

Beate Jung[1] Bernd Heinrich[2]

In this talk we present a combination of the Fourier-finite-element method with the Nitsche-finite-element method (as a mortar method). The approach is applied to the Dirichlet problem of the Poisson equation in three-dimensional axisymmetric domains with re-entrant edges entailing singularities of the solution. We use a non-tensor product representation of singularities.
The approximating Fourier method yields a splitting of the 3D-problem into 2D-problems. For solving the 2D-problems on the meridian plane Ω_a, the Nitsche-finite-element method with non-matching meshes is applied. In order to improve the accuracy of the method in presence of singularities, these meshes are provided with local grading. The solution of the 3D-problem is obtained by Fourier synthesis of the 2D-solution.
The rate of convergence in some H^1-like norm is proved to be of the type $\mathcal{O}(h^\alpha + N^{-1})$ (h: mesh size on Ω_a, N: length of the Fourier sum), where $\alpha = 1$ in case of appropriate mesh grading, i.e. the same convergence rate as for a regular solution of the BVP can be achieved. Moreover, we prove that the convergence rate in the L_2-norm is of the order $\mathcal{O}(h^{2\alpha} + N^{-2})$.

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$\mathcal{H}^2$ matrix based Wavelet Galerkin BEM

Ulf Kähler[1]

This talk is devoted to the fast solution of boundary integral equations on unstructured meshes by the Galerkin scheme. To avoid the quadratic costs of traditional discretizations with their densely populated system matrices it is necessary to use fast techniques such as hierarchical matrices, the multipole method or wavelet matrix compression, which will be the topic of the talk.

On the given, possibly unstructured, mesh we construct a wavelet basis providing vanishing moments with respect to the traces of polynomials in the space. With this basis at hand, the system matrix in wavelet coordinates can be compressed to $\mathcal{O}(N \log N)$ relevant matrix coefficients, where N denotes the number of unknowns.

For the computation of the compressed system matrix with suboptimal complexity we will present a new method based on the strong similarities of substructures of the $\mathcal{H}^2$ matrices and the used wavelet basis.

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Adaptive Finite Element Algorithms of Optimal Complexity for the Stokes Problem.

Yaroslav Kondratyuk[1]

Nowadays adaptive finite element algorithms are recognized as powerful techniques for solving PDEs. The general structure of the loop of an adaptive algorithm is Solve - Estimate - Refine, Derefine. Especially the analysis of the last step of this loop is important for showing the optimality of the method. In "Adaptive Finite Element Methods with Convergence Rates" [Numer. Math., 97,(2004), pp.219-268], Binev, Dahmen and DeVore and in "An Optimal Adaptive Finite Element Method" [to appear in SIAM J. Numer. Anal.], Stevenson showed optimality of adaptive FEM algorithms for elliptic problems.

Concerning the solution of mixed variational problems, the situation is more complecated, and we are not aware of any theoretical study of optimality of finite element algorithms.

In "An Adaptive Uzawa FEM for the Stokes Problem: Convergence without the Inf-Sup Condition" [SIAM J. Numer. Anal., 40, (2002), pp. 1207-1229], Bänch, Morin and Nochetto introduced an adaptive FEM algorithm for the Stokes problem. Although they proved convergence of the algorithm, and numerical experiments showed (quasi-) optimal triangulations for some values of the parameters, a theoretical analysis whether the algorithm is optimal is missing.

In this talk, we present a detailed design of adaptive FEM algorithms for the Stokes problem, and an analysis of their computational complexity. We apply a fixed point iteration to an infinite dimensional Schur complement operator, where to approximate the inverse of the elliptic operator we use a convergent adaptive finite element method. Further, we apply a Chebyshev acceleration of this fixed point iteration, and show that the overall method has optimal computational complexity.

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AN ADAPTIVE FINITE ELEMENT / BOUNDARY ELEMENT COUPLING METHOD FOR ELECTROMAGNETIC PROBLEMS

Florian Leydecker[1] Matthias Maischak[2] Ernst P. Stephan[3]

We present an *hp*-version of the finite element / boundary element coupling method to solve time-harmonic scattering problems and eddy current problems in $I\!R^3$. We use $\mathbf{H}(\mathrm{rot}, \Omega)$–conforming vector-valued polynomials to approximate the electric field in the conductor Ω and $\mathbf{H}(\mathrm{div}_\Gamma, \Gamma)$–conforming polynomials on the boundary Γ of Ω to approximate the twisted tangential trace of the magnetic field. We present both a priori and a posteriori error estimates together with an adaptive algorithm to compute the fem/bem coupling solution on suitably refined meshes. We present numerical results.

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Anisotropic meshes and streamline-diffusion stabilization

Torsten Linß[1]

We study a convection-diffusion problem with dominant convection. Anisotropic streamline aligned meshes with high aspect ratios are recommended to resolve characteristic interior and boundary layers and to achieve high accuracy. We address the question of how the stabilization parameter in the streamline-diffusion FEM (SDFEM) should be chosen inside the layers. Using a residual free bubbles approach, we show that within the layers the stabilization must be drastically reduced.

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FENFLOSS - a parallel implementation of the FEM in CFD-Engineering

Felix Lippold[1] Stefan Borowski[2]

1 FENFLOSS - a parallel implementation of the FEM in CFD-Engineering

Simulation of flow phenomena in engineering applications gained more and more importance in the last two decades. The limiting factor in most cases was the available computing time and storage capacity. Nowadays, very complex flow problems can be simulated within acceptable time. However, the demand for more computing power still lasts, and simulation codes and algorithms have be adapted to the respective architectures.

The unsteady Reynolds averaged Navier Stokes solver FENFLOSS (**F**inite **E**lement based **N**umerical **FLO**w **S**imulation **S**ystem) is being developped at the University of Stuttgart, Institute of Fluid Mechanics and Hydraulic Machinery (IHS), since early 80s. Main applications are steady and unsteady turbulent flow problems of incompressible fluids in complex three dimensional geometries. To model the physical problem, a Q1P0 Petrov-Galerkin-formulation on hexahedral elements is applied. A Richardson-iteration folded by a time loop is used to solve the global non-linear problem. The linearised equations are solved by an iterative BICGStab-solver. In order to appropriately model turbulence, two-equation models or enhanced, adaptive turbulence models are available. Furthermore, a special formulation for rotating frames of reference is implemented.

Today, the typical problem size is about one to ten million or more grid points which means up to 60 million unknowns. Besides special matrix storage methods, this requires an appropriate size of available computing time and memory. In this case, the best way to reduce the absolute time to obtain a solution is parallel processing.

FENFLOSS uses a distributed memory (DMP) approach based on MPI. The domain decomposition technique is based on the METIS-library to guarantee good load balancing between the single processes. Communication is applied directly in the matrix-vector and scalar product of the solver. The main advantage of this approach, besides a very good speed-up ratio, is the independence of solution from the number of partitions. This allows the usage of massively parallel architectures such as PC-clusters.

In order to exploit the power of highly specialised vector computer architectures, such as the new NEC SX-8 installed at the HPC-Centre in Stuttgart, the code provides special storage schemes and loop orderings for vector processing. Though already vectorised, the solver of FENFLOSS is still further optimised and matrix reorderings yield another improvement in performance. Another way to use modern hybrid SMP-DMP architectures is the combination of shared memory parallisation (SMP) and DMP.

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Performance measurements on the new SX-8 vector system for the diffent code optimisation steps will be discussed for a chosen example. Furthermore, the changes made in the code will be presented in detail and the issue of indirect addressing in vector computing will be addressed.

References:

[1] 1. NEC:*NEC SX-Series Programming Environment - Ready Reference*
[2] 2. MAIHÖFER:
[3] *Effiziente Verfahren zur Berechnung dreidimensionaler Strömungen mit nichtpassenden Gittern*, Dissertation, Universität Stuttgart, IHS 2002.
[4] 3. RUPRECHT, A. *Finite Elemente zur Berechnung dreidimensionaler turbulenter Strömungen in komplexen Geometrien.*
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[6] 4. VAN DER VORST, H. A. *BI-CGSTAB: A fast and smoothly converging variant of BI-CG for the solution of nonsymmetric linear systems.*
[7] SIAM J.Sci.Stat.Comp, Vol.13(2), 1992.

New Approaches for Generating Adaptive Numerical Grids

Vladimir Liseikin[1] A.H. Glasser[2] I.A. Kitaeva, Yu.V. Likhanova[3]

The paper presents recent results related to the development of algorithms and codes for generating both structured and unstructured grids with the use of operator Beltrami. An original description of the method was given in the monograph V.D. Liseikin Ä Computaional Differential Geometry Approach to Grid Generation", 2004, Berlin, Springer. Control of grid properties is realized by monitor metrics introduced in the physical geometry under consideration. The metrics for generating grids adapting to vector fields, gradients, and/or values of physical quantities are presented. Applications of adaptive grids to fluid dynamics and plasma related problems are demonstrated.

The work over the paper and participation in conferences are supported by CRDF (grant RU-M1-2579).

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Finite element methods for parabolic problems with emphasis on the singularly perturbed case

Gert Lube[1]

In the main part of the talk, we consider the linear parabolic advection-diffusion-reaction model

$$\partial_t u - \epsilon \nabla \cdot (a \nabla u) + (b \cdot \nabla) u + cu = f \quad \text{in} \quad (0,T) \times \Omega \subset \mathbf{R} \times \mathbf{R}^d \tag{1}$$

with $\epsilon \in (0,1]$. The singularly perturbed case $0 < \epsilon \ll 1$ is often of special interest in applications. A plain FEM-semidiscretization in space leads to a very large stiff and dissipative ODE-system. A proper implicit discretization in time gives a large set of algebraic equations to be solved within each time step, see [1]. Typical requirements are stability of the time discretization (A-stability, eventually B-stability) , high accuracy in time and space, adaptive time step control (hopefully with adaptive control of the spatial mesh) and efficient solvability of the algebraic systems.

First we discuss these aspects for the standard θ-scheme as an example of a low-order scheme in time, see [2]. Then we consider higher-order schemes in time, in particular B-stable Runge-Kutta methods and discontinuous Galerkin methods in time [3]. From the view-point of adaptivity, we propose to consider the time discretization in an outer loop, see also [4]. In the singularly perturbed case, one is also interested in robustness of a-priori and a-posteriori estimates with respect to the parameter ϵ. We will discuss difficulties which appear if standard residual-based stabilization techniques (like streamline upwinding) are applied. Recent stabilization methods, e.g. the edge-stabilization or local projection schemes, avoid some of these problems.

In applications, the model problem (1) will appear only as an auxiliary problem. In the final part of the talk, we will briefly discuss a suitable approach to time-dependent, thermally-coupled, incompressible and turbulent flow problems [5].

References

[1] V. Thomee: Galerkin Finite Element Methods for Parabolic Problems, Springer 1997

[2] R. Verfürth: A posteriori error estimates for linear parabolic equations, Ruhr-Universität Bochum, Fakultät für Mathematik, Preprint 2004

[3] K. Svadlenka, M. Feistauer: Space-time discontinuous Galerkin method for solving non-stationary convection-diffusion reaction, Charles University Prague, Preprint MATH-knm-2005/2

[4] J. Lang: Adaptive Multilevel Solution of Nonlinear Parabolic PDE systems, Springer 2001

[5] T. Knopp, G. Lube, R. Gritzki, M. Rösler: A near-wall strategy for buoyancy-affected turbulent flows using stabilized FEM with applications to indoor air flow simulation, Comput. Methods Appl. Mech. Engr. 194 (2005), 3797-3816

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Solving the Navier-Stokes equations by multigrid methods using quasi divergence free functions

Gunar Matthies[1] Friedhelm Schieweck[2]

We consider higher order finite element discretisations for solving the Navier–Stokes problem by means of discontinuous elements for the pressure and suitable conforming elements for the velocity such that the global and the local inf-sup condition are satisfied.

Higher order finite element discretisations have proved to be very efficient for the numerical solution of incompressible flow problems. However, the block Gauss-Seidel smoothers of existing coupled multi-level solvers become quite expensive for higher order discretisations, especially in the 3D case.

We will present a new multigrid solver that allows to use a smoother with low computational costs. The idea is to switch inside of the multigrid method to a new velocity basis which leads to a system with a much lower number of unknowns as well as a very small number of couplings between them. We call this new basis quasi divergence free since most of the basis functions are discretely divergence free which implies that they do not have any coupling to the pressure. The quasi divergence free basis functions can be constructed locally during the assembling process of the stiffness matrix by means of local projection operators.

The discrete problem which uses the quasi divergence free basis functions is decomposed into two subproblems. The first one is a problem for the element bubble part of the velocity solution. It can be solved independently from the remaining part in an element-wise way already during the assembling process of the stiffness matrix. The second problem of the decomposition is a reduced problem for the piecewise constant part of the pressure solution and the remaining velocity part. This system has a much smaller dimension than the original discrete Ossen problem. The remaining pressure part can be computed at the end by an element-wise post-processing procedure.

Furthermore, we will show how the multigrid solver constructed for the Oseen equations can be used for solving a discrete problem of a streamline diffusion method inside of a modified Picard-type iteration.

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Domain decomposition preconditioning for elliptic problems with jumps in coefficients

Sergey V. Nepomnyaschikh[1]

In this talk, we propose an effective iterative preconditioning method to solve elliptic problems with jumps in coefficients. The algorithm is based on the additive Schwarz method (ASM). First, we consider a domain decomposition method without cross points on interfaces between subdomains and the second is the cross points case. In both cases the main computational cost is an implementation of preconditioners for the Laplace operator in whole domain and in subdomains. Iterative convergence is independent of jumps in coefficients and mesh size.

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On the computation of singularity exponents

Cornelia Pester[1]

In this talk we give an introduction to boundary value problems with singular behaviour of the solution. Singularities occur, for example, near concave corners in the domain, at points of changing boundary conditions or when the differential operator is discontinuous. In three-dimensional domains, we have to distinguish in addition between edge and corner singularities and interacting edge and corner singularities. We present strategies for the computation of the singularities near two- or three-dimensional corners and discuss the convergence behaviour of the Finite Element Method.

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A comparison of time-discretization/linearization approaches for the incompressible Navier-Stokes equations

Joachim Rang[1] Volker John[2] Gunar Matthies[3]

This talk presents a numerical study of two ways for discretizing and linearizing the time-dependent incompressible Navier-Stokes equations. One approach consists in first applying a semi-discretization in time by a fully implicit θ-scheme. Then, in each discrete time, the equations are linearized by a fixed point iteration. The number of iterations to reach a given stopping criterion is a priori unknown in this approach. In the second approach, Rosenbrock schemes with s stages are used as temporal discretization. The non-linearity of the Navier-Stokes equations is treated internally in the Rosenbrock methods. In each discrete time, exactly s linear systems of equations have to be solved. The numerical study considers five two-dimensional problems with distinct features. Four implicit time stepping schemes and five Rosenbrock methods are involved.

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On the numerical verification of optimality conditions for optimal control problems

Arnd Rösch[1] Daniel Wachsmuth[2]

Optimality conditions are the base of all numerical methods. For instance, the first-order necessary optimality conditions can be solved by Newton-type algorithms. The second-order sufficient optimality condition (definiteness, coercivity) ensure the local quadratic convergence of such methods. However, the verification of second-order sufficient optimality condition is still a challenge.

In this talk, we will shed light on the numerical verification of optimality conditions. We will present interesting cases where numerical solutions guarantee the existence of a solution of the undiscretized problem in a well determined neighborhood of the numerical solution.

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The Finite Element Method for the Boundary Value Problem with Strong Singularity of Solution

V.A. Rukavishnikov[1] H.I. Rukavishnikova[2]

Mathematical models for a number of physical processes lead to the differential problems in which the strong singularity of solution is caused by the singularity of initial data (the coefficients of the equation, the right hand sides of the equation and boundary conditions). For the boundary value problem of this type, for which the generalized (weak) solution can not be defined, or it does not have necessary regularity, we offered to define the solution as the R_ν-generalized one. Such a concept of solution led to distinction of two classes of boundary value problems: the problems with co-ordinated and non-co-ordinated degeneration of initial data. For these classes of problems this approach allowed to investigate the existence, uniqueness, coercivity, differential properties of the R_ν-generalized solution in the weighted Sobolev spaces. We construct and investigate the h-version and the $h-p$-version of the finite element method for these problems. We introduce the special regularizor and the finite element space which contains the singular functions, having the singularity depending on the space, to which the R_ν-generalized solution of the problem belongs. Using these elements we prove the estimate of the rate of convergence of the approximate solution to the exact R_ν-generalized solution in the norm of the weighted space. Numerical analysis of the modeling problems with singularity was made with elements of parallelizing the process of computing.

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An LQR approach to tracking control for parabolic systems

Jens Saak[1] Peter Benner[2]

We present a linear-quadratic regulator design for tracking reference states of parabolic systems. It is shown that the solution strategy is closely related to an earlier approach where the LQR approach was used to achieve asymptotic zero stabilization. That means, here we want to regulate the state to a given stationary state. We discuss theoretical extensions to the earlier approach needed to complete this task and compare numerical results for both approaches.

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On the reference mapping for quadrilateral and hexahedral elements on multilevel adaptive grids

Friedhelm Schieweck[1] Gunar Matthies[2]

We study the properties of a general non-affine family of quadrilateral and hexahedral meshes with possibly hanging nodes which are typically generated by an adaptive finite element method starting from a regular coarse mesh. It turns out that for such meshes the reference mapping, which maps a fixed reference element to an arbitrary element of the mesh, behaves nearly like an affine mapping up to a perturbation of the magnitude of the mesh-size. This result may be useful for the finite element analysis since it allows to generalize by means of a perturbation argument some existing results that are proved in the literature only for the special case of an affine equivalent quadrilateral and hexahedral finite element mesh. However, from the practical point of view, the assumption of an affine equivalent mesh is too restrictive for quadrilateral and hexahedral mesh cells since it would admit only parallelograms or parallelepipeds. As an application we show how the local inf-sup condition for the (Q_r, P_{r-1}) element can be proved via transformation from a known inf-sup condition on the unit cube.

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Mixed hp-adaptive FEM of the eddy current model

Kersten Schmidt[1]

We are interested in the electromagnetic field generated by an alternating current density, in the computational domain Ω with dielectric media. In many situations the quasi-static eddy current model is reliable. The E-field is determined in $H(\mathrm{curl}, \Omega)$ only up to gradients of potential functions ϕ in $H^1(\Omega_0)$, where Ω_0 is the sub-domain of non-conducting materials. However, by introducing additional constraints a uniquely solvable mixed formulation for E and ϕ in $H(\mathrm{curl}, \Omega) \times H^1(\Omega_0)$ results.

The space $H(\mathrm{curl}, \Omega) \times H^1(\Omega_0)$ is discretised by $W \times S$, consisting of fully hp-adaptive edge and nodal element spaces on a quadrilateral mesh. To ensure unique solvability of the discrete problem the space of the discrete gradients of the potentials have to coincide with the kernel of the discrete curl operator applied to W. This implies relations of the polynomial degrees of W and S and enforces a so-called minimum rule.

The talk focuses on developing an algorithm, which delivers small supported basis functions satisfying the minimum rule.

In the presented numerical results interface effects are accurately resolved by anisotropic polynomial degrees and non-conforming meshes at low computational costs. Extension to three dimensions and other mixed formulations follows similarly.

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Wavelets for linear scaling computation in electronic structure calculation

Reinhold Schneider[1]

In the present talk we consider effective one particle models for the ground state calculation of the electronic Schrödinger equation for molecular systems with N electrons, like Kohn-Sham equations based on density functional theory as well as the classical Hartree-Fock model. Instead of computing the orbitals, we compute the so called *density matrix* which represents the kernel function in $\mathbb{R}^6$ the spectral projection operator. We consider systematic basis functions subordinated to different scales e.g. wavelets for the discretisation. We exploit the potential of wavelets for hyperbolic cross approximation in high dimensional spaces together with their ability for sparse representation of nonlocal operators to achieve *linear scaling* with respect to the number of particles and basis functions (in a suitable setting). Optionally a new concept of Kronecker-product approximation introduced by Beylkin et al. and Tyrtyshnikov et al. of operators will be presented.

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Optimal control of PDEs – from optimality conditions to numerical methods

Fredi Tröltzsch[1]

The talk surveys basic numerical ideas for solving optimal control problems governed by elliptic equations. Necessary optimality conditions and related numerical methods are explained in parallel for problems with increasing difficulty. Starting from convex problems for linear elliptic equations without additional constraints, finally nonconvex problems with semilinear equation and some inequality constraints are considered. In particular, gradient methods, primal-dual active set strategies, SQP-and interior point methods are addressed.

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Subspace cg-techniques for innner-domain-restrictions

Roman Unger[1]

Subspace-cg-techniques with projection methods are useful for an easy extension of an arbitrary finite element code with error estimation and adaptive strategies to an algorithm for solving restricted problems like contact problems between an elastic body and obstacles.

In this talk the usage of this method to apply restrictions in the inner domain of an elastic body, not on the boundary will considered.

Some practical applications of this method and numerical examples will be shown.

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Optimal Control Problem on non-convex Domains

Gunter Winkler[1] Thomas Apel[2] Arnd Rösch[3]

In a recent paper Meyer and Rösch prove superconvergence properties in the control variable for linear-quadratic optimal control problems in convex domains. We generalize these results for non-convex domains. The corner singularities are treated by a-priori mesh grading such that we are able to prove results of the same quality as in the case of regular solutions. Numerical examples are presented.

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Hybrid discretization techniques for variational inequalities

Barbara Wohlmuth[1]

Hybrid discretization techniques provide a powerful tool for the numerical approximation of variational inequalities. Variational inequalities such as contact problems can be easily analyzed within the abstract framework of saddle point problems. A priori results for the displacements and the stresses can be obtained. The Lagrange multiplier plays the role of the contact pressure and enters as additional variable in the weak formulation. In terms of a local basis transformation, static condensation can be carried out. Numerical examples include incompressible materials, Coulomb friction, non-linear material laws, large deformations and thermo-mechanical coupling.

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