FAKULTÄT FÜR
MATHEMATIK

Chemnitz FEM-Symposium 2010

Programme

Collection of abstracts

List of participants

Chemnitz FEM Symposium

TECHNISCHE UNIVERSITÄT CHEMNITZ
1836-2011
175 Jahre

Chemnitz, September 27 - 29, 2010

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

- Adaptive Methods
- Eigenvalue Approximation for Differential Operators
- Singularly Perturbed Problems

Invited Speakers:

Kunibert Siebert (Universität Duisburg-Essen)

Klaus Neymeyr (Universität Rostock)

Martin Stynes (University College Cork)

Anders Logg (University of Oslo)

Scientific Committee:

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

Organising Committee:

F. Schmidt, J. Rückert, H. Schmidt, T. Hein, M. Pester, K. Seidel

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TECHNISCHE UNIVERSITÄT CHEMNITZ

Fakultät für Mathematik

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Chemnitz, September 27 - 29, 2010

Programme for Monday, September 27, 2010

9:00 **Opening**
A. Meyer
Room: “Aula”

Eigenvalues
Chairman: A. Meyer
Room: “Aula”

9:05 K. Neymeyr 7
On optimal complexity gradient type solvers for elliptic eigenvalue problems.

9:55 G. Unger 8
Convergence analysis of iterative methods for algebraic nonlinear eigenvalue problems.

10:20 A. Zeiser 9
On the optimality of the inexact inverse iteration coupled with adaptive finite element methods.

10:45 *Tea and coffee break*

Eigenvalues
Chairman: K. Neymeyr
Room: “Aula”

11:10 O. Steinbach 10
Coupled FE/BE formulations for the fluid-structure interaction.

11:35 T. Mach 11
Preconditioned inverse iteration for $\mathcal{H}$-matrices.

12:00 C. Engstroem 12
On the computation of resonances in absorptive photonic crystals with the interior penalty method.

12:25 C. Effenberger 13
Linearization of rational eigenvalue problems arising in band structure computations for photonic chrystals.

Identification and Optimization
Chairman: H. Harbrecht
Room: “Sachsenburg”

11:10 P. Steinhorst 14
Test of a crack plane identification method using FEM-data of cracked domains.

11:35 L. Banz 15
Hp-time discontinuous Galerkin method for american put option pricing.

12:00 G. Haase / A. Kucher 16
GPU accelerated best curve approximation in pill identification.

12:50 *Lunch*

Adaptivity
Chairman: A. Rösch
Room: "Aula"

14:30	K. G. Siebert Convergence and optimality of adaptive finite elements.	17
15:20	F.-T. Suttmeier An adaptive low-order FE-scheme for Stokes flow with cavitation.	18
15:45	H. Egger On a posteriori estimates for hybrid discontinuous Galerkin methods.	19
16:10	*Tea and coffee break*	

	Adaptivity *Chairman*: K. G. Siebert *Room*: "Aula"		**A Priori Error Estimates** *Chairman*: G. Haase *Room*: "Sachsenburg"	
16:35	H. Harbrecht On error estimation in finite element methods without having Galerkin orthogonality.	20	J. Rückert Basic modelling for large deformation of plates.	24
17:00	R. Schneider Adaptive anisotropic mesh refinement based on a new adaptivity paradigm.	21	S. Ganesan Operator-split finite element method for high-dimensional population balance equations.	25
17:25	A. Große-Wöhrmann A posteriori control of modelling and discretization errors in thermoelasticity.	22	P. Skrzypacz Superconvergence results for Brinkman–Forchheimer–extended Darcy equation.	26
17:50	M. Bürg *Hp*-adaptivity in higher space-dimensions.	23	Y. Zhu Numerical modeling eutectic solidification by multiphase field technique.	27
19:00	*Conference Dinner (in* **"Schloßgasthaus"***)*			

Programme for Tuesday, September 28, 2010

Singularly Perturbed Problems
Chairman: T. Apel
Room: "Aula"

9:00	M. Stynes . . . . . 28 Finite element methods for stationary convection-diffusion problems.
9:50	M. Bause . . . . . 29 On stabilized higher order approximation of time dependent problems.
10:15	S. Franz . . . . . 30 SDFEM with non-standard higher-order finite elements for a convection-diffusion problem.
10:40	*Tea and coffee break*

	Adaptivity *Chairman*: F. Suttmeier *Room*: "Aula"	**Solver** *Chairman*: O. Steinbach *Room*: "Sachsenburg"
11:05	C. Waluga . . . . . 31 A posteriori error estimation for a hybridized discontinuous Galerkin method for incompressible flow.	C. Pechstein . . . . . 35 Weighted Poincare inequalities and robust domain decomposition solvers.
11:30	S. Ronnas . . . . . 32 Implementation of hp-adaptive FEM in HiFlow3.	C. Augustin . . . . . 36 Modeling the mechanics of nonlinear biological tissue with finite element and domain decomposition methods.
11:55	M. Baumann . . . . . 33 Goal oriented adaptivity for tropical cyclones.	M. Kolmbauer . . . . . 37 A frequency-robust solver for eddy current problems.
12:20	R. Müller . . . . . 34 A posteriori analysis for phase field simulations in the sharp interface limit.	M. Neumüller . . . . . 38 A hybrid DG space-time method.

12:45	*Conference Photo*
13:00	*Lunch*
14:00	*Excursion*
18:00	*Meeting of the Scientific Committee*

Programme for Wednesday, September 29, 2010

Special Guest
Chairman: R. Herzog
Room: "Aula"

9:00 A. Logg 39
Automated Scientific Computing.

9:50 *break for change of rooms*

	Singularly Perturbed Problems *Chairman*: M. Stynes *Room*: "Aula"	**Optimal Control** *Chairman*: R. Herzog *Room*: "Sachsenburg"
9:55	P. Knobloch .... 40 Local projection stabilization for convection-diffusion problems.	S. Beuchler .... 43 Boundary concentrated finite elements for optimal boundary control problems of elliptic PDEs.
10:20	G. Matthies .... 41 Variational time discretisations for unsteady convection-diffusion equations.	V. Dhamo .... 44 Numerical analysis of a quasilinear Neumann equation under minimal regularity of the data.
10:45	C. Reibiger .... 42 A system of singularly perturbed convection-diffusion equations related to optimal control.	J. Pfefferer .... 45 Finite element error estimates on the boundary and its application to optimal control.

11:10 *Tea and coffee break*

	Optimal Control *Chairman*: S. Beuchler *Room*: "Aula"	**Singularly Perturbed Problems** *Chairman*: G. Matthies *Room*: "Sachsenburg"
11:35	T. Apel .... 49 Finite element analysis for $H^{(2,1)}$-elliptic equations.	
12:00	S. Steinig .... 50 An application of FEM methods to an elliptic optimal control problem with state constraints.	S.-B. Savescu .... 46 A posteriori optimization of parameters in stabilized methods for convection-diffusion problems.
12:25	L. John .... 51 Stabilized FEM for the Stokes problem and an application to optimal control.	N. Ahmed .... 48 Finite element methods of an operator splitting applied to population balance equations.

12:50 *break for change of rooms*

12:55 **Closing**
A. Meyer
Room: "Aula"

13:05 *Lunch*

On optimal complexity gradient type solvers for elliptic eigenvalue problems

Klaus Neymeyr[1]

The topic of this talk is the numerical solution of eigenvalue problems for self-adjoint elliptic partial differential operators. Various gradient iterations can be applied to the finite element discretization in order to compute some of the smallest eigenvalues and its corresponding eigenfunctions.

First we present new convergence estimates for a class of (non-preconditioned) gradient iterations [1]. The analysis is based on a theorem which shows that poorest convergence within Krylov subspaces is attained in invariant subspaces of small dimensions. Then sharp convergence estimates for the Rayleigh-Ritz approximations are proved by means of a *mini-dimensional analysis*. However, these simple gradient iterations show a mesh-dependent convergence rate.

In a second step *preconditioning* is introduced by changing the geometry underlying these gradient iterations. With suitable multigrid preconditioners optimal complexity solvers are attainable which allow the numerical approximation of a fixed number of the smallest eigenvalues and the corresponding eigenfunctions with costs that increase linearly in the number of unknowns. These solvers can be derived systematically by a comparison of the boundary value and of the eigenvalue problem for the same partial differential operator. Until now only a small number of convergence rate estimates are known for these iterations. Only for the simplest solver - the fixed step size preconditioned gradient iteration - sharp convergence estimates are known. A new *gradient-flow-analysis* [2] is presented which allows to derive sharp convergence rate estimates in a significantly simpler and shorter way compared to the original proof.

References:

[1] K. N. and M. Zhou: *Convergence analysis of gradient iterations for the symmetric eigenvalue problem*, Technical report 2010.
[2] A. Knyazev and K. N.: *Gradient flow approach to geometric convergence analysis of preconditioned eigensolvers*, SIAM J. Matrix Analysis 31 (2009), 621–628.

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Convergence analysis of iterative methods for algebraic nonlinear eigenvalue problems

Gerhard Unger[1]

The convergence analysis of iterative methods for algebraic nonlinear eigenvalue problems is in the most cases restricted to simple eigenvalues. In this talk the convergence order for multiple eigenvalues for several methods as the inverse iteration and Kummer's method is analyzed. We use the Smith form of matrix functions to characterize the multiplicity of the eigenvalues. The key tool of our analysis is a special representation of the resolvent close to an eigenvalue as Laurent series which was introduced by Keldysh for polynomial eigenvalue problems and extended by Gohberg and Sigal for meromorphic ones. We show that the convergence rate of the methods depends on which order the eigenvalues have as pole of the resolvent. For the inverse iteration and Kummer's method local quadratic convergence is obtained if the eigenvalue is semi-simple. For defective eigenvalues both methods have only a local linear convergence order.

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On the optimality of the inexact inverse iteration coupled with adaptive finite element methods

Andreas Zeiser[1]

In this talk we study the convergence of the inverse iteration where the intermediate problems are solved only approximately. In particular we are interested in finding an approximation of an eigenvector corresponding to the smallest eigenvalue of an elliptic operator L. We show that this inexact inverse iteration converges if the tolerances are chosen appropriately. As a direct consequence using adaptive finite element methods (AFEM) for the approximate solution of the intermediate elliptic problems yields a convergent algorithm. Moreover we will show that under mild assumptions on the operator L the inexact inverse iteration coupled with AFEM exhibits quasi-optimal convergence rates governed by the approximability of the eigenvector. This is surprising since in general the convergence rates of the intermediate elliptic problems deteriorate from convergence rate of the inexact inverse iteration. This is due to the fact that the exact solutions of the intermediate problems are in general not in the same approximation class as the eigenvectors.

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Coupled FE/BE formulations for the fluid-structure interaction

Olaf Steinbach[1]

We present and discuss several coupled finite and boundary element formulations in vibro-acoustics. All formulations are based on the different use of standard boundary integral equations. Besides a direct simulation we also focus on the solution of the related eigenvalue problem.

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Preconditioned inverse iteration for $\mathcal{H}$-matrices

Thomas Mach[1] Peter Benner[2]

We will present a method of almost linear complexity to approximate some (inner) eigenvalues of symmetric differential operators. Using $\mathcal{H}$-arithmetic the discretisation of the operator leads to a large hierarchical ($\mathcal{H}$-) matrix M. We assume that M is symmetric, positive definite. Then we will compute the smallest eigenvalues with Preconditioned Inverse Iteration (PINVIT), which was extensively investigated by Knyazev and Neymeyr.

Hierarchical matrices were introduced by W. Hackbusch in 1998. They are data-sparse and require only $\mathcal{O}(nk \log n)$ storage. There is an approximative inverse, beside other matrix operations, within the set of $\mathcal{H}$-matrices, which can be computed in linear-polylogarithmic complexity. We will use the approximative inverse as preconditioner in the PINVIT.

Further we will combine the PINVIT with the folded spectrum method to compute inner eigenvalues M. We apply PINVIT to the matrix

$$M_\mu = (M - \mu I)^2 .$$

The matrix M_μ is symmetric, positive definite, too.

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On the computation of resonances in absorptive photonic crystals with the interior penalty method

Christian Engstroem[1]

Photonic crystals are promising materials for controlling and manipulating electromagnetic waves [1]. The spectral parameter is usually related to the time frequency and the Floquet-Bloch wave vector is a parameter. This leads to a rational spectral problem when the frequency dependence of a Lorentz material model is included [2,3]. A different approach is based on a quadratic spectral problem in the amplitude of the Floquet-Bloch wave vector [4].

We use a high-order interior penalty method with curved elements to discretize the quadratic and the rational eigenvalue problem. The resulting matrix problems are transformed into linear eigenvalue problems and approximate eigenpairs are computed with a Krylov space method. The limitations of the used linearization and the connection between the two approaches will be discussed.

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[1] K. Sakoda, Optical properties of photonic crystals, Springer-Verlag, Heidelberg, 2001.
[2] C. Engstroem, *On the spectrum of a holomorphic operator-valued function with applications to absorptive photonic crystals*, To appear in Mathematical Models and Methods in Applied Sciences, 2010.
[3] C. Engstroem and M. Wang, *Complex dispersion relation calculations with the symetric interior penalty method*, To appear in International Journal for Numerical Methods in Engineering, 2010.
[4] C. Engstroem and M. Richter, *On the spectrum of an operator pencil with applications to wave propagation in periodic and frequency dependent materials*, SIAM Journal on Applied Mathematics, **70** (1), 231-247, 2009.

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Linearization of rational eigenvalue problems arising in band structure computations for photonic chrystals

Cedric Effenberger[1] Christian Engstroem[2] Daniel Kressner[3]

This talk is concerned with numerical methods for nonlinear eigenvalue problems of the form $T(\lambda)x = 0$, $x \neq 0$, where the entries of the matrix T are rational functions in λ. This is motivated by electronic band structure calculations for photonic chrystals, where the nonlinear dependence on the eigenvalue parameter arises from a frequency-dependent material model.

The most straightforward approach to solve such eigenvalue problems is to multiply the entries of T by their common denominator and apply a standard linearization to the resulting polynomial eigenvalue problem. However, with an increasing number of poles, the degree of the intermediate polynomial eigenvalue problem quickly becomes large, leading to a severe magnification of the problem size during the linearization process.

In this talk, an alternative approach is proposed based on recent work by Bai and Su. This approach leads to significantly smaller linearizations, especially when the coefficient matrices associated with the rational terms are of low rank. This approach is combined with structure-exploiting Krylov subspace techniques and applied to photonic chrystals composed of Lorentz materials, where a discontinuous Galerkin scheme is used to discretize the underlying PDE eigenvalue problem.

References:

[1] C. Engstroem and M. Wang. Complex dispersion relation calculations with the symetric interior penalty method. International Journal for Numerical Methods in Engineering, 2010. To appear.
[2] Y. Su and Z. Bai. Solving Rational Eigenvalue Problems via Linearization. Technical Report CSE-2008-13, Department of Computer Science, University of California, Davis, 2008

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Test of a crack plane identification method using FEM-data of cracked domains

Peter Steinhorst[1]

In a wide spectrum of technical applications, cracks in materials can involve crucial effects like loss of functionality or even destruction of a device. Especially, undesirably cracking occurs in materials which are rather brittle like piezoelectric ceramics, and under situations with extreme or cyclic loads. So, the detection of cracks is an important problem in material control. If the crack does not touch the boundary, a simple visual control is not sufficient to determine it. The goal is, to use nondestructive techniques for the detection of inner cracks. Beside some possibilities of radiation and image processing, a basic idea is the use of outer boundary measurements under certain loads to get informations about the inner geometry of a device or even cracks. From the mathematical point of view, this leads to an inverse problem.

In the literature some approaches are discussed in this sense. Andrieux, Ben Abda et.al. introduced a method which identifies planar cracks using the reciprocity principle in the case of electrostatics (Laplace equation) and also in isotropic linear elasticity. We look on a generalisation of the first part of this method, the identification of the crack plane, to linear piezoelectric material behaviour.

Instead of the use of real data from experimental measurements, FEM allows to compute approximate solutions of boundary value problems in a cracked domain. Using only the FEM-solution on the outer boundary (and no informations about inner geometry) in postprocessing as input data, the correctness of the crack plane identification can be tested. This computation approach further enables to get informations about what measurement resolution levels are sufficient for a adequate accuracy of the inverse detection. It also allows numerical sensitivity studies of the method to data noise, which may offer important informations for practical use.

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Hp-time discontinuous Galerkin method for american put option pricing

Lothar Banz[1] Ernst P. Stephan[2]

High order methods are very efficient to obtain high accuracy with only moderate degrees of freedom. Hence they are well suited for problems where the computational time and the total error are crucial properties. The "fair" price of an American put option can be obtained by solving a parabolical obstacle problem, a modification of the original Black-Scholes PDE.
In this talk we present a *hp*-FE time discontinuous Galerkin method for the parabolical obstacle problem of pricing American put options. The non-penetration condition is resolved using a Lagrange multiplier yielding a mixed formulation. Its Lagrange multiplier space is spanned by basis functions (in space and time variables) which are biorthogonal to the corresponding basis functions for the primal variable. This biorthogonality allows a component-wise decoupling of the weak contact constraints and can therefore be equivalently rewritten in finding the root of a semi-smooth penalized Fischer-Burmeister non-linear complementary function. The arising system of non-linear equations are solved by a globalized semi-smooth Newton algorithm which is proven to converge locally Q-quadratic. Our numerical examples confirm the superiority of this method in terms of error reduction and computational time.

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[1] L. Banz and E. P. Stephan. Hp-time-discontinuous Galerkin for pricing American put options. (submitted 2010).
[2] S. Hüeber. Discretization techniques and efficient algorithms for contact problems. PhD thesis, Universität Stuttgart, 2008.
[3] B. P. Lamichhane and B. Wohlmuth. Biorthogonal bases with local support and approximation properties. *Mathematics of Computation*, **76**, 233–249, (2007).

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GPU accelerated best curve approximation in pill identification

Gundolf Haase[1] Andreas Kucher[2] Craig C. Douglas[3]

The increasing success of general purpose GPUs in general computing and also in high performance computing is unquestioned. We will present the suitability of GPUs in the "pill identification problem", (see [1], [2] and [3]), which might be considered as a representative example for parallelization of many identical sequential optimization problems. For this purpose we will examine a sub problem on a GPU and then compare the performance of the "parallel pill identification algorithm" (see [4]) implemented as C++ CPU-only version using openMPI and as C++ CPU/GPU version using openMPI and CUDA It turned out, that the CPU/GPU approach, under some restrictions, is faster than the CPU-only approach by a factor between 60 and 200.

The curve approximation itself is based alternatively on polynomial approximation or circular splines [5] and the best curve for the given 3D data point should result in a linear regression between the arc length of the curve (wrt. projected data points) [6] and the concentration value assigned to that point. The resulting functional for one curve is minimized by a Quasi-Newton method with an Inverse-BFGS-Update [7]. Instead of performing a line search with the commonly used strategies, a rather naive approach prove to be much more efficient for our use on GPUs.

References:

[1] C. Douglas, L. Deng, Y. Efendiev, G. Haase, A. Kucher, R. Lodder, G. Qin, Advantages of Multiscale Detection of Defective Pills During Manufacturing, HPCA 2010, LNCS 5938, pp. 8–16. Springer, Heidelberg (2010)

[2] C. Douglas, L. Deng, G. Haase, H. Lee, R. Loder, Data-Driven Pill Monitoring, Elsevier, Procedia Computer Science (2010), submitted

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[7] J. Nocedal, S. J. Wright, Numerical optimization, Springer, New York (1999)

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Convergence and optimality of adaptive finite elements

Kunibert G. Siebert[1]

Adaptive finite elements are successfully used since the 1970s for the efficient approximation of solutions to partial differential equations. The typical adaptive iteration is a loop of the form

$$\mathsf{SOLVE} \quad \rightarrow \quad \mathsf{ESTIMATE} \quad \rightarrow \quad \mathsf{MARK} \quad \rightarrow \quad \mathsf{REFINE}.$$

Traditional a posteriori error analysis was mainly concerned with the step ESTIMATE by deriving computable error bounds for the true error. During the last years there is an increasing interest in proving convergence of the above iteration, this means that the sequence of discrete solutions converges to the exact solution. Once convergence is established, we would like to show that the discrete solutions provide quasi-optimal approximations in terms of degrees of freedom.

In this talk we give a brief overview of the current state of the art in the convergence and optimality analysis of conforming adaptive finite element discretizations.

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An adaptive low-order FE-scheme for Stokes flow with cavitation

Franz-Theo Suttmeier[1] Frank Gimbel[2] Peter Hansbo[3]

In this note we derive a posteriori error bounds for FE-discretisations for a fluid problem with cavitation. The underlying model is the Stokes system together with an inequality constraint for the pressure. In order to avoid suboptimal behavior of the error bounds we propose to employ a Lagrange setting yielding an improved estimate. Numerical tests confirm our theoretical results.

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On a posteriori estimates for hybrid discontinuous Galerkin methods

Herbert Egger[1]

We discuss a class of a-posteriori error estimators for hybrid discontinuous Galerkin methods. As two particular instances, we derive an estimator of residual-type, and a second estimator based on equilibration. Both methods yield certified upper bounds for the error without generic constants.

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On error estimation in finite element methods without having Galerkin orthogonality

Helmut Harbrecht[1] Reinhold Schneider[2]

In this talk we present computable bounds to estimate the distance of finite element approximations to the solution of the Poisson equation. If the finite element approximation is a Galerkin solution, the derived error estimator coincides with the standard element and edge based estimator. If Galerkin orthogonality is not satisfied, the discrete residual additionally appears in terms of the BPX preconditioner. A consequence of the present analysis is the proof of the reliability and efficiency of hierarchical error estimation.

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Adaptive anisotropic mesh refinement based on a new adaptivity paradigm

Rene Schneider[1]

We propose a new paradigm for adaptive mesh refinement. Instead of considering local mesh diameters and their adaption to solution features, we propose to evaluate the benefit of possible refinements in a direct fashion, and to select the most profitable refinements. We demonstrate that based on this approach a directional refinement of triangular elements can be achieved, allowing arbitrarily high aspect ratios. With the help of an edge swapping criterion, even the mesh re-alignment with arbitrary error directions is achieved. Numerical experiments demonstrate the utility of the proposed anisotropic refinement strategy.

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A posteriori control of modelling and discretization errors in thermoelasticity

André Große-Wöhrmann[1] Heribert Blum[2] Marcus Stiemer[3]

The concept of adaptive error control for finite element Galerkin discretizations has more recently been extended from the pure treatment of the discretization errors [1], [2] also to the control of modelling errors [4], [5]. These techniques can be employed for a rigorous justification of the local choice of the model out of a given hierarchy with increasing complexity. In the present talk the concept is exemplified by a hierarchy of models arising out of the scope of thermoelasticity [6]. Significant reduction of the computational complexity can be achieved by a proper choice of the model in different subdomains, automatically chosen by the error estimators. Several error indicators are investigated in the context of goal oriented error estimation. Their efficiency is compared by means of finite element simulations [3].

This project is supported by the Deutsche Forschungsgemeinschaft (DFG) under grant SFB-TR 73 "Sheet-Bulk Metal Forming" (https://www.tr-73.de).

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[6] P. G. Ciarlet and J.L. Lions (Editors): Handbook of Numerical Analysis (Volume VI): J.C. SIMO: Numerical Analysis and Simulation of Plasticity, North Holland 1998.

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Hp-adaptivity in higher space-dimensions

Markus Bürg[1]

Nowadays a posteriori error estimation is an expected and assessed feature in scientific computing. It is used for adaptively creating approximation spaces and to assess the accuracy of numerical solutions. The performance of the finite element method can be improved by mesh refinement (h-FEM) or the use of higher oder ansatz spaces (p-FEM). Taking a combination of both (hp-FEM) can lead to exponentially fast convergence with respect to the number of degrees of freedom. For the h-FEM adaptive mesh creation is widely discussed in literature. For the p- and hp-FEM there have been proposed several strategies for adaptively creating problem-dependent meshes. In [1] an hp-adaptive refinement strategy, which is based on the solution of local boundary value problems, was proposed and also its convergence was shown.
In this talk we present this refinement strategy shortly. Further we show first results of the application of this adaptive strategy to problems with boundary layers.

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Basic modelling for large deformation of plates

Jens Rückert[1] Arnd Meyer[2]

We investigate large deformations of plates with nonlinear elastic material. Therefore we consider a model using the Kirchhoff assumption locally, avoiding any further simplifications. This way of modelling leads to a two-dimensional strain tensor, which depends essentially on the two fundamental forms of the differential geometry of the deformed midsurface. The desperate ambitious Newton linearization of the arising equation is analytically very expensive. So we examine replacements by some modified Newton linearizations.

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Operator-split finite element method for high-dimensional population balance equations

Sashikumaar Ganesan[1]

Simulations of population balance systems can be used to study the behavior of crystallization, polymerization, pharmaceutical productions, dispersed phase, etc. A population balance system (PBS) consists of the time-dependent Navier-Stokes equations to describe the flow field, a couple of nonlinear convection-diffusion-reaction equations for describing chemical reactions, transport of temperature and concentrations, and a population balance equation (PBE). The PBE depends not only the time and physical space but also the properties of the particles. Thus, the PBE is posed on high-dimensional domain than other equations in the PBS.

In this talk, we present the recently developed operator-split finite element method for high-dimensional PBE. In the operator-split finite element method, we first split the single high-dimensional PBE into a collection of low-dimensional equations using an operator-splitting method. Then, we solve each low-dimensional equation separately. In addition, the splitting facilitates to use different finite element discretizations such as the standard Galerkin and SUPG for different low-dimensional equations. The stability and convergence analysis of the operator-split finite element discretization of the PBE will be presented. Further, a new algorithm based on the nodal points of the finite elements to implement the operator-split finite element method will also be presented.

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Superconvergence results for Brinkman–Forchheimer–extended Darcy equation

Piotr Skrzypacz[1] Gunar Matthies[2] Lutz Tobiska[3]

It is well known that the piecewise polynomial conforming finite element solution of Poisson equation approximates the interpolant to a higher order than the solution itself. This type of superconvergence is established for a nonstandard interpolant of the (Q_2, P_1^{disc}) element applied to the nonlinear Brinkman–Forchheimer–extended Darcy equation which describes the flow behaviour in porous media. After stating the optimal convergence for the family of $(Q_{k+1}, P_k^{\text{disc}})$ elements, $k \in \mathbb{N}$, the supercloseness results are presented. Applying (Q_3, P_2^{disc}) post-processing technique, we can state a superconvergence property for the discretisation error of the post-processed discrete solution to the solution itself. Numerical experiments verify the predicted convergence rates.

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Numerical modeling eutectic solidification by multiphase field technique

Yaochan Zhu[1] Eckart Schnack[2]

Here the multiphase field model[1,2] is studied which is extensively applied in simulation of microstructure evolution during phase transformations such as solid-solid transition, solidification, grain growth. Depending on problem itself, the model is openly coupled by a set of partial different equations which is of property of conserved nonlinear parabolic equations (Cahn-Hilliard type[3]) for temperature or composite and nonconversed hyperbolic equations (Cahn-Allen type[4]) for phase field order parameters. The basic physic meaning behind multiphase phase field model is that supposing the system free energy tends toward minimization by the response of phase field order parameters to the driving force. As a diffusive interface model, the movement of interfaces/boundaries which involved in complex microstructure evolution during transformation/grain growth is implicitly tracked by multi-phase field parameters, which changes smoothly across a spatial diffuse interface/boundary from one constant to another within finite width. This character greatly facilitates dealing with free boundary problem (e. g. eutectic solidification), which is mathematically described as a sharp interface model requiring explicit tracking interfaces/boundaries with great difficulty by numerical method.

The finite difference method is of advantage over other numerical method such as finite element method, spectral method that it is conceptually intuitive and easy to implement, and consequently, it is most frequently employed for numerical work with multiphase field model[5]. Here this method is applied to discretize the set of partial differential equations of the multiphase model for eutectic solidification and it is analyzed including its consistence, stability and convergence. The detailed discretization error analysis is made. One numerical example of multiphase phase field modeling is supplied to show this process.

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Finite element methods for stationary convection-diffusion problems

Martin Stynes[1]

The nature of solutions of steady-state convection-diffusion problems (where convection dominates) will be described. Standard numerical methods have difficulty in providing accurate solutions to such problems. Finite element methods that are specially designed for convection-diffusion will be described. The use of special meshes in the solution of these problems will also be considered.

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On stabilized higher order approximation of time dependent problems

Markus Bause[1]

$$\partial_t u_i + \boldsymbol{b} \cdot \nabla u_i - \nabla \cdot (\boldsymbol{A}_i \nabla u_i) + r_i(\boldsymbol{u}) = f_i\,, \qquad i = 1, \dots, m\,, \tag{1}$$

with $\boldsymbol{u} = (u_1, \dots, u_m)$ are studied in various technical and environmental applications. The reliable approximation of such systems is still a challenging task. The model equations are strongly coupled such that inaccuracies in one unknown directly affect all other unknowns. In large chemical systems with complex interactions numerical artifacts can lead to wrong predictions. Higher order finite element methods reduce the effect of numerical diffusion leading to an artifical mixing of chemical species.

In the convection- and/or reaction-dominated case with solutions having sharp layers, standard finite element methods cannot be applied. Modified finite element approaches are required that are able to prevent unphysical oscillations. Here, we analyze approximating the system (1) in space by higher order finite element methods with *streamline upwind Petrov-Galerkin (SUPG)* and *(an-)isotropic shock capturing stabilization*. The shock capturing terms further reduce spurious localized oscillations in crosswind-direction. Recently, these stabilization techniques were studied for linear finite element methods. However, in combination with higher finite element methods the stabilizations show to be more efficient. The design of the various stabilization parameter is considered carefully.

For a steady nonlinear model problem the error estimate

$$|||u - u_h|||^2 + \sum_{T \in \mathcal{T}_h} \tau_T(u_h) \left\| \boldsymbol{D}_{\mathrm{sc}}^{1/2} \nabla u_h \right\|_{L^2(T)}^2 \le C_{\mathrm{SC}} \sum_{T \in \mathcal{T}_h} \frac{h_T^{2(l_T-1)}}{p_T^{2(k_T-1)}} M_T^{\mathrm{opt}} \|u\|_{H^{k_T}(T)}^2$$

is shown within an *hp* finite element framework. The efficiency and robustness of the discretization schemes is studied and illustrated by numrous numerical experiments.

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SDFEM with non-standard higher-order finite elements for a convection-diffusion problem

Sebastian Franz[1]

Considering a singularly perturbed problem with exponential and characteristic layers, we show convergence for non-standard higher-order finite elements using the streamline diffusion finite element method (SDFEM). Moreover, for the standard higher-order space $\mathcal{Q}_p$ supercloseness of the numerical solution w.r.t. an interpolation of the exact solution in the streamline diffusion norm of order $p + 1/2$ is proved.

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A posteriori error estimation for a hybridized discontinuous Galerkin method for incompressible flow

Christian Waluga[1] Herbert Egger[2]

We present a hybridized discontinuous Galerkin method for incompressible flow, that naturally allows for locally varying polynomial degrees and nonconforming h-refinements. Furthermore, the number of unknowns can be significantly reduced by static condensation on the element level. We present optimal a-priori estimates and also analyze a posteriori error estimates based on a H(div)-conforming flux reconstructions.

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Implementation of hp-adaptive FEM in HiFlow3

Staffan Ronnas[1] Martin Baumann[2]

The finite element method is popular among scientists and engineers who need to solve PDEs and integral equations arising from problems in a large number of areas. As the complexity of models being solved using FEM increases, the need for adaptive algorithms that can construct accurate approximations using a small number of degrees of freedom becomes apparent. At the same time, the use of high-performance parallel computing on distributed-memory machines remains necessary to be able to tackle many problems.

hp-adaptivity is one of the most powerful approaches to adaptive finite element discretization. By combining local mesh refinements close to irregularities of the solution with the use of higher-order elements where the solution is smooth, this technique often yields very high convergence rates and reduces the computation time significantly.

In this talk, we will present some aspects of how support for parallel hp-adaptivity was implemented in HiFlow3, a general purpose C++ library designed to assist in the construction of parallel finite element solvers.

Of primary importance is the support for different cell types and refinement strategies in both conforming and non-conforming meshes, which forms the basis for adaptation of the discretization space. Another central issue is the numbering of degrees of freedom, and the identification of additional constraints in the presence of hanging nodes and local variations of polynomial orders. Finally, the use of parallel data structures for representing the computational mesh makes it possible for algorithms to scale to a large number of processors, without being limited by memory constraints.

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Goal oriented adaptivity for tropical cyclones

Martin Baumann[1] Vincent Heuveline[2] Sarah Jones[3] Leonhard Schenk[4]

Many meteorological and environmental phenomena are influenced by processes on a large range of scales in space and time. For such multi-scale problems the numerical modelling and solution is challenging since not all scales can be resolved adequately due to memory or CPU time restrictions. Often a certain physical quantity of the solution is of interest. In such cases goal oriented adaptivity is a promising approach as only features that are relevant for the determination of the quantity of interest – described by some goal functional J – need to be considered.

By means of the dual-weighted residual method (DWR) ([EEHJ95] and [BR03]) the error in J can be estimated and the mesh can be adapted accordingly. The sensitivity information with respect to the goal functional required for the error estimator is obtained as solution of a so-called dual problem. In a time-varying context the dual problem is posed backward in time and requires the solution of the original problem in each time step. Therefore the estimation of the error and adaption process is expensive in terms of memory consumption and CPU time. The recently proposed local dual-weighted residual method [Huertas08] is suitable for a certain class of goal functionals and presents a compromise between classical error estimators and the DWR method.

In this paper we present specific adaptive schemes based on goal oriented adaptivity techniques for the simulation of tropical cyclones. It turns out that the definition of goal functionals for meteorological applications is a non-trivial task. In this contribution we propose adaptive methods based on several goal functionals which lead to economical meshes with error control both in space and time. We further address the issue of the efficient computation of the dual problem by means of interpolated higher-order solutions.

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A posteriori analysis for phase field simulations in the sharp interface limit

Rüdiger Müller[1] Sören Bartels[2]

Phase field equations are widely used to approximate the evolution of free moving interfaces. The diffuse interface width ϵ is related to a singular perturbation leading to nonlinear parabolic equations.

Efficient finite element simulations of phase field problems require a fine grid resolution only close to the moving fronts. Therefore, adaptive mesh refinement and coarsening is highly desirable. Unfortunately, conventional a posteriori error estimators depend exponentially on the inverse ϵ^{-1} of the interface parameter and become useless in the sharp interface limit $\epsilon \to 0$.

We derive robust and fully computable error estimators that depend on ϵ^{-1} only in a low order polynomial. They are based on the numerical evaluation of the principal eigenvalue of the linearized operator. Numerical results show that robust error control is possible, even if the phase field solution undergoes topological changes, which causes a blow–up of the principal eigenvalue when $\epsilon \to 0$.

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Weighted Poincare inequalities and robust domain decomposition solvers

Clemens Pechstein[1] Robert Scheichl[2]

Robust solvers for problems with high-contrast coefficients are currently an important and active area of research. In this talk we present weighted Poincaré inequalities of the form

$$\inf_{c\in\mathbb{R}} \int_\Omega \alpha(x)\, |u(x)-c|^2\, dx \;\le\; C_P\ \mathrm{diam}(\Omega)^2 \int_\Omega \alpha(x)\, |\nabla u(x)|^2\, dx$$

for functions u in $H^1(\Omega)$ or in a finite element space. For a certain class of piecewise constant and positive weight functions $\alpha(x)$, we can get the constant C_P independent of the values of α, i. e. of high contrast in α.

As a simple example consider the case where α takes two different values on two connected subregions $\Omega^{(k)}$ of Ω. For this situation we can even give estimates on how C_P depends on the subregions $\Omega^{(k)}$. Generalizations to the multi-subregion case are also possible.

Finally, we give some applications in domain decomposition methods, in particular for FETI (finite element tearing and interconnecting) type methods. With our inequalities we can show condition number estimates that are robust for certain high contrast coefficients, including cases where the subdomain partitioning does not resolve coefficient jumps.

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Modeling the mechanics of nonlinear biological tissue with finite element and domain decomposition methods

Christoph Augustin[1] Olaf Steinbach[2]

In this talk the focus will be on the structural model for the nonlinear elastic behavior of biological tissues, in particular arterial walls. Arteries are treated as an anisotropic material consisting of several layers. I present the governing equations of an arterial wall model and outline the main steps to the finite element model.

Matters of existence and uniqueness of a solution are discussed as well as difficulties in the numerical simulation.

A way to treat the very complex algorithms resulting from the nonlinear models is the strategy of parallel computing. One possibility to achieve such a parallelization is to apply domain decomposition methods, which are also motivated by the composition in layers of most biological tissues. I outline the main ideas of one particular approach, the finite element tearing and interconnecting (FETI) method and its application to the artery model.

Finally numerical examples are included.

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A frequency-robust solver for eddy current problems

Michael Kolmbauer[1] Ulrich Langer[2]

In many practical applications in computational electromagnetics, the excitation is time-harmonic. Due to the time-harmonic excitation, we can switch from the time domain to the frequency domain. At least in the case of linear problems, this allows us to replace the expensive time-integration procedure by the solution of a linear system for the amplitudes belonging to the sine- and to the cosine-excitation. The fast solution of the corresponding linear system of finite element equations is crucial for the competitiveness of this method. J. Schöberl and W. Zulehner (2007) proposed a new parameter-robust MinRes preconditioning technique for saddle point problems. This method allows us to construct a frequency-robust preconditioned MinRes solver.

The application of this MinRes preconditioning technique to linear time-harmonic eddy current problems in electromagnetics is not straight forward. Due to the non-trivial kernel of the curl operator we have to perform an exact regularization of the frequency domain equations, in order to provide a theoretical basis for the application of the MinRes preconditioner.

Furthermore we have to find appropriate parameter robust preconditioners for the inversion of the diagonal blocks in (2).

$$\frac{1}{\omega}\begin{pmatrix} \omega\mathbf{M}_{\sigma,h} + \mathbf{A}_h & 0 \\ 0 & \omega^2(\omega\mathbf{M}_{\sigma,h} + \mathbf{A}_h) \end{pmatrix} \tag{2}$$

The multigrid preconditioner by Arnold, Falk and Winther (2000) and the domain decomposition preconditioner by Hu and Zou (2004) are candidates for σ being constant and σ being piecewise constant respectively.

Finally, we discuss the application of this solver to linear eddy current problems with non-harmonic excitation and to non-linear problems in the framework of the multiharmonic technique.

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A hybrid DG space-time method

Martin Neumüller[1] Olaf Steinbach[2]

DG space-time methods have been applied to several model problems in the last view years. In this talk we consider the time dependent heat equation as a model problem. For a spatial domain $\Omega \in \mathbb{R}^d, d = 1, 2, 3$ the heat equation will be discretized in the space time cylinder $Q = \Omega \times (0, T) \in \mathbb{R}^{d+1}$. This approach results in a large system of linear equations. To handle such a large system, a hybrid version in the space time domain will be presented. This approach allows the application of parallel solution algorithms to solve the large system of linear equations.

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Automated Scientific Computing

Anders Logg[1]

Increasingly complex mathematical models are being solved in large computer simulations to answer questions of scientific and industrial relevance. Often, these models come in the form of differential equations that may be solved by means of standard numerical methods such as the finite element method.

However, the implementation of a numerical method to solve a given differential equation is a both difficult and time-consuming task. Furthermore, the output of a computer simulation is an approximate numerical solution that may or may not be close to the exact solution. Mathematical techniques exist for assessing the accuracy of a computed numerical solution, but this too is a difficult and time-consuming task that requires manual labor.

In this talk, I demonstrate how one may automate the solution of differential equations and remove the need for any manual labor. The key to this automation is automated code generation, where computer code is automatically generated to solve a given problem with a prescribed accuracy.

Examples are presented that range from simple model problems like the Poisson equation to complex nonlinear fluid-structure interaction problems.

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Local projection stabilization for convection-diffusion problems

Petr Knobloch[1]

We apply the local projection stabilization to finite element discretizations of convection-diffusion and convection-diffusion-reaction problems. We shall present error estimates and stability results and demonstrate the properties of the method by means of various numerical experiments.

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Variational time discretisations for unsteady convection-diffusion equations

Gunar Matthies[1] Friedhelm Schieweck[2]

We will give an overview on variational time discretisation methods for unsteady convection-diffusions equations. In particular, the discontinuous Galerkin method (dG) and the continuous Galerkin-Petrov method (cGP) will be considered. Both classes allow to construct A-stable time discretisations of arbitrarily high order.

A comparison of both classes concerning the order of convergence, stability properties and computational costs will be presented. Moreover, we discuss the superconvergence of both types of methods at the discrete time points.

Furthermore, the idea of a new C1GP(r)-method will be presented. One feature of this method is that the discrete solution satisfies the unsteady convection-diffusion equation at the discrete time points exactly. Moreover, the close relation to the cGP(r-1)-method will be shown.

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A system of singularly perturbed convection-diffusion equations related to optimal control

Christian Reibiger[1] Hans-Görg Roos[2]

We consider an optimal control problem with an 1D singularly perturbed differential state equation. For solving such problems one uses the enhanced system of the state equation and its adjoint form. Thus, we obtain a system of two convection-diffusion equations. Using linear finite elements on adapted grids we treat the effects of two layers arising at different boundaries of the domain. We proof uniform error estimates for this method on meshes of Shishkin type. We present numerical results supporting our analysis.

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Boundary concentrated finite elements for optimal boundary control problems of elliptic PDEs

Sven Beuchler[1]

We investigate the discretization of optimal boundary control problems for elliptic equations by the boundary concentrated finite element method. We prove that the discretization error $\|u^* - u_h^*\|_{L^2(\Gamma)}$ decreases like N^{-1}, where N is the total number of unknowns. This makes the proposed method favorable in comparison to the h-version of the finite element method, where the discretization error behaves like $N^{-3/4}$. Moreover, we present an algorithm that solves the discretized problem in almost optimal complexity. The talk is complemented with numerical results. This is a joint work with Clemens Pechstein (JKU Linz) and Daniel Wachsmuth (RICAM, Linz).

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Numerical analysis of a quasilinear Neumann equation under minimal regularity of the data

Vili Dhamo[1] Eduardo Casas[2]

We consider the finite element approximation of the following quasilinear Neumann problem

$$\begin{cases} -\operatorname{div}\left[a(x,u(x))\nabla u(x)\right] + f(x,u(x)) &= 0 \quad \text{in } \Omega\,, \\ a(x,u(x))\partial_\nu u(x) &= g(x) \quad \text{on } \Gamma\,. \end{cases} \tag{3}$$

The consideration is restricted to polygonal domains of dimension two and polyhedral domains of dimension three. For numerical purposes we discretize Ω by a regular triangulation and the mesh on Γ is induced by that on Ω. We approximate the PDE (3) by linear and continuous finite elements.

In spite that f is considered monotone nondecreasing with respect to u, the above equation is not monotone because of the dependence of the coefficients of the operator with respect to the function u. This lack of monotonicity causes the main difficulty in the numerical analysis of the above equation: the uniqueness of a solution of the discretized version of (3) is an open question, even though (3) has a unique solution. This non-monotonicity also complicates the discussion of any linearization of (3) which is needed, in particular, to apply the well-known Aubin-Nitsche trick for optimal L^2 error estimates for the approximation of (3).

In contrast to well-known results in the literature, the C^2 regularity and the boundedness of the coefficient a are not necessary to derive error estimates. In most of the cases it suffices to require only a local Lipschitz property of a.

The boundary datum g is supposed to be in $L^s(\Gamma)$ $(s \geq 2)$, therefore the regularity of the solution u of (3) cannot be $H^2(\Omega)$ but only $H^{3/2}(\Omega)$. Because of this lower regularity of u, the analysis becomes more difficult than in the regular case.

The assumption on Ω introduces a new difficulty: the regularity of elliptic equations in corner domains needs special care. For this reason, we distinguish two cases: whether Ω is convex or not. These two different situations yield different order of convergence for the discretization of equation (3) in the $L^2(\Omega)$ norm.

The main aims of this talk are twofold. First, error estimates in different function spaces are presented and second the issue of uniqueness of a solution to the approximate discrete equation is addressed.

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Finite element error estimates on the boundary and its application to optimal control

Johannes Pfefferer[1] Thomas Apel[2]

In this talk we consider a priori error estimates for an elliptic linear-quadratic Neumann boundary control problem with pointwise inequality constraints on the control. The domain is assumed to be polygonal and maybe non-convex. For discretizing the state linear finite elements are used, the control is approximated by piecewise constant ansatz functions. Approximations of the optimal control of the continuous problem are constructed in a postprocessing step by a projection of the discrete adjoint state into the set of admissible controls. For the proof of approximation rates for this optimal control problem, finite element error estimates in the L^2-norm on the boundary are essential, but it turned out that optimal ones are only available for domains with a maximum interior angle smaller than $\pi/2$. We prove that a convergence order close to 2 can also be obtained up to an interior angle of $2\pi/3$. For domains with larger interior angles we use mesh grading techniques to overcome the negative effects of corner singularities. We apply this result to the optimal control problem and show nearly second order convergence for the approximations of the solution. The theoretical results are illustrated by numerical examples.

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A posteriori optimization of parameters in stabilized methods for convection-diffusion problems

Simona-Blanca Savescu[1] Volker John[2] Petr Knobloch[3]

Stabilized finite element methods for convection-dominated problems require appropriate choices of stabilization parameters. Only asymptotic choices of these parameters are currently available in the numerical analysis literature. We present a general framework for optimizing the stabilization parameters with respect to the minimization of a target functional and apply this framework to the SUPG finite element method and the minimization of residual based error estimators and error indicators. We illustrate by numerical examples the benefits and the shortcomings of our approach.

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Nitsche-mortaring for singularly perturbed convection-diffusion problems

Martin Schopf[1] Hans-Görg Roos[2] Torsten Linß[3]

A finite element method for a singularly perturbed convection-diffusion problem with exponential boundary layers is analysed. Using a mortaring technique we combine an anisotropic triangulation of the layer region (into rectangles) with a shape regular one of the remainder of the domain. This results in a possibly non-matching (and hybrid), but layer adapted mesh of Shishkin type. We study the error of the method allowing different asymptotic behavior of the triangulations and prove uniform convergence and a supercloseness property of the method. Numerical results supporting our analysis are presented.

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Finite element methods of an operator splitting applied to population balance equations

Naveed Ahmed[1] Gunar Matthies[2] Hehu Xie[3] Lutz Tobiska[4]

In population balance equations, the distribution of the entities depends not only on space and time but also on their own properties referred as internal coordinates.

The operator splitting method is used to transform the whole problem into two unsteady subproblems of smaller complexity. The first subproblem is a time dependent convection-diffusion problem while the second one is a transport problem with pure advection.

We use the backward Euler method to discretise the subproblems in time. Since the first problem is convection-dominated, the local projection method is applied as stabilisation in space.

The transport problem in the one-dimensional internal coordinate is solved by a discontinuous Galerkin method.

The unconditional stability of the method will be presented. In the L^2 norm, error estimates are given which are of optimal order. The theoretical results are confirmed by numerical tests.

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Finite element analysis for $H^{(2,1)}$-elliptic equations

Thomas Apel[1] Thomas Flaig[2]

The convergence of finite element methods for linear elliptic equations of second or fourth order is well understood. In this paper we discuss the finite element approximation of linear elliptic equations of mixed second and fourth order in a two-dimensional rectangular domain. We establish an estimate for the finite element error of a conforming approximation of this equation.

This type of equation appears in the optimal control of parabolic partial differential equations if one eliminates the state or the control in the first order optimality conditions.

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An application of FEM methods to an elliptic optimal control problem with state constraints

Simeon Steinig[1]

In this talk we examine a discretisation of an elliptic optimal control problem with state constraints, using finite element spaces.
The continuous problem consists of the following task:
We minimise a quadratic functional

$$J(y,u) = \frac{1}{2}\left\|y - y_d\right\|^2_{L^2(\Omega)} + \frac{\nu}{2}\left\|u\right\|^2_{L^2(\Omega)},$$

depending on the control u and the state $y = y(u)$, given as the solution of the Poisson equation with u as the right-hand side and homogeneous Dirichlet boundary data on the smooth domain Ω. y_d is a given function, $\nu > 0$ a fixed parameter. There are further constraints on u given by real numbers a, b and the pointwise inequality $a \leq u(x) \leq b$. Besides, there is the pointwise state constraint $y \geq y_c$ with given smooth function y_c.
We discretise this problem with the aid of piecewise constant functions for the control u and piecewise linear functions for the state y. This leads to an a-priori error estimate for the approximation of the unique global solution u to the above problem in the L^2-norm. As it turns out, we arrive at an order of $\mathcal{O}(h^{3/4})$, which was also tested numerically.

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Stabilized FEM for the Stokes problem and an application to optimal control

Lorenz John[1] Olaf Steinbach[2]

We will consider different stabilized finite element methods for the Stokes problem where we mainly focus on lowest order elements. In particular we will discuss different stabilization strategies and we comment on related numerical results. Furthermore the application of stabilized finite elements to related Dirichlet control problems will be presented. Here we consider the maximization of the lift force where the boundary control will be realized either in $L_2(\Gamma)$ or in the energy space $H^{1/2}(\Gamma)$.

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Notes:

Internet access:

A laptop with internet connection is available in front of the "Aula".

username:	"fem10"
password:	"chemnitz"

Wireless network is available for free, please contact reception for your personal login-information.

Food:

The conference fee includes:

- Lunch on all three days of the symposium (one soft drink is included)
  Further drinks are on your own expense.
- The conference dinner on Monday ("Schlossgasthaus").
- Tea, coffee, soft drinks and snacks during breaks.

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

Recreation:

The hotel offers for free (contact reception):

- sauna,
- solarium,
- gym.

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