

Chemnitz FEM-Symposium 2012

Programme

Collection of abstracts

List of participants

25th

Chemnitz

FEM

Symposium



TECHNISCHE UNIVERSITÄT
CHEMNITZ

Chemnitz, September 24 - 26, 2012

Internet access:

In most rooms of the Chemnitz University wireless networks are accessible via:

eduroam : If your home institution participates to the **eduroam** project and your computer is properly configured

special : secure wireless network with WPA2 and pre-shared key
PSK:

camo : Open radio network with highly restricted access;
no internet, only www.tu-chemnitz.de

More information: www.tu-chemnitz.de/urz/netz/wlan/ssid.html.

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Food:

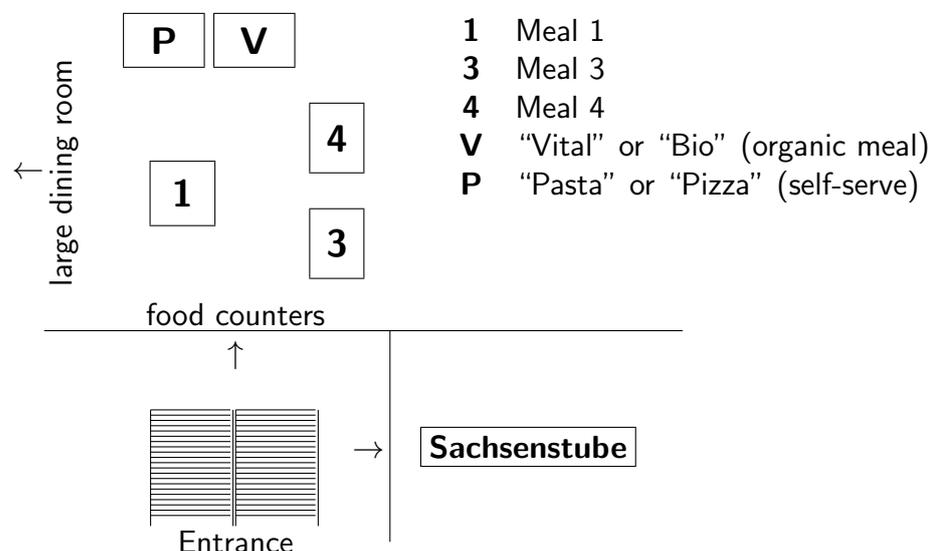
The conference fee includes:

- Lunch on all three days of the symposium (soft drink included)
- Tea, coffee, soft drinks and snacks during breaks.
- Snacks and finger-food during the poster session on Monday.
- The conference dinner on Tuesday.

You have luncheon vouchers for the refectory ("Neue Mensa") opposite the lecture building. The vouchers are valid to choose any one of the 3-5 meals available on the imprinted day, see also: <http://www.swcz.de/bilderspeiseplan/>.

There is a special room ("Sachsenstube") reserved for participants of the FEM Symposium on Monday and Tuesday. On Wednesday we will have a few tables in the large dining room.

Lunch location:



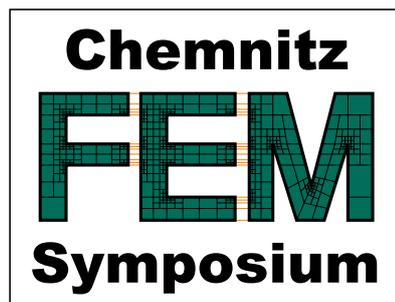
(food counters opened: 11:00 – 13:30)



TECHNISCHE UNIVERSITÄT CHEMNITZ

Fakultät für Mathematik

Chemnitz FEM-Symposium 2012



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Chemnitz, September 24 - 26, 2012

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

- Domain Decomposition
- Plates and Shells

Invited Speakers:

Martin J. Gander (University of Geneva)

Manfred Bischoff (Universität Stuttgart)

Jubilee:

The 25th Finite Element Symposium is dedicated to the **60th birthdays** of

Ulrich Langer and **Arnd Meyer**

Scientific Committee:

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

Organising Committee:

A. Günnel, J. Rückert, H. Schmidt, M. Pester, K. Seidel, A.-K. Glanzberg

<http://www.tu-chemnitz.de/mathematik/fem-symposium/>

Programme for Monday, September 24, 2012

9:00 **Opening**

Room: N111

9:10 Thomas Apel

History of the Chemnitz Finite Element Symposia.

Domain Decomposition

Chairman: T. Apel

Room: N111

9:35 Martin J. Gander 8
On the origins of domain decomposition methods

10:25 *Tea and coffee break*

Domain Decomposition

Chairman: H. Harbrecht

Room: N111

10:50 Heiko Andrä 9
Two-level domain decomposition preconditioners for multi-phase elastic composites.

11:15 Zdenek Dostal 10
Scalable TFETI/TBETI algorithms for contact problems with variationally consistent discretization and optional preconditioning.

11:40 André Massing 11
Nitsche-based overlapping and fictitious domain methods for the Stokes problem.

12:05 Steffen Weißer 12
Finite Element Method with local Trefftz basis functions on polygonal/polyhedral meshes.

Error Analysis

Chairman: S. Bartels

Room: N101

Herbert Egger 13
hp estimates for hybrid DG methods for incompressible flow.

Dietmar Gallistl 14
A posteriori error estimates for nonconforming finite element methods for fourth-order problems on rectangles.

Lennard Kamenski 15
How a non-convergent Hessian recovery works in mesh adaptation.

Mira Schedensack 16
Comparison results for first-order FEMs.

12:30 *Lunch*

Solver*Chairman:* G. Of*Room:* N111

- 14:00 Helmut Harbrecht 17
Combination technique based k -th
moment analysis of elliptic problems
with random diffusion.
- 14:25 Lorenz John 18
Fast solvers for the Navier–Stokes
equations with applications in arte-
rial blood flow.
- 14:50 Boris Khoromskij 19
Tensor numerical methods for multi-
dimensional PDEs.
- 15:15 Martin Neumüller 20
A parallel space-time multigrid
method.

Flow*Chairman:* M. Braack*Room:* N101

- Tobias Köppl 21
Reduced one-dimensional modelling
and numerical simulation for mass
transport in fluids.
- Jens Lang 22
Adaptive and higher order methods
in computational fluid dynamics.
- Gunar Matthies 23
A two-level local projection stabili-
sation on uniformly refined triang-
ular meshes.
- Piotr Skrzypacz 24
Composite non-conforming elements
and local projection stabilization for
transport dominated flow problems.

15:40

*Tea and coffee break***Maxwell***Chairman:* H. Egger*Room:* N111

- 16:15 Antti Hannukainen 25
Analysis of preconditioned iterative
methods for the Helmholtz equation.
- 16:40 Lothar Nannen 26
Hardy space infinite elements for ex-
terior Maxwell problems.
- 17:05 Viktor Rukavishnikov 27
The weighted edge finite element
method for Maxwell equations with
strong singularity.

Optimal Control*Chairman:* R. Herzog*Room:* N101

- Thomas Flaig 28
Crank-Nicolson discretization for
parabolic optimal control problems
with terminal observation.
- Christian Reibiger 29
Optimal control subject to sin-
gularly perturbed convection-diffu-
sion-equations.
- Fredi Tröltzsch 30
On an optimal control problem for
magnetic fields.

17:30

Poster Session

Martina Balg	31
Compressible and incompressible material under large deformations.	
Gundolf Haase	32
AMG accelerated elasticity solver on GPU-clusters.	
Katharina Hofer	33
High-order finite element methods for optimal control problems.	
Sven-Joachim Kimmerle	34
Optimal control of coupled systems of ordinary and partial differential equations with algebraic constraints.	
Uwe Köcher	35
Numerical simulation of elastic wave propagation in composite material.	
Günther Of	36
Non-symmetric coupling of finite and boundary element methods for the heat equation.	
Johannes Pfefferer	37
Dirichlet boundary control problems: finite element discretization and error estimates.	
Jens Rückert	38
Modelling and numerical experiments for Kirchhoff plates using finite strain.	
Jens Saak	40
Non-conforming finite elements and Riccati-based feedback stabilization of the Stokes equations.	
Hansjörg Schmidt	41
On adaptive FEM for viscoelasticity at large strain deformations.	
Olaf Steinbach	42
Coupling of finite and boundary element methods: Do we need the symmetric formulation.	
Carina Suciu	43
A numerical method for the simulation of uni- and bivariate population balance systems.	

20:00

Meeting of the Scientific Committee

Programme for Tuesday, September 25, 2012

Plates and Shells	
<i>Chairman:</i> C. Wieners	
<i>Room:</i> N111	
9:00	Manfred Bischoff 44 Computational modeling of shells - Classical strategies and recent developments

Plates and Shells	Flow
<i>Chairman:</i> C. Wieners	<i>Chairman:</i> J. Lang
<i>Room:</i> N111	<i>Room:</i> N101
9:55	Andreas Günnel 45 Numerical aspects of plates under large deformations.
10:20	Michael Weise 46 An a posteriori error estimator for laminated Kirchhoff plates.
10:45	<i>Tea and coffee break</i>

Mechanics	Flow
<i>Chairman:</i> M. Jung	<i>Chairman:</i> G. Matthies
<i>Room:</i> N111	<i>Room:</i> N101
11:15	Sören Bartels 49 Finite element approximation of large bending isometries.
11:40	Jörg Frohne 50 FEM-Simulation of elasto-plastic deformations with contact.
12:05	Christian Wieners 51 Robust discretization and reliable and efficient error control for general first-order systems.
12:30	<i>Conference Photo</i>
12:40	<i>Lunch</i>
15:00	<i>Ceremonial Event</i> <i>on the occasion of the 60th birthdays of Ulrich Langer and Arnd Meyer</i> <i>Room: N112</i>

S. Rjasanow Adaptive cross approximation with applications to real world problems	
J. Schöberl Domain decomposition methods for Hybrid Discontinuous Galerkin Methods	
18:00	<i>Conference dinner and more informal events</i>

Programme for Wednesday, September 26, 2012

Advanced Finite Element Methods and Applications

Chairman: T. Apel

Room: N111

- 9:00 Anke Bucher 55
Towards the direct and inverse adaptive mixed finite element formulations for nearly incompressible elasticity at large strains.
- 9:20 Vadim Korneev 56
Fast domain decomposition solvers for discrete problems with chaotically sub-domain wise variable orthotropism.
- 9:40 Michael Kuhn 57
Non-sequential optical field tracing.
- 10:00 Boniface Nkemzi 58
An iterative finite element method for boundary value problems in domains with geometric singularities: Computing the coefficients of the singularities.
- 10:20 Frank Rabold 59
Procrack: A software for simulating three-dimensional fatigue crack growth.

10:40 *Tea and coffee break*

Advanced Finite Element Methods and Applications

Chairman: O. Steinbach

Room: N111

- 11:10 Rene Schneider 60
Implementation of Schur-complement-preconditioners for the Stokes and Navier-Stokes Equations.
- 11:30 Peter Steinhorst 61
Application of the reciprocity principle for the determination of planar cracks in piezoelectric material.
- 11:50 Michael Theß 62
Multilevel preconditioners for temporal-difference learning methods related to recommendation engines.
- 12:10 Gerhard Unger 63
Coupled FE-BE eigenvalue problems for fluid-structure interaction.
- 12:30 Sabine Zaglmayr 64
Sensitivity analysis for Maxwell eigenvalue problems in industrial applications.
- 12:50 **Closing**

Lunch

On the Origins of Domain Decomposition Methods

Martin J. Gander¹

Domain decomposition methods have been developed in various contexts, and with very different goals in mind. I will start my presentation with the historical inventions of the Schwarz method, the Schur methods and Waveform Relaxation. I will show for a simple model problem how all these domain decomposition methods function, give precise results for the model problem, and also explain the most general convergence results available currently for these methods. I will conclude with the parareal algorithm as a new variant for parallelization of evolution problems in the time direction.

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Two-level domain decomposition preconditioners for multi-phase elastic composites

Heiko Andrä¹ Marco Buck² Oleg Iliev³

We analyse two-level overlapping Schwarz domain decomposition methods for a finite element discretization of the PDE system of linear elasticity. The focus in our study lies in the application to particle-reinforced composites with nearly incompressible and very stiff inclusions with large jumps in their material coefficients. We present explicit bounds for the condition number of the two-level additive Schwarz preconditioned linear system. Thereby, we do not require that the coefficients are resolved by the coarse mesh. The bounds show a dependence of the condition number on the energy of the coarse basis functions, the coarse mesh, and the width of the overlap. Similar estimates have been developed for scalar elliptic PDEs by Graham, Lechner and Scheichl (2007). The coarse spaces of our method are assumed to contain the six rigid body modes and can be considered as generalizations of the space of piecewise linear vector valued functions on a coarse triangulation. The developed estimates provide a concept for the construction of coarse spaces which can lead to preconditioners which are robust w.r.t. discontinuities in the elasticity coefficients of the underlying composite.

In our numerical tests, we extend the linear multiscale finite element method as formulated by Hou and Wu (1997) to the system of linear elasticity. For isolated inclusions of high contrast in the interior of coarse elements, the condition number bound does not depend on variations in the Young's modulus and the Poisson's ratio for the multiscale coarse space. By using oscillatory boundary conditions of the multiscale basis functions, the method is robust also in cases where inclusions cross coarse element boundaries. Furthermore, linear and energy minimizing coarse spaces are discussed.

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Scalable TFETI/TBETI algorithms for contact problems with variationally consistent discretization and optional preconditioning

Zdenek Dostal¹ Tomas Kozubek² Tomas Brzobohaty³

The results related to the development of theoretically supported scalable algorithms for the solution of large scale transient contact problems of elasticity will be reviewed. The algorithms combine the Total FETI/BETI based domain decomposition methods adapted to the solution of 2D and 3D multibody contact problems of elasticity with optional preconditioning by conjugate projector or dual scaling with our in a sense optimal algorithms for the solution of resulting quadratic programming problems. Rather surprisingly, the theoretical results are qualitatively the same as the classical results on scalability of FETI/BETI for linear elliptic problems, i.e., the inequality constraints are treated in a sense for free. We also discuss the effect of implementation of the nonpenetration condition by the variationally consistent discretization introduced recently by B. I. Wohlmuth. The numerical and parallel scalability of the method is demonstrated by the results of numerical experiments with parallel solution of 2D and 3D contact problems of elasticity discretized by millions of nodal variables.

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Nitsche-based overlapping and fictitious domain methods for the Stokes problem

André Massing¹ Mats G. Larson² Anders Logg³ Marie R. Rognes⁴

Overlapping and fictitious domain methods offer many advantages over standard finite element methods that require the generation of a single high-quality mesh conforming to computational domain. For instance, with overlapping mesh methods, the computational domain may instead be decomposed into different subdomains which then may be meshed independently. Fictitious domain methods, on the other hand, allow to embed complex geometries only described by their boundary surfaces into a structured background mesh. Both approaches require a special treatment of the imposed boundary and interface conditions.

Nitsche's method provides a general approach to weakly imposing boundary and interface conditions in a Lagrange multiplier-free way. Recently, the ideas behind Nitsche's method have been extended to propose overlapping [1] and fictitious domains [2] formulations. Here, a main challenge is to design the methods to be insensitive with regard to the interface and boundary position.

In this work, we present Nitsche-based formulations for a class of stabilized finite element methods for the Stokes problem posed on fictitious [3] and overlapping domains [4]. We address various ways to make the formulation robust and to avoid ill-conditioned linear algebra systems by adding certain so-called ghost-penalties in the vicinity of the boundary and interface. As a consequence, the resulting methods are inf-sup stable and optimal order *a priori* error estimates can be established. Moreover, the condition number of the resulting stiffness matrix is shown to be bounded independently of the location of the boundary and interface. Finally, we present numerical examples in three spatial dimensions confirming the theoretical results and illustrating the applicability of the methods to complex 3D geometries.

References:

- [1] A. Hansbo, P. Hansbo, M. Larson, A finite element method on composite grids based on Nitsche's method, *ESAIM, Math. Model. Numer. Anal.* 37 (2003) 495–514.
- [2] E. Burman, P. Hansbo, Fictitious domain finite element methods using cut elements: II. A stabilized Nitsche method, *Appl. Numer. Math.* 62 (2012) 328–341.
- [3] A. Massing, M. G. Larson, A. Logg, M. E. Rognes, A stabilized Nitsche fictitious domain method for the Stokes problem, submitted for publication.
- [4] A. Massing, M. G. Larson, A. Logg, M. E. Rognes, A stabilized Nitsche overlapping mesh method for the Stokes problem, submitted for publication.

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Finite Element Method with local Trefftz basis functions on polygonal/polyhedral meshes

Steffen Weißer¹ Sergej Rjasanow²

In the development of numerical methods for boundary value problems, the requirement of flexible mesh handling gains more and more importance. D. Copeland, U. Langer and D. Pusch proposed a new kind of conforming finite element method on polygonal/polyhedral meshes in 2009. The idea is to use basis functions which are defined implicitly as local solutions of the underlying homogeneous problem with constant coefficients. The local problems are treated by means of boundary integral equations and are approximated by the use of the boundary element method in the numerics. Therefore, this promising strategy is also called BEM-based finite element method.

In the last years, there have been several developments concerning residual error estimates and extensions with higher order basis functions on polygonal meshes in two space dimensions. The challenging part is to handle polygonal elements and to get the constants in the approximation estimates independent of the polygonal shapes. Following recent ideas, error estimates can be proven which guarantee optimal rates of convergence in the H^1 -norm as well as in the L_2 -norm for a model problem. Concerning higher order approximations, the basic method has to be modified to work with a continuous approximation of the material coefficient.

After a short review of recent results, a generalization to three space dimensions is discussed. All theoretical results are confirmed and illustrated by several numerical experiments.

References:

- [1] D. Copeland, U. Langer, D. Pusch: From the boundary element domain Decomposition methods to local Trefftz finite element methods on polyhedral meshes. Domain Decomposition Methods in Science and Engineering XVIII, 315–322, 2009
- [2] S. Weißer: Residual error estimate for BEM-based FEM on polygonal meshes. Numerische Mathematik, 118:765–788, 2011
- [3] S. Rjasanow, S. Weißer: Higher order BEM-based FEM on polygonal meshes. Preprint 297, Fachrichtung 6.1 Mathematik, Universität des Saarlandes, Germany, September, 2011

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hp estimates for hybrid DG methods for incompressible flow

Herbert Egger¹ Christian Waluga²

We discuss a hybrid discontinuous Galerkin method for incompressible flow. Besides the usual coercivity and boundedness estimates, we establish the inf-sup stability for the discrete incompressibility constraint with a constant which is only sub-optimal by one half order of the polynomial degree of approximation. This result holds on irregular and hybrid meshes in two and three spatial dimensions, and its proof is based on a new stability estimate for the L^2 projection on simplex elements. The sharp estimate for the inf-sup constants in turn allows to derive a-priori estimates which are optimal with respect to the mesh-size and only slightly sub-optimal with respect to the polynomial degree. In addition to the a-priori results, we also present a rigorous *hp* analysis of a residual-type a-posteriori error estimator. Reliability and efficiency are proven and the explicit dependence of the estimates on the polynomial approximation order is elaborated. The validity of the theoretical results is demonstrated in numerical tests.

References:

- [1] H. Egger and C. Waluga, *hp-Analysis of a Hybrid DG Method for Stokes Flow*, IMANUM, 2012.

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A posteriori error estimates for nonconforming finite element methods for fourth-order problems on rectangles

Dietmar Gallistl¹ C. Carstensen² J. Hu³

The a posteriori error analysis of conforming finite element discretisations of the biharmonic problem for plates is well established, but nonconforming discretisations are more easy to implement in practice. The a posteriori error analysis for the Morley plate element appears very particular because two edge contributions from an integration by parts vanish simultaneously. This miracle does not arise for popular rectangular nonconforming finite element schemes like the nonconforming rectangular Morley finite element, the incomplete biquadratic finite element, and the Adini finite element. This talk introduces a novel methodology and utilises some conforming discrete space on macro elements to prove reliability and efficiency of an explicit residual-based a posteriori error estimator for two of these methods. An application to the Morley triangular finite element shows the surprising result that *all* averaging techniques yield reliable error bounds. Numerical experiments confirm the reliability and efficiency for the established a posteriori error control on uniform and graded tensor-product meshes.

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How a non-convergent Hessian recovery works in mesh adaptation

Lennard Kamenski¹ Weizhang Huang²

A typical use of gradient/Hessian recovery in adaptive mesh computation is to compute an approximation to the gradient/Hessian of the exact solution based on the computed solution on the current mesh and then to generate a new mesh based on the recovered gradient/Hessian. Obviously, the convergence of such adaptive mesh computation relies crucially on the convergence of the recovery.

It is known that some gradient recovery methods are convergent on general meshes and even superconvergent for mildly structured meshes and for a type of adaptive meshes. The analysis of the Hessian recovery, on the other hand, receives much less attention and little is known except for special situations. Moreover, a convergent Hessian recovery cannot be obtained from the linear finite element approximation on general, non-uniform meshes. On the other hand, it has been observed that adaptive meshes generated by means of a non-convergent Hessian recovery still result in optimal order of error reduction.

In this talk we will try to explain why a non-convergent recovered Hessian works in mesh adaptation. We consider piecewise linear interpolation error and show that the interpolation error converges at a theoretically predicted order if the recovered Hessian satisfies some mild closeness conditions.

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Comparison results for first-order FEMs

Mira Schedensack¹ Carsten Carstensen² Daniel Peterseim³

This talk establishes the equivalence of conforming Courant finite element method, nonconforming Crouzeix-Raviart finite element method, and several first-order discontinuous Galerkin finite element methods in the sense that the respective energy error norms are equivalent up to generic constants and higher-order data oscillations in a Poisson model problem. The Raviart-Thomas mixed finite element method is better than the previous methods whereas the conjecture of the converse relation is proved to be false.

This talk completes the analysis of comparison initiated by Braess in *Calcolo* (2010).

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Combination technique based k -th moment analysis of elliptic problems with random diffusion

Helmut Harbrecht¹ Michael Peters² Markus Siebenmorgen³

We consider the efficient deterministic solution of elliptic boundary value problems with random diffusion matrix. Assuming random perturbations with known k moments, we derive, to leading order in the random perturbation's amplitude, deterministic equations for k moments of the random solution. The solution's k -th moment satisfies a k -fold tensor product boundary value problem on the k -fold product domain which can efficiently be discretized in sparse tensor product spaces. By defining the complement spaces via Galerkin projections, the related system of linear equations decouples and can be solved by standard multilevel finite element solvers. Numerical results for $k = 2$ are presented to validate and quantify our theoretical findings.

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Fast solvers for the Navier–Stokes equations with applications in arterial blood flow

Lorenz John¹ Olaf Steinbach²

We present an overview on different preconditioners for the Navier–Stokes equations. In particular we focus on preconditioning techniques for high Reynolds number flows, which arise in problems for arterial blood flow. Further, preconditioners for stabilized finite element methods for the Navier–Stokes equations are discussed. Some numerical results with applications in arterial blood flow will be given.

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Tensor numerical methods for multi-dimensional PDEs

Boris Khoromskij¹

Most common in computational practice separable representations of functions and operators combine the canonical, Tucker, tensor train (TT) and the quantized-TT (QTT) formats. The QTT tensor format, invented in 2009 [1], makes it possible to represent the multivariate functions, operators and dynamical systems in quantized tensor spaces with logarithmic complexity scaling in the size of the full tensor. QTT approximation applies to the quantized images, obtained by reshaping up to the 'indivisible' mode size '2', that represents a *quant* of information (reminiscent quantum bits, i.e. qubits in quantum computations). The numerical efficiency is justified by the remarkable QTT-approximation properties proven for the wide class of functions and operators. We focus on the main approximation and complexity results in the quantized tensor formats recently applied to the solution of d -dimensional elliptic and parabolic equations [2]. Numerical tests indicate the logarithmic computational complexity of the QTT-tensor method in application to the parametric elliptic PDEs, computational quantum chemistry and to the multi-dimensional dynamics.

References:

- [1] B.N. Khoromskij. *$O(d \log N)$ -Quantics Approximation of N -d Tensors in High-Dimensional Numerical Modeling*. J. Constr. Approx. v. 34(2), 257-289, 2011.
- [2] B.N. Khoromskij, *Introduction to Tensor Numerical Methods in Scientific Computing*. Lecture Notes, Preprint 06-2011, University of Zuerich, Institute of Mathematics, 2011, pp. 1 - 238. http://www.math.uzh.ch/fileadmin/math/preprints/06_11.pdf.

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A parallel space-time multigrid method

Martin Neumüller¹ Olaf Steinbach²

For evolution equations we present a space-time method based on Discontinuous Galerkin finite elements. Space-time methods have advantages when we have to deal with moving domains and if we need to do local refinement in the space-time domain. For this method we present a multigrid approach based on space-time slaps. This method allows the use of parallel solution algorithms. First numerical examples will be given.

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Reduced one-dimensional modelling and numerical simulation for mass transport in fluids

Tobias Köppl¹ Barbara Wohlmuth²

Based on the Navier–Stokes equations in three space dimensions and a convection-diffusion equation, we use a nonlinear system of three hyperbolic PDEs in one space dimension to simulate mass transport. In this talk we focus on the modelling of mass transport through an arterial network. For the numerical treatment of the hyperbolic PDE system, we use stabilised discontinuous Galerkin (DG) approximations with a Taylor basis. Higher order discontinuous Galerkin approximations together with a suitable time integration method enable us to simulate wave propagations for many periods avoiding excessive dispersion and dissipation effects. However higher order polynomials in standard discontinuous Galerkin approximations tend to create non-physical oscillations at sharp fronts and thus stabilisation techniques are required. Finally we present some numerical results illustrating the robustness of our model and the numerical discretisation.

References:

- [1] D. Kuzmin, Slope limiting for discontinuous Galerkin approximations with possibly non-orthogonal Taylor basis, *Int. J. Numer. Meth. Fluids*, 2011 (1), pp.1-12
- [2] S. J. Sherwin, L. Formaggia, J. Piero and V. Franke, Computational modelling of 1D blood flow with variable mechanical properties and its application to the simulation of wave propagation in the human arterial system. *Int. J. for Numerical Methods in Fluids*, 2003 (43), pp. 673-700
- [3] L. Formaggia, A. Quarteroni and A. Veneziani, *Cardiovascular Mathematics-Modelling and simulation of the circulatory system*. Springer, Italia, Milano, 2009
- [4] T. Köppl and B. Wohlmuth and R. Helmig, *Reduced one-dimensional modelling and numerical simulation for mass transport in fluids*

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Adaptive and higher order methods in computational fluid dynamics

Jens Lang¹

In this talk, I will summarize our recent activities in constructing higher order variable timestep integrators for computational fluid dynamics and adaptive moving meshes in large eddy simulation (LES) for turbulent flows.

I will focus on two-step peer methods which were first developed for ODEs and subsequently applied to parabolic PDEs. Their main advantage over one-step methods lies in the fact that even in the application to PDEs no order reduction is observed. Our aim is to investigate whether the higher order of convergence of the two-step peer methods equipped with variable timesteps pays off in practically relevant CFD computations. In turbulent flows, the characteristic length scale of the turbulent fluctuation varies substantially over the computational domain and has to be resolved by an appropriate numerical grid. We propose to adjust the grid size in an LES by adaptive moving meshes. The main advantage of mesh moving methods is that during the integration process the mesh topology is preserved and no new degrees of freedom are added and therefore the data structures are preserved as well. This makes the method an attractive add-on for the many fluid flow solvers available. I will present results for meteorological applications.

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A two-level local projection stabilisation on uniformly refined triangular meshes

Gunar Matthies¹ Lutz Tobiska²

The local projection stabilisation (LPS) has been successfully applied to scalar convection-diffusion-reaction equations, the Stokes problem, and the Oseen problem.

A fundamental tool in its analysis is that the interpolation error of the approximation space is orthogonal to the discontinuous projection space. It has been shown that a local inf-sup condition between approximation space and projection space is sufficient to construct modifications of standard interpolations which satisfy this additional orthogonality.

There are different versions of the local projection stabilisation on the market; we will consider the two-level approach based on standard finite element spaces Y_h on a mesh \mathcal{T}_h and on projection spaces D_h living on a macro mesh \mathcal{M}_h . Hereby, the finer mesh is generated from the macro mesh by a certain refinement rules. In the usual two-level local projection stabilisation on triangular meshes, each macro triangle $M \in \mathcal{M}_h$ is divided by connecting its barycentre with its vertices. Three triangles $T \in \mathcal{T}_h$ are obtained. Then, the pairs $(P_{r,h}, P_{r-1,2h}^{\text{disc}})$, $r \geq 1$, of spaces of continuous, piecewise polynomials of degree r on \mathcal{T}_h and discontinuous, piecewise polynomials of degree $r - 1$ on \mathcal{M}_h satisfy the local inf-sup condition and can be used within the LPS framework.

One disadvantage of this refinement technique is however that \mathcal{T}_h contains simplices with large inner angles even in the case of a uniform decomposition \mathcal{M}_h into isosceles triangles. Another drawback is that this refinement rule leads to non-nested meshes and spaces whereas the common refinement technique of one triangle into 4 similar triangles (called red refinement in adaptive finite elements) results into nested meshes and spaces.

We will show that in the two-dimensional case the pairs $(P_{r,h}, P_{r-1,2h}^{\text{disc}})$, $r \geq 2$, satisfy the local inf-sup condition with the refinement of one triangle into 4 triangles. Consequently, the LPS can be also applied on sequences of nested meshes and spaces and keeping the same error estimates. Finally, we compare the properties of the two resulting LPS methods based on the different refinement strategies by means of numerical test examples for convection-diffusion problems with dominating convection.

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Composite non-conforming elements and local projection stabilization for transport dominated flow problems

Piotr Skrzypacz¹ Friedhelm Schieweck²

We consider composite non-conforming elements which are suitable for solving both, convection-diffusion and Oseen equations, respectively. Numerical experiments show that the usual Local Projection Stabilization (LPS) fails in the case of non-conforming elements. This drawback can be cured by adding a modified LPS-term to the discrete bilinear form. In contrast to the known one-level LPS approach, the proposed discrete space of composite non-conforming elements does not need special enrichments. One advantage of the composite non-conforming elements compared to known conforming quadrilateral elements like the Taylor-Hood elements is that they guarantee a better local mass conservation. Another advantage is that the matrices for the coupling between pressure and velocity are much more sparse for the composite non-conforming elements. Furthermore, the low order non-conforming element (Crouzeix-Raviart element) leads to a diagonal mass matrix which is advantageous for time dependent problems. We present several numerical experiments which show optimal approximation and good stability properties for our proposed non-conforming elements and the modified LPS.

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Analysis of preconditioned iterative methods for the Helmholtz equation

Antti Hannukainen¹

The finite element discretization of time-harmonic wave propagation problems, such as the Helmholtz equation or the Maxwell equations, leads to a solution of large, complex valued, indefinite, non-hermitian and non-normal linear systems. These systems are typically solved with a suitable preconditioned iterative method. Due to indefiniteness and non-normality of the linear system, a rigorous convergence analysis of such iterative solution methods is still a challenge.

Because of the non-normality, the eigenvalues alone do not give information of the convergence. In addition, due to indefiniteness, the interesting eigenvalue is the one closest to the origin. This eigenvalue cannot be bounded using techniques familiar from convergence analysis of elliptic problems. In this talk we discuss these difficulties and possible solutions to them. As a model problem, we use the Helmholtz equation discretized with the standard first order finite element method, and solved using the preconditioned GMRES method.

The non-normality can be handled in analysis by using a suitable convergence criterion. For GMRES, two possibilities exist, estimating the location of the field of values or the pseudospectrum. The FOV based convergence criterion has been used to study Laplace preconditioners for Helmholtz equation with losses. The major shortcomings of FOV based convergence criterion are in handling the indefiniteness of the linear system. These problems with FOV based criterion motivate us to study a pseudospectrum based criterion. The pseudospectrum is well suited for handling indefinite problems. We demonstrate this for the Helmholtz equation with absorbing boundary conditions.

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Hardy space infinite elements for exterior Maxwell problems

Lothar Nannen¹ Joachim Schöberl²

In this talk we present an infinite element method for solving electromagnetic scattering and resonance problems posed on unbounded domains. As our motivation is to solve Maxwell's equations we take care that these infinite elements fit into the discrete de Rham diagram, i.e. they span discrete spaces, which together with the exterior derivative form an exact sequence.

The theoretical framework of the method is the so called *pole condition*, which characterizes radiating solutions via the poles or singularities of the Laplace transformed solutions: The Laplace transform in radial direction of an outgoing wave belongs to a certain Hardy space of holomorphic functions, while the Laplace transform of an incoming wave does not. Hence, the Hardy space infinite elements are constructed using tensor products of Hardy space basis functions with standard finite element surface basis functions.

Numerical tests indicate super-algebraic convergence in the number of additional unknowns per degree of freedom on the coupling boundary.

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The weighted edge finite element method for Maxwell equations with strong singularity

Viktor Rukavishnikov¹

Maxwell equations are used in mathematical models of electromagnetic fields, for example, in plasma physics, electrodynamics and engineering of high-frequency devices. As a rule, in practical problems the computational domain is nonconvex with reentrant corners or edges on its boundary. Such geometry singularities leads to strong electromagnetic fields in their neighborhood, and a solution of Maxwell equations is strongly singular, i.e. it does not belong to the Sobolev space $H^1(W_2^1)$. In the present talk we develop the weighted edge finite element method (FEM) based on the conception of R_ν -generalized solution (see, example, [1-3]) of the Maxwell equations with strong singularity due to a reentrant corner on the boundary. Numerical experiments of model problems showed that the rate of convergence of the numerical solution to the exact one is more than one and a half times better in comparison with the results established in papers of other mathematicians. Another advantage of this method is simplicity of the solution determination which is an additional benefit for numerical experiments.

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Crank-Nicolson discretization for parabolic optimal control problems with terminal observation

Thomas Flaig¹

Crank-Nicolson schemes are often used for the time discretization of parabolic partial differential equations. In this talk we present a second order discretization scheme for optimal control problems with terminal observation. The discretization is based on the Crank-Nicolson scheme with different time discretizations for state y and adjoint state p so that discretization and optimization commute.

As the scheme can be explained as the Störmer-Verlet method, we can also interpret the method in the context of geometric numerical integration of Hamilton systems as parabolic optimal control problems are Hamilton systems. This Hamiltonian structure is also discussed in this presentation. Further we point out that the scheme may also be obtained as a Galerkin method. We prove second order convergence of the scheme.

Finally we present the analytic solution of the optimal control problem as eigenfunction expansion with respect to the eigenfunction of the spatial operator. In a numerical example second order convergence in time is observed.

We discuss an optimal control problem with an inhomogenous initial condition for the state y . The resulting optimality system also contains an inhomogenous terminal condition for the adjoint state p .

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Optimal control subject to singularly perturbed convection-diffusion-equations

Christian Reibiger¹ Hans-Görg Roos²

We consider the optimal control problem

$$\min_{y,u} J(y, u) := \min_{y,u} \left(\frac{1}{2} \|y - y_0\|_0^2 + \frac{\lambda}{2} \|u\|_0^2 \right)$$

subject to a convection dominated differential state equation

$$\begin{aligned} Ly &:= -\varepsilon y'' + ay' + by = f + u \text{ in } (0, 1), \\ y(0) &= y(1) = 0. \end{aligned}$$

The solutions of such singularly perturbed differential equations typically exhibit boundary layers. The optimality condition leads to the enhanced system of the state equation and its adjoint form. The change of sign of the convection term in the adjoint equation induces a boundary layer of the adjoint state at the opposite side of the domain compared to the primal state. By the coupling of the two differential equations via the optimality system those layers lead to additional boundary layers of a weaker form in the other part of the solution. Our analysis shows the layer structure of the solution of such an optimality system.

Using linear finite elements on adapted grids of Shishkin type we treat the effects of the arising layers at the boundaries of the domain. Furthermore we proof uniform error estimates with respect to the perturbation parameter ε . We show that the weak boundary layers also have an impact on the quality of numerical algorithms for solving the optimality system. Numerical results supporting our analysis are presented.

Moreover, we discuss extensions to the case of box constraints for the control u .

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On an optimal control problem for magnetic fields

Fredi Tröltzsch¹ Kristof Altmann² Serge Nicaise³ Simon Stingelin⁴

An optimal control problem is considered for a coupled Maxwell integrodifferential model. The problem is related to an industrial application, where a time-optimal switching between magnetic fields of different polarization is needed. In the talk, the well-posedness of an associated system of degenerated parabolic integrodifferential equations, first-order necessary optimality conditions for the optimal control, and their numerical application are sketched. Numerical results are presented for a simplified 3D geometry.

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Compressible and incompressible material under large deformations

Martina Balg¹ Arnd Meyer²

In the development of new mechanical components the efficient usage of material resources is very important. Therefore one needs a fast and highly accurate simulation to predict the actual material deformations, that are caused by external loads and the material behaviour.

In this talk we want to focus on incompressible materials, see [1] and derive a possibility to numerically simulate this material in the context of large deformations. Although these rubber like materials are widely used in the industry the efficient simulation of such parts is still an open problem due to their special material properties. Since incompressible materials have an infinite bulk modulus they may change their shape but they keep their constant volume during any deformation. In our approach we treat this speciality by introducing a new variable, the hydrostatic pressure and by working with a mixed formulation.

From the equilibrium of forces in the deformed domain we develop the nonlinear weak form in the known initial domain. For linearisation we apply a modified Newton's method with incremental load steps. This yields a linear saddle point problem in every step. By means of the finite element method with a mixed ansatz via the Taylor Hood element we get a linear system of equations. Its structure invites the usage of an adjusted Bramble-Pasciak conjugate gradient method with suitable preconditioning. This simulation can be improved by using an adaptive mesh refinement with a residuum based error estimator and parallel strategies (e.g. with openMP).

Finally we want to present some results that show the combination of incompressible and compressible material.

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AMG accelerated elasticity solver on GPU-clusters

Gundolf Haase¹ Aurel Neic² Gernot Plank³ Patrick Ditz⁴ Manfred Liebmann⁵

Recent developments in graphics hardware by NVidia and ATI, and associated software development tools as CUDA (and OpenACC recently) enable us to transfer numerical solver components on the recent generation of graphics processing units (GPUs).

Originating from potential problems we solve systems of linear equations with sparse unstructured system matrices derived from f.e. discretizations of PDEs and we present the adaption of an algebraic multigrid solver (AMG) used as preconditioner in a conjugate gradient solver on these GPUs. We achieve an accelerations of 10 wrt. to one CPU core in various practical applications ranging from engineering to medical technology based on fully unstructured discretizations.

The step from the potential problem to elasticity seems to be quite straight forward. But as always, the challenges are hidden in the details. Applying the AMG for the potential problems works in the first place at the cost of high iteration counts. Replacing the inappropriate potential solver components in smoother and intergrid transfer operations by appropriate 3×3 block components, i.e., taking into account the underlying energy norm/physics, reduces the number of iterations significantly.

Stepping forward from one GPU to clusters of GPUs is non-trivial even with a fast interconnect between the compute nodes. Here, even minor imbalances in a small subset of the code cause dramatic efficiency losses. A rescheduling of communication and operations on the boundary nodes was necessary to improve the efficiency of the parallel solver. Together with the new extension of all solver components to blocks systems, e.g., elasticity, we are able to run most parts of the CARP simulation software on clusters of GPUs now [1]. The Cardiac Arrhythmia Research Package (CARP) simulation software is used worldwide for the simulation of cardiovascular phenomena, see <http://carp.meduni-graz.at> .

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High-order finite element methods for optimal control problems

Katharina Hofer¹ Sven Beuchler² Daniel Wachsmuth³

Considered is a linear-quadratic elliptic boundary control problem on two-dimensional polygonal domains, where the observation domain for the state is either the whole domain Ω or a part of the boundary $\partial\Omega$. For solving these problems the boundary concentrated finite element method (BC-FEM), a high-order finite element method, can be used. After getting a general idea of the BC-FEM, a discretization error estimate for the case, where the observation domain is a part of the boundary, is given.

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Optimal control of coupled systems of ordinary and partial differential equations with algebraic constraints

Sven-Joachim Kimmerle¹ Matthias Gerdts² Roland Herzog³

In the modelling of multi-body systems we find ODEs representing the interactions between the centers of mass, algebraic equations (AE) from constraining forces and elliptic PDEs modelling mechanical deformations within the bodies. Another typical example for coupled ODE, PDE and AE are free boundary problems, where, for example, the ODE describes the motion of the free interface between two phases and the PDE the evolution or quasi-stationary solution of quantities inside the phases. This might be coupled to constraints representing global conservation of mass. We discuss the well-posedness of these kind of problems shortly and are finally interested in the optimal control of these systems.

For solving the PDEs finite element methods are well applicable. Special attention has to be given to the finite elements in the neighbourhood of points or surfaces where forces are applied or whenever free boundaries occur. For several examples, e.g. an elastic crane, an elastic tyre-damper system, phase transitions and a fluid-elastomer interaction, the problems and first results are presented. The research on the elastic crane and elastic tyre is joint work with Matthias Gerdts and Roland Herzog.

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Numerical simulation of elastic wave propagation in composite material

Markus Bause¹ Uwe Köcher²

Composites are one of the most promising materials to build light-weight structures for several fields of application, e.g. for wind energy plants and aerospace applications. Piezoelectric induced ultrasonic waves can be used for the development of structural health monitoring (SHM) systems. But, there are still a lot of open questions, especially regarding the application of ultrasonic waves in layered composite structures. Numerical simulation can help to understand wave propagation in heterogeneous and composite media. The reliable prediction of structural damages requires accurate numerical schemes.

Recently, there has been an increased interest in applying the discontinuous Galerkin method (DGM) to wave propagation. Some of the advantages of the finite element method are the flexibility with which it can accommodate the underlying geometry, discontinuities in the model and boundary conditions, and the ability to approximate the wavefield with high-degree polynomials. The DGM has the further advantage that it can accommodate discontinuities, not only in the media parameters, but also in the wavefield, it can be energy conservative, and it is suitable for parallel implementation.

In this contribution we study the application of continuous and discontinuous Galerkin methods for analyzing elastic wave propagation in heterogeneous media. A symmetric interior penalty discontinuous Galerkin method is used. An error analysis of this scheme is given in [1] for the acoustic wave equation. For the integration in time the second order-accurate method of Crank-Nicolson and the Newmark-Schemes are used. Precisely, we consider solving the linear-elastic wave equation without damping [2].

In our numerical results we study the performance and accuracy properties of continuous and discontinuous Galerkin methods for predicting wave propagation phenomena. In particular, a positive impact of higher order discontinuous approximations for heterogeneous materials will be illustrated; cf. also [3] for the application of higher order techniques to convection-dominated transport problems. Wave propagation in various composite materials and the potential of using guided waves for detecting structural damages is considered further.

The implementations were done by using the finite element toolbox `deal.II` [4].

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Non-symmetric coupling of finite and boundary element methods for the heat equation

Günther Of¹ Martin Neumüller² Olaf Steinbach³

We present some coupling formulations of continuous and discontinuous Galerkin finite element methods with boundary element methods for the heat equation. In particular, we consider the non-symmetric coupling. This enables us to use even discontinuous basis functions on the interface between the subdomains represented by the finite element and boundary element methods while other formulations require continuity. We will address the error and stability analysis and show the stability and efficiency of the proposed approach for some numerical examples.

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Dirichlet boundary control problems: finite element discretization and error estimates

Johannes Pfefferer¹ Thomas Apel²

This presentation is concerned with the unconstrained Dirichlet boundary control problem

$$\begin{aligned} \min J(y, u) &= \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Gamma)}^2, \\ \text{s.t.} \quad & -\Delta y = f \text{ in } \Omega, \\ & y = u \text{ on } \Gamma, \end{aligned}$$

where the state equation has in general to be understood in the very weak sense. In order to solve this problem the state and adjoint state are discretized by linear finite elements and also the control is discretized by piecewise linear and continuous functions. For convex domains finite element error estimates of this problem are proven by May, Rannacher and Vexer (2009). However, numerical tests suggest that these results are not sharp. First theoretical results are presented, which fit to the observations. In addition, Dirichlet boundary control problems in non-convex domains are attacked. These are more sophisticated compared to the convex ones, since the optimal state does not belong to the space $H^1(\Omega)$. Thus, the weak formulation is not well defined. Instead one has to deal with the very weak formulation.

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Modelling and numerical experiments for Kirchhoff plates using finite strain

Jens Rückert¹ Arnd Meyer²

In the simulation of deformations of plates it is well known that we have to use a special treatment of the thickness dependence. Therewith we achieve a reduction of dimension from $3D$ to $2D$.

For linear elasticity and small deformations several techniques are well established to handle the reduction of dimension and achieve acceptable numerical results. In the case of large deformations of plates with non-linear material behaviour there exist different problems. One of these is the impossibility of analytical integration over the thickness of the plate due to the non-linearities arising from the material law and the large deformations themselves. There are several approaches to introduce a hypothesis for the treatment of the plate thickness from the strong Kirchhoff assumption on one hand up to some hierarchical approaches on the other hand.

Here we consider a model of using the Kirchhoff assumption. Therewith, a fibre that is straight and perpendicular to the midsurface of the undeformed plate has to be straight and rectangular to the midsurface of the deformed plate, as well. A possible change in length of the fibre is not considered in this hypothesis. From now on, it is important that we avoid any further simplifications, which could be crucial for large strain.

We are aware of the fact, that the Kirchhoff assumption is well suited for small deformations and linear material laws. However, we want to investigate the deformation of thin plates with isotropic nonlinear material as a numerical experiment. Particularly we are interested in bending dominated real $3D$ - deformations. As a result we get a heavily deformed shell but without change in thickness.

This way of modelling leads to a two-dimensional strain tensor, which depends essentially on the first two fundamental forms of the deformed midsurface. By minimizing the resulting deformation energy we end up with a nonlinear equation, defining the unknown displacement vector \mathbf{U} . The aim of the presentation is to combine incremental Newton technique with the finite element discretisation. The first derivative of the energy functional is relatively easy to obtain (our nonlinear equation to solve), but its second derivative, for performing Newton's method, is analytically ambitious and leads to time consuming element routines. Nevertheless we demonstrate the practicability, due to the fast convergence of the Newton linearization.

We will present the total theory and give first numerical results for comparisons.

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The finite element method for Dirichlet problem with degeneration of solution on the boundary

Elena Rukavishnikova¹

The first-boundary-value problem for the second-order elliptic equation with degeneracy of input data whose solution has weak singularity on the curvilinear boundary of a two-dimensional convex domain is considered. There exists a unique generalized solution of this problem in the Sobolev weighted space. We construct and investigate the finite element method for this problem. We created an algorithm and program for automated triangular elements to the boundary. It was established that the approximation to the exact generalized solution has first-order convergence in the norm of the Sobolev weighted space and second-order convergence in the norm of the Lebesgue space.

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Non-conforming finite elements and Riccati-based feedback stabilization of the Stokes equations

Jens Saak¹ Peter Benner² Heiko K. Weichelt³ Friedhelm Schieweck⁴ Piotr Skrzypacz⁵

We investigate the problem of feedback stabilization of the Stokes equations. Following recent results by Raymond our goal is to apply a Riccati-based boundary feedback stabilization. Here the main difficulty is that a standard finite element discretization of this type of problems usually leads to a discrete differential-algebraic model of differential index two. It is, therefore, necessary to project the system to the space of divergence-free functions and apply the numerical methods for solving the Riccati equation to the resulting projected state space ODE system. However, it is prohibitive to form that system explicitly due to memory and complexity restrictions.

Here we consider non-conforming finite elements, which guarantee that an application of the spatially semi-discretized PDE operators always give a discrete divergence-free solution. So they do not provide the state space representation of the system, without algebraic constraints, but in the matrix based solver framework the projection of the solution never needs to be performed explicitly. As a second important ingredient of our solver, we show in a proof of concept implementation that the solver framework can in principle be implemented matrix-free, i.e., all steps of the underlying algorithms are expressed in terms of PDE operators, such that all applications of matrices are mapped to function calls within the finite element code.

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On adaptive FEM for viscoelasticity at large strain deformations

Hansjörg Schmidt¹ Arnd Meyer²

Following the derivation in [1] we arrive at the following (non-linear) weak formulation for large deformations

$$0 = \int_{\Omega_0} \overset{2}{T} : E(U(t); V) \, d\Omega_0 - \int_{\Omega_0} \rho_0 \vec{f}(t) \cdot V \, d\Omega_0 - \int_{\Gamma_N} \vec{g}(t) \cdot V \, d\mathcal{S}_0 \quad \forall V \in \mathbb{V}, \quad \forall t \in [0, t_{end}].$$

The dependence of the second Piola-Kirchhoff stress tensor $\overset{2}{T}$ on the displacement U and potential other quantities has to be specified. Polymers and soft tissues are often modelled as viscoelastic continua which are characterised by a spontaneously elastic and dissipative viscous behaviour. There are at least two different models for viscoelasticity. In [2, p. 242] the model of fading memory is used to arrive at the stress-strain relation

$$\overset{2}{T}(t, U) = \mathfrak{h}_e(C(U(t))) + \int_0^\infty \mathfrak{G}(C(U(t)); s) : (\Delta C(t-s, t) - I) \, ds$$

with a function $\mathfrak{G}(C; \cdot)$ which is pointwise a fourth order material tensor and where the right Cauchy-Green tensor $C(U(t))$ depends solely on the current displacement, but $\Delta C(t-s, t)$ depends on the whole history of the displacement U . This stress-strain relation is accurate for large strain deformations which are slow with respect to the properties of the considered material. Another model for the stress-strain relation is based on thermodynamic with internal state variables, [3], and results in

$$\overset{2}{T}(t, U) = 2 \left. \frac{\partial \psi(C, G)}{\partial C} \right|_{C(U(t)), G(t)} \quad \text{subject to} \quad \mathcal{F}(t, G, \dot{G}, C) = 0,$$

with a differential(-algebraic) equation describing the evolution of the internal variable G .

The aim is to improve the simulation of these materials, to achieve results with a higher accuracy with lower computational cost. We give some remarks about the discretisation and adaptivity in time and space.

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Coupling of finite and boundary element methods: Do we need the symmetric formulation

Olaf Steinbach¹

While the symmetric coupling of finite and boundary element methods is stable for an almost arbitrary choice of finite and boundary elements, its implementation requires a Galerkin formulation and the discretization of the hypersingular boundary integral operator. This is why engineering and industrial applications in most cases still rely on the use of the classical one-equation coupling which also allows the use of a collocation boundary element method. Here we give an overview on recent stability results on the one-equation coupling of finite and boundary element methods.

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A numerical method for the simulation of uni- and bivariate population balance systems

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Crystallization processes are fundamental operations in obtaining particulate products in the chemical industry. Such processes can be modeled by a *population balance system* describing different mechanical phenomena, e.g. nucleation, growth, aggregation, breakage and transport of particles. This system consists of the incompressible Navier–Stokes equations for describing the flow field in the domain $\Omega \subset \mathbb{R}^3$ and scalar convection-diffusion equations which model the energy balance (temperature) and the concentration of dissolved species. Coupled to these equations, there is an equation for the particle size distribution.

Altogether, a population balance system contains equations which are defined in domains with different dimensions. In fact, the flow field, the concentrations of dissolved species and temperature are defined in a three-dimensional spatial domain, while the PSD depends also on the *internal* coordinates, which describe additional properties of the particles (e.g. *diameter, volume*) resulting in uni-variate models. More geometrical properties of the particles are often needed to characterize the particles for crystallization processes. Thus, extensions to the multivariate models yield more trustful models of such processes, improving the accuracy of simulations.

In particular, **uni-variate** and **bi-variate** population balance models are based on one- and two-dimensional geometrical characterization of the individual particles (*diameter, volume, or main axis in case of anisotropic particles*), resulting in four-dimensional (4D) and five-dimensional (5D) PSD systems.

The talk presents an approach for the simulations of the population balance systems (e.g. the synthesis of urea for the uni-variate model, the production of potassium dihydrogen phosphate for the bi-variate model). This approach is based on implicit time-stepping schemes, finite element, and finite difference discretizations.

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Computational modeling of shells – Classical strategies and recent developments

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The first generally accepted theory for analysis of shells has been presented by August E.H. Love 124 years ago. Its theoretical structure and principal ideas are still utilized today. Nevertheless, research on shell theories and solution methods has been an extraordinarily active field ever since and still today significant progress seems to be possible. Particularly the advent of computational methods, like the finite element method, in the second half of the past century has triggered an enormous variety of shell models and formulations.

The concept of degeneration and, more recently, formulation of three-dimensional shell models have received a great deal of attention. So-called 'continuum-shell' elements are available in commercial codes since a couple of years. In this context, shell theory may as well be regarded as a semi-discretization of the spatial domain in thickness direction.

One of the prominent issues of finite element technology for shells is the problem of 'locking' arising from the bad conditioning of the equations governing mechanical behavior of thin-walled structures. Here, recent developments in the field of spline-based finite element formulations along with the so-called isogeometric concept offer both new challenges and possibilities. An intrinsically locking-free isogeometric shell formulation, developed at the Institute of Structural Mechanics in Stuttgart is presented and some numerical experiments demonstrate its features.

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Numerical aspects of plates under large deformations

Andreas Günnel¹

Elastic material behavior of plates, more precisely thin and plane mechanical structures, often leads to large deformations. Still today, the elastic material models are mainly phenomenological, that is suggested formulas for the stored elastic energy Ψ are verified by experiments. Instead of starting from the balance of forces, we base our model on a stored energy minimisation $\Psi \rightarrow \min$ which leads to an equivalent variational equation as the balance of forces. The advantage of this approach lies in the use of optimisation strategies like line-search methods to improve the convergence of the newton-solver. To simulate very thin structures like plates, one approach is a reduction to the two-dimensional mid-surface by restricting the deformation in a certain way. We use a polynomial ansatz over the thickness η^3 , e.g.

$$x(\eta^1, \eta^2, \eta^3) = X(\eta^1, \eta^2, \eta^3) + U(\eta^1, \eta^2) + \eta^3 \theta_1(\eta^1, \eta^2) + (\eta^3)^2 \theta_2(\eta^1, \eta^2) + (\eta^3)^3 \theta_3(\eta^1, \eta^2).$$

We insert this special deformation in our three-dimensional model and get a non-linear two-dimensional PDE. This reduction allows more complex deformations than the Midlin-Reisner or Kirchhoff-model, especially change in thickness and shear. We present numerical experiments (implemented in FEniCS) and discuss the how the polynomial degree of the ansatz effects the solution and how the integration over the thickness is realized.

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An a posteriori error estimator for laminated Kirchhoff plates

Michael Weise¹ Arnd Meyer²

Lightweight construction plays an important role in modern engineering. Fibre reinforced polymers (FRP) are in common use in this field. Strong fibres (e. g. glass fibres, carbon fibres) are combined with a weaker polymer which holds the fibres in place. This gives a composite material which features high stiffness and strength in fibre direction while having a relatively low specific weight. The material can be described as a continuum featuring transversely isotropic material behaviour, a special case of anisotropy, see [1].

FRP structures are often constructed as a thin shell, e.g. parts of the bodies of planes or cars. Since the material is only strong in fibre direction, multiple layers with different fibre directions are combined into a laminate to account for different load cases. Our goal is to simulate such structures. As a simplification we restrict ourselves to plates, that means we only consider structures with a flat mid-surface.

Using the Kirchhoff plate model and assuming constant materials over the thickness one gets a plate equation decoupled from the in-plane deformation of the mid-surface. In the given problem this only holds true for a symmetric laminate sequence over the thickness but not in the general asymmetric case. Here in-plane deformations can cause out-of-plane deformations and vice versa.

A precise simulation of FRP components is the basis for efficient design of lightweight structures. A fast as well as highly accurate computation can be achieved using the adaptive finite element method with its solution-dependent automatic mesh refinement, based on local error estimation.

In our talk we present an a posteriori error estimator for the specified problem. It considers element residuals and edge jump terms of the arising plate, membrane and couple parts of the equation.

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Numerical studies of Galerkin-type time discretizations applied to transient convection-diffusion-reaction equations

Naveed Ahmed¹ Gunar Matthies²

It is well known that the Galerkin finite element method is unstable for the numerical solution of convection-dominated problems since the solution is typically polluted by spurious oscillations. To enhance the stability while keeping the accuracy of the Galerkin method, several stabilization techniques have been developed. We consider the streamline upwind Petrov-Galerkin (SUPG) method and local projection stabilization (LPS) method to stabilize the Galerkin discretization. The SUPG formulation is strongly consistent whereas, the LPS method lies in the class of symmetric stabilizations and weakly consistent.

We shall employ the combination of SUPG and LPS methods in space with the variational type time-discretization schemes for the numerical solution of time-dependent convection-diffusion-reaction equations. In particular, we consider the discontinuous Galerkin (dG) and continuous Galerkin-Petrov (cGP) method to discretize the problem in time. Several numerical tests have been performed to assess the accuracy of the higher order time-discretization schemes. For the smooth solution, optimal order of convergence for cGP and dG-methods are obtained. Furthermore, numerical comparison of SUPG and LPS methods for the smooth solution shows that both stabilization techniques perform quite similar and no difference among them can be appreciated. Finally, the dependence of the results on the stabilization parameters are discussed for smooth and non-smooth solution.

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Directional-do-nothing condition for the Navier-Stokes equations

Malte Braack¹ Piotr Boguslaw Mucha² Wojciech M. Zajączkowski³

The numerical solution of flow problems usually requires bounded domains although the physical problem may take place in an unbounded or substantially larger domain. In this case, artificial boundaries are necessary. A well established artificial boundary condition for the Navier-Stokes equation discretized by finite elements is the “do-nothing” condition. The reason for this is the fact that this condition does appear automatically due to partial integration of the viscous term and the pressure gradient. This condition is one of the most established outflow conditions for Navier-Stokes but there are very few analytical insight into this boundary condition. We address the question of existence and stability of weak solutions for the Navier-Stokes equations with a “directional do-nothing” condition. In contrast to the usual “do-nothing” condition this boundary condition has enhanced stability properties. In the case of pure outflow, the condition is equivalent to the original one, whereas the new boundary condition has a dissipative effect in the case of inflow. We show existence of weak solutions and illustrate the effect of this boundary condition by computation of steady and for non-steady flows.

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Finite element approximation of large bending isometries

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The mathematical description of the elastic deformation of thin plates can be derived by a dimension reduction from three-dimensional elasticity and leads to the minimization of an energy functional that involves the second fundamental form of the deformation and is subject to the constraint that the deformation is an isometry. We discuss two approaches to the discretization of the second order derivatives and the treatment of the isometry constraint. The first one relaxes the second order derivatives via a Reissner-Mindlin approximation and the second one employs discrete Kirchhoff triangles that define a nonconforming second order derivative. In both cases the deformation is decoupled from the deformation gradient and this enables us to employ techniques developed for the approximation of harmonic maps to impose the constraint on the deformation gradient at the nodes of a triangulation. The solution of the nonlinear discrete schemes is done by appropriate gradient flows and we demonstrate their energy decreasing behaviours under mild conditions on step sizes. Numerical experiments show that the proposed schemes provide accurate approximations for large vertical loads as well as compressive boundary conditions.

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FEM-Simulation of elasto-plastic deformations with contact

Jörg Frohne¹

From the mathematical point of view modeling of elasto-plastic deformations of a solid with contact builds the main issue of my talk. Beside the appearance of external forces of friction and lubricant pressures the strains will be caused by a movable rigid obstacle. To take into consideration the history of loads, we use the Prandtl-Reuss-Law. The temporary changes of the stresses will be approximated by means of a Backward-Euler-Method. At every particular time this leads to a variational problem with nonlinear operator and nontrivial inequality conditions. Based on concepts of SQP-methods we design a robust, adaptive damped method for the handling of this continuous problem. This leads to a sequence of quadratic minimization problems, which will be efficiently solved via projection-techniques (CG-PSSOR) after Galerkin-discretisation on local refined FE-Grids.

Alternatively, it is possible to use a primal-dual active set strategy to solve the quadratic minimization problems. The advantage of this method is the possibility to parallelize the AMG preconditioner we used for this method, which is necessary to compute further more expensive, coupled simulations.

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Robust discretization and reliable and efficient error control for general first-order systems

Christian Wieners¹ Barbara Wohlmuth²

We discuss a class of discontinuous Petrov-Galerkin schemes obtained by substructuring. The method allows to discretize very general differential operators and yields a solution procedure where only positive definite linear systems have to be solved. These systems arise from the reduction to interface values of the skeleton corresponding to a domain decomposition. In the subdomains, in analogy to an inexact Trefftz method a dual problem is solved with higher accuracy. It is shown that this corresponds to local least squares problems in negative norms. The method coincides with the DPG method introduced by Demkowicz et al. Here, we extend the numerical analysis of this method and we consider new applications. Moreover, the method comes along with full error control with efficient and reliable bounds.

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Numerical modeling of fluid flow and species transport by a coupled finite element/finite volume approach.

Jürgen Fuhrmann¹ Alexander Linke² Hartmut Langmach³

We present a coupled discretization approach for species transport in an incompressible fluid. The Navier-Stokes equations for the flow are discretized by the point-wise divergence-free Scott-Vogelius element. The convection-diffusion equation describing the species transport is discretized by the Voronoi finite volume method on boundary conforming Delaunay meshes. This approach guarantees that the discrete species concentration fulfills discrete global and local maximum principles. We report convergence results for the coupled scheme and an application of the scheme to the interpretation of limiting current measurements in an electrochemical flow cell.

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A high order discontinuous Galerkin method for the Boltzmann equation

Gerhard Kitzler¹ Joachim Schöberl²

The Boltzmann equation is a statistical model for gases. The density distribution function $f(t, x, v)$ describes the probability to find a particle at time t near the spatial position x and which has the velocity close to v . The time evolution of f is given by the Boltzmann equation. The collision of particles is formulated in terms of the collision operator $Q(f)$ which is local in x and t . We perform a Petrov-Galerkin method in the spatial domain Ω and velocity domain \mathbb{R}^3 . In the v domain the solution is expanded as a sum over multivariate Lagrange polynomials $l_j(x)$ times an appropriate gaussian peak. In space we discretize by a high order discontinuous Galerkin method with natural upwind fluxes.

Due to this expansion, the Boltzmann transport operator decouples when using Gauß-Hermite integration rules of appropriate order into transport operators for the individual components.

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A nonlinear LPS FEM for convection-diffusion-reaction equations

Petr Knobloch¹ Gabriel R. Barrenechea² Volker John³

This contribution is devoted to the numerical solution of convection-diffusion-reaction equations by means of the finite element method (FEM). It is well known that the standard Galerkin discretization is inappropriate if convection dominates diffusion since the approximate solution is usually globally polluted by large spurious oscillations. The usual way of treating dominating convection consists in adding extra terms to the Galerkin formulation, aimed at enhancing the stability of the approximate solution. Among such stabilized FEMs, the local projection stabilization (LPS) method has received some attention over the last decade. Originally proposed for the Stokes problem and extended to the Oseen equations, the LPS method has also been used recently to treat convection-diffusion equations.

We introduce an extension of the LPS FEM and analyze it both in the steady-state and transient settings. In addition to the standard LPS method, a nonlinear crosswind diffusion term is introduced, which accounts for the reduction of spurious oscillations. The time-dependent equation is discretized in time with an implicit one-step θ -scheme. We prove the existence of a solution and, depending on the choice of the stabilization parameter, also its uniqueness. To our best knowledge, this is the first nonlinear discretization for convection-diffusion-reaction equations for which both existence and uniqueness of a solution can be shown. Moreover, we derive error estimates which are supported by numerical studies. These studies demonstrate also a reduction of the spurious oscillations.

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Towards the direct and inverse adaptive mixed finite element formulations for nearly incompressible elasticity at large strains

Anke Bucher¹ Uwe-Jens Görke² Reiner Kreißig³

This contribution presents advanced numerical models for the solution of the direct and inverse problems of nearly incompressible hyperelastic processes at large strains. The discussed mixed finite element approach contributes to the numerical simulation of coupled multiphysics problems, including the calibration of appropriate material models (parameter identification). The presented constitutive approach is based on the multiplicative decomposition of the deformation gradient resulting in a two-field formulation with displacement components and hydrostatic pressure as primary variables. The ill-posed inverse problem of parameter identification analyzing inhomogeneous displacement fields is solved using deterministic trust-region optimization techniques. Within this context, a semi-analytical approach for sensitivity analysis represents an efficient and accurate method to determine the gradient of the objective function. The mixed boundary value problem is based on the spatial discretization of the weak formulations of the linear momentum balance and the incompressibility condition. Its linearization serves as basis for the solution of the direct problem, while the implicit differentiation of the weak formulations with respect to material parameters provides the necessary relations for the semi-analytical sensitivity analysis. Adaptive mesh refinement and mesh coarsening are realized controlled by a residual a posteriori error estimator. Efficiency and accuracy of the presented direct and inverse numerical techniques are demonstrated on a typical example.

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Fast domain decomposition solvers for discrete problems with chaotically subdomain wise variable orthotropism

Vadim Korneev¹ Michael Jung²

The second order elliptic equation is considered in the domain, composed of some shape and size irregular rectangles, which are nests of the orthogonal nonuniform decomposition mesh. The matrix of coefficients of the elliptic operator, written in the divergent form, is diagonal and its nonzero coefficients in each subdomain are arbitrary positive numbers. The orthogonal finite element mesh satisfies only one condition: it is uniform on each subdomain. No other conditions on the coefficients of the elliptic equation and on variable step sizes of the discretization and decomposition meshes are imposed. For the resulting discrete finite element problem, we present the DD (domain decomposition) preconditioner of the Dirichlet-Dirichlet type, in which d.o.f.'s at nodes of the decomposition mesh are split from others, and it is assumed that the contribution of the subproblem, related to these d.o.f.'s, to the computational cost of the DD solver is secondary. Essential components of DD preconditioner are the same as in the paper of Korneev, Poborchii & Salgado (2007). However, here we remove weak dependence of the relative condition number of the DD preconditioner on some measure of the local orthotropism of the discretization. We show that the DD solver has linear complexity, independently of the aspect ratios of the three types of orthotropism listed above. The result became possible due to the special way of the interface preconditioning by means of the inexact solver employing the preconditioner-multiplicator and the preconditioner-solver. The interface preconditioning makes also the main difference from other authors works on fast DD solvers for similar problems, *e.g.*, of Khoromskij & Wittum (1999,2004) and Kwak, Nepomnyaschikh & Pyo (2004).

Range of applications of the designed DD solver includes discretizations of a class of elliptic equations with non-matched deterioration of coefficients, a simple representative of which is $\mathcal{L}u \equiv y^2 \partial^2 u / \partial x^2 + x^2 \partial^2 u / \partial y^2$, $(x, y) \in \Omega = (0, 1) \times (0, 1)$, $u|_{\partial\Omega} = 0$. According to Korneev & Jensen (1997), the matrix of finite-difference analogue of \mathcal{L} on the uniform square grid of size h can be also used for efficient preconditioning of the internal stiffness matrix of the reference p -element. In DD solvers for such problems, the number of subdomains, maximal over subdomains edge ratios and aspect ratios of orthotropism grow at $h \rightarrow \infty$. We show that nevertheless the linear complexity of DD solver is retained. At that the independent block of the DD preconditioner, related to the nodes of the decomposition mesh, can be preconditioned by the diagonal matrix.

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Non-sequential optical field tracing

Michael Kuhn¹ Frank Wyrowski² Christian Hellmann³

Optical field tracing methods generalize ray tracing methods by considering harmonic fields instead of ray bundles. This allows the smooth combination of different modeling techniques in different subdomains of the system. Based on tearing and interconnecting ideas, the paper introduces the basic concepts of non-sequential field tracing and derives the corresponding operator equations and a solution formula for the simulation task. The evaluation requires the solution of local Maxwell problems (tearing) and the continuity of the solution across boundaries is achieved along with the convergence of the iterative procedure (interconnecting). The number of local problems to be solved is optimized by a newly introduced light path tree algorithm. Finally some examples for the selection of local Maxwell solvers and numerical results are presented.

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An iterative finite element method for boundary value problems in domains with geometric singularities: Computing the coefficients of the singularities

Boniface Nkemzi¹ Michael Jung²

Many problems in physics and engineering can be modeled mathematically using elliptic boundary value problems. Most of the time the physical domains associated with these problems are non-smooth, in the sense that they may entail corners, edges, cracks, conic vertices, etc. Physical experiments as well as mathematical analysis have shown that the gradient of the solutions (stress or flux) may become unbounded (singularity) in the vicinity of such geometric singularities and near points where there is a change in boundary conditions. Thus the lifespan of the physical system depends highly on its behavior near these geometric singularities.

Standard numerical schemes, for example, finite element, boundary element, finite difference methods, for computing the solution of the boundary value problems may severely lose accuracy when the solution entails singularities.

In this presentation we introduce a new iterative finite element method for accurate computation of the coefficients of the singularities and the solutions for boundary value problems for the Laplace operator in two-dimensional domains with corners and three-dimensional domains with edges. The results are illustrated with numerical examples.

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Procrack: A software for simulating three-dimensional fatigue crack growth

Frank Rabold¹

A finite element software for automated simulation of fatigue crack growth in arbitrarily loaded three-dimensional components is presented. The criterion, direction and amount of crack propagation are controlled by concepts of linear elastic fracture mechanics. The fracture mechanical parameters are calculated by means of a special submodelling technique in combination with the interaction integral technique. In the adaptive crack growth step, the updated crack front position is determined and the mesh in the crack region is automatically adapted. The preprocessing and main FEM-analysis of the cracked structure are done using the commercial software ABAQUS. Two application examples show the capability of the simulation program.

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Implementation of Schur-complement-preconditioners for the Stokes and Navier-Stokes Equations

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Finite Element discretisation of the Stokes or the linearised Navier-Stokes equations result in block structured systems of linear equations. For these various Schur-complement preconditioners have been proposed, yielding very good performance, see e.g. [1].

In this talk we discuss various implementation issues, which result from attempts to implement these block preconditioners using efficient inexact solution methods for the building blocks of the preconditioners. Especially in the Navier-Stokes setting, it is non-trivial to maintain good scaling as the Reynolds number increases.

Numerical examples demonstrating these issues will be given.

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Application of the reciprocity principle for the determination of planar cracks in piezoelectric material

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The functionality of piezoelectric devices can be strongly reduced by cracks. Due to the brittle material behaviour of piezoelectric ceramics, the question if cracks exist and of their position and size if existing, is of significant interest in engineer applications. We examine the question, how it is possible to test devices for inner cracks (not visible) in a nondestructive manner. We focus to the inverse method of measurements of boundary data under different loads like described by ANDRIEUX ET. AL. e.g. in [1] and [2]. This approach uses overdetermined information on boundary data to reconstruct inner geometry properties, especially cracks. We utilize a first generalization [3] of the approach in [1] to anisotropic elastic material. Some results of the reconstruction method are demonstrated by numerical experiments in 2D. Sensitivity studies show at the one hand that the reconstruction works well in principle in the case of a single straight crack, but also the limited scope by examining examples with perturbed data, different crack lengths and slightly nonplanar cracks.

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Multilevel preconditioners for temporal-difference learning methods related to recommendation engines

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In many areas of retail and especially e-business recommendation engines are applied to increase the usability of the store or portal. Advanced recommendation engines use approaches from control theory for adaptive learning. At the forefront of these algorithms reinforcement learning is applied which however requires large transaction numbers to converge. To overcome this problem, we propose a hierarchical approach of reinforcement learning for recommendation engines by combining a multilevel preconditioner with the temporal-difference learning method, the most important algorithm class of reinforcement learning. The multilevel preconditioner works on a combined hierarchy of states and actions. We describe the preconditioner, prove its convergence and present results on real-life data.

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Coupled FE-BE eigenvalue problems for fluid-structure interaction

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In this talk we present a coupled finite and boundary element eigenvalue problem formulation for the simulation of the vibro-acoustic behavior of elastic bodies submerged in unbounded fluid domains as submarines in the sea. Usually the fluid is assumed to be incompressible and hence modeled by the Laplace equation. In contrast, we do not neglect the compressibility of the fluid but model it by the Helmholtz equation. The resulting coupled eigenvalue problem for the fluid-structure interaction is then nonlinear since the frequency parameter appears nonlinearly in the boundary integral formulation of the Helmholtz equation. We analyze this eigenvalue problem and its discretization in the framework of eigenvalue problems for holomorphic Fredholm operator-valued functions. For the numerical solution of the discretized eigenvalue problem we use the contour integral method which reduces the algebraic nonlinear eigenvalue problem to a linear one. The method is based on a contour integral representation of the resolvent operator and it is suitable for the extraction of all eigenvalues which are enclosed by a given contour. The dimension of the resulting linear eigenvalue problem corresponds to the number of eigenvalues inside the contour. The main computational effort consists in the evaluation of the resolvent operator for the contour integral which requires the solution of several linear systems involving finite and boundary element matrices.

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Sensitivity analysis for Maxwell eigenvalue problems in industrial applications

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In this presentation we focus on the sensitivity analysis of Maxwell's eigenvalue problem, where the derivatives of the eigenvalues are calculated with respect to design parameters (i.e., material or geometrical parameters). Utilizing the adjoint approach the derivatives can be calculated at almost no additional cost. The challenge consists in the computation of the required derivatives (i.e., derivatives of bilinear forms with respect to the design parameters) from a higher order, curved finite element discretization. Numerical studies show the application for a real life electromagnetic filter application where the sensitivities of the eigenvalues give a better insight into the characteristics of the underlying filter. The benefit is apparent if the adjoint method is compared to a standard finite difference approach.

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