ENUMATH 2007

10. - 14.09.07
Graz, Austria

Final Program and Abstracts

INSTITUTE FOR MATHEMATICS AND SCIENTIFIC COMPUTING

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TU Graz
Graz University of Technology

In cooperation with:
Institute for Computational Mathematics
http://www.numerik.math.tu-graz.ac.at

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TU Graz

ENUMATH: Final Program and Abstracts

Welcome

The Organizing Committee is delighted to welcome you to the ENUMATH 2007 conference in Graz.

The ENUMATH conferences started in Paris in 1995 in order to provide a forum for discussion on recent aspects of numerical mathematics on the highest level of international expertise. Subsequent ENUMATH conferences were held at the universities of Heidelberg (1997), Jyvaskyla (1999), Ischia Porto (2001), Prague (2003) and Santiago de Compostela (2005).

Recent results and new trends in the analysis of numerical methods as well as their application to challenging scientific and industrial problems will be discussed. Apart from theoretical aspects, a major part of the conference will be devoted to numerical techniques for interdisciplinary applications.

With ten invited talks, nine minisymposia and fifty four sessions of contributed talks ENUMATH 07 assembles an impressive cross-section of numerical analysts. Enjoy the math and the city of Graz !

For the organizing committee, *Karl Kunisch*

Sponsors

Bundesministerium für Wissenschaft und Forschung

Gesellschaft für Angewandte Mathematik und Mechanik

Graz University of Technology

Land Steiermark

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University of Graz

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Sunday, September 9

16:00 - 18:00. *LS 15.03*
Registration

Under Construction:

This program is subject to change. Check the "Program Updates" posted on the bulletin board located in the registration area or check from 8:45-9:00 in HS 15.03.
Changes are posted daily.

Monday, September 10

8:00 - 16:00. *LS 15.03*
Registration

8:45 - 9:00. *HS 15.03*
Opening Remarks

9:00 - 10:00. *HS 15.03*
IP1 Imaging in Random Media
G.Papanicolaou, Stanford University,USA

10:00 - 10:30. *RESOWI Center*
Coffee Break

10:30 - 12:30. Concurrent Sessions.

MS1 Level-Set Methods, Hamilton-Jacobi Equations and Applications *HS 15.03*

MS2 Liquid Vapor Phase Transitions *HS 15.02*

CT1 Fluid-Structure Interaction. *HS 15.12*

CT2 Inverse Problems. *HS 15.01*

CT3 Discontinuous Galerkin. *HS 11.01*

CT4 Adaptive Methods. *HS 11.02*

CT5 Singular Perturbation. *LS 15.01*

12:30 - 14:00. Lunch Break

14:00 - 15:00. *HS 15.03*
IP2 Parametric Approximation of Geometric Evolution Equations
J. Barrett, Imperial College, UK

15:00 - 16:00. Concurrent Sessions.

CT7 Domain Decomposition. *HS 11.02*

CT8 Optimal Control with Applications *HS 15.03*

CT9 Discontinuous Galerkin. *HS 15.12*

CT10 Boundary Elements. *HS 15.02*

CT11 Adaptive Methods. *HS 15.01*

16:00 - 16:15. *RESOWI Center*
Coffee Break

16:15 - 18:15. Concurrent Sessions.

MS3 Model Reduction, POD. *HS 15.02*

MS4 Geometric PDEs. *HS 15.03*

CT12 Fluid-Structure Interaction *HS 15.12*

CT13 Inverse Problems. *HS 15.01*

CT14 Waves. *LS 15.01*

CT15 Discontinuous Galerkin. *HS 11.01*

CT16 Interface Problems and Free Boundary Problems. *HS 11.02*

Tuesday, September 11

8:00 - 16:00. *LS 15.03*
Registration

8:45 - 9:00. *HS 15.03*
Remarks/Changes

9:00 - 10:00. *HS 15.03*
IP3 Discontinuous Galerkin elements for Reissner-Mindlin plates
D. Marini, University of Pavia, Italy

10:00 - 10:30. *RESOWI Center*
Coffee Break

10:30 - 12:30. Concurrent Sessions.

MS5 Level-Set Methods, Hamilton-Jacobi Equations and Applications *HS 15.03*

MS6 Model Reduction, POD. *HS 15.02*

CT17 Navier-Stokes. *HS 11.01*

CT18 Inverse Problems. *HS 15.12*

CT19 Optimal Control with Applications *HS 15.01*

CT20 Multiscale Methods. *HS 15.01*

CT21 Numerical Methods in Finance. *LS 11.02*

12:30 - 14:00. Lunch Break

14:00 - 15:00. *HS 15.03*
IP4 Boundary and Finite Element Domain Decomposition Methods
U. Langer, University of Linz, Austria

15:00 - 15:15. *RESOWI Center*
Coffee Break

15:15 - 17:15. Concurrent Sessions.

MS7 Modelling in Medicine. *HS 15.02*

MS8 Inverse Problems. *HS 15.12*

MS9 Geometric PDEs. *HS 15.03*

CT22 Navier-Stokes. *HS 11.01*

CT23 Optimal Control with Applications *HS 15.01*

CT24 Multiscale Methods. *HS 11.02*

CT25 Convection-Diffusion Problems *LS 15.01*

17:15 - 17:30. *RESOWI Center*
Coffee Break

17:30 - 18:30 *HS 15.03*
PL1 Public Lecture
Mathematics in Facial Surgery Planning
P. Deuflhard, Zuse-Institut Berlin, Germany

19:00. *Old University*

Reception by the Governor of Styria

Wednesday, September 12

8:15 - 13:00. *LS 15.03*
Registration

8:45 - 9:00. *HS 15.03*
Remarks/Changes

8:30 - 9:30. *HS 15.03*
IP5 On the numerical solution of higher-dimensional partial differential equations
M. Griebel, University of Bonn, Germany

9:30 – 10:30. *HS 15.03*
IP6 Open boundary conditions for wave propagation problems on unbounded domains
A. Arnold, TU Wien, Austria

10:30 - 10:45. *RESOWI Center*
Coffee Break

10:45 - 12:45. Concurrent Sessions.
MS10 Fluid-Structure Interaction. *HS 15.02*
MS11 Modelling in Medicine. *HS 15.03*
MS12 Inverse Problems. *HS 15.12*
CT26 Navier-Stokes. *HS 11.01*
CT27 Hyperbolic Equations. *HS 15.01*
CT28 Domain Decomposition. *HS 11.02*
CT29 Interface Problems and Free Boundary Problems. *LS 15.01*

13:30 - 18:00. Excursion

Rein Monastery and
Guided Tour of the City of Graz

19:00. *Aula - University of Graz*

Reception by the Rector of the University of Graz and the Rector of the Technical University of Graz

Thursday, September 13

8:30 - 16:00. *LS 15.03*
Registration

8:45 - 9:00. *HS 15.03*
Remarks/Changes

9:00 - 10:00. *HS 15.03*
IP7 Transparent boundary conditions, wave propagation and periodic media
P. Joly, INRIA, France

10:00 - 10:30. *RESOWI Center*
Coffee Break

10:30 - 12:30. Concurrent Sessions.
MS13 Fluid-Structure Interaction. *HS 15.02*
MS14 Optimal Control with PDEs. *HS 15.12*
MS15 Fast Methods for Nonlocal Operators. *HS 15.03*
CT30 Hyperbolic Equations. *HS 11.01*
CT31 Nonlinear PDEs. *HS 11.02*
CT32 Domain Decomposition. *HS 15.01*
CT33 Electromagnetism. *LS 15.01*

12:30 - 14:00. Lunch Break

14:00 - 15:00. *HS 15.03*
IP8 Geometric Integration, in particular of Euler's Rigid Body Equation
G. Wanner, University of Geneva, Switzerland

15:00 - 16:00. Concurrent Sessions.
CT34 Numerical Linear Algebra. *LS 15.01*
CT35 Nonlinear PDEs. *HS 11.02*
CT36 Domain Decomposition. *HS 15.01*
CT37 Nonlinear Mechanics. *HS 15.12*
CT38 Hyperbolic Equations. *HS 11.01*
CT39 Optimal Control with Applications. *HS 15.02*
CT40 Navier-Stokes *HS 15.03*

16:00 - 16:15. *RESOWI Center*
Coffee Break

16:15 - 18:15. Concurrent Sessions.
MS16 Fluid-Structure Interaction. *HS 15.02*
MS17 Optimal Control with PDEs. *HS 15.03*
MS18 Fast Methods for Nonlocal Operators. *HS 15.12*
CT41 Nonlinear PDEs. *HS 11.02*
CT42 Numerical Linear Algebra. *HS 15.01*
CT43 hp-Finite Elements. *LS 15.01*
CT44 Electromagnetism. *HS 11.01*

Friday, September 14

8:00 - 14:30. *LS 15.03*
Registration

8:45 - 9:00. *HS 15.03*
Remarks/Changes

8:30 - 9:30. *HS 15.03*
IP9 Robust Interactive Methods for PDEs with Rough Coefficients
J. Xu, Pennsylvania State University, USA

9:30 - 10:30. *HS 15.03*
IP10 The worst scenario method: a red thread running through various approaches to problems with uncertain input data
J. Chleboun, Academy of Sciences, Czech Republic

10:30 - 10:45. *RESOWI Center*
Coffee Break

10:45 - 12:45. Concurrent Sessions.
MS19 Optimal Control with PDEs. *HS 15.03*
CT45 Navier-Stokes. *HS 15.02*
CT46 Convection-Diffusion Problems. *HS 15.12*
CT47 hp-Finite Elements. *HS 15.01*
CT48 ODEs and Fractional Step Methods. *HS 11.01*
CT49 Electromagnetism. *HS 11.02*
CT50 Modelling in Medicine. *LS 15.01*

12:45 - 13:00. *RESOWI Center*
Coffee Break

13:00 - 15:00. Concurrent Sessions.
CT53 Optimal Control with Applications. *HS 15.02*
CT54 Convection-Diffusion Problems. *HS 15.12*

Monday, September 10

Registration

8:00 - 16:00
Room: LS 15.03

Opening Remarks

8:45 - 9:00
Room: HS 15.03

Schedule

Time	Talk	Room
9:00 - 10:00	**IP1**	HS 15.03
10:00 - 10:30	**Coffee Break**	
10:30 - 12:30	**MS1** **MS2** **CT1** **CT2** **CT3** **CT4** **CT5**	HS 15.03 HS 15.02 HS 15.12 HS 15.01 HS 11.01 HS 11.02 LS 15.01
12:30 - 14:00	**Lunch**	
14:00 - 15:00	**IP2**	HS 15.03
15:00 - 16:00	**CT7** **CT8** **CT9** **CT10** **CT11**	HS 11.02 HS 15.03 HS 15.12 HS 15.02 HS 15.01
16:00 - 16:15	**Coffee Break**	
16:15 - 18:15	**MS3** **MS4** **CT12** **CT13** **CT14** **CT15** **CT16**	HS 15.02 HS 15.03 HS 15.12 HS 15.01 LS 15.01 HS 11.01 HS 11.02

Monday, Sept. 10

IP1

Imaging in Random Media

9:00 - 10:00
Room: HS 15.03

I will present an overview of some recently developed methods for imaging with array and distributed sensors when the environment between the objects to be imaged and the sensors is complex and only partially known to the imager. This requires modeling and analysis in random media, and the use of statistical algorithms which increase the overall computational complexity. Imaging is done by backpropagating local correlations rather than traces (interferometry). I will illustrate the theory with applications from nondestructive testing and from other areas.

George Papanicolaou
Stanford University, USA

Monday, Sept. 10

IP2

Parametric Approximation of Geometric Evolution Equations

14:00 – 15:00
Room: HS 15.03

Geometric flows, in which hypersurfaces move such that an energy, involving surface and bending terms, decreases appear in many situations in the natural sciences and in geometry. Classic examples are mean curvature, surface diffusion and Willmore flows. Computational methods to approximate such flows are based on one of three approaches (i) parametric methods, (ii) phase field methods or (iii) level set methods. The first tracks the hypersurface, whilst the other two implicitly capture the hypersurface. A key problem with the first approach, apart from the fact that it is does not naturally deal with changes of topology, is that in many cases the mesh has to be redistributed after every few time steps to avoid coalescence of mesh points.
In this talk we present a new variational formulation of the parametric approach, which leads to an unconditionally stable, fully discrete finite element approximation. In addition, the scheme has very good properties with respect to the distribution of mesh points, and if applicable volume conservation. We illustrate this for (anisotropic) mean curvature and (anisotropic) surface diffusion flows of closed curves in $\mathbb{R}^2$. We extend these flows to curve networks in $\mathbb{R}^2$. Here the triple junction conditions, that have to hold where three curves meet at a point, are naturally approximated in the discretization of our variational formulation. Moreover, we extend this approximation to flows on closed hypersurfaces in $\mathbb{R}^3$.

John Barrett
Imperial College, UK

Monday, Sept. 10

MS1

Level-set Methods, Hamilton-Jacobi Equations and Applications I

10:30 – 12:30
Room: HS 15.03

The goal of this Minisymposium is to present some recent advances in this field and to show how they can be effective in several fields of application including image processing, granular materials, dislocation dynamics, homogenization and shape optimization.

Organizer:
M. Falcone

10:30 - 10:55
Fast Marching Semi-Lagrangian Methods for Hamilton-Jacobi Equations
Maurizio Falcone, Dipartimento di Matematica SAPIENZA - Universita' di Roma, Italy

11:00 - 11:25
Discretization of Hamilton-Jacobi Equations on Unstructured Triangulations
Folkmar Bornemann, Technische Universität München, Germany

11:30 - 11:55
Recent Advances on Large Time-Step Schemes for Degenerate Second-Order Equations and Mean Curvature Motion
Roberto Ferretti, Dipartimento di Matematica, Universitá di Roma Tre, Italy

12:00 - 12:25
A Generalized Fast Marching Method Applied to Dislocations Dynamics
Elisabetta Carlini, Dipartimento di Matematica, Università di Roma, "La Sapienza", Italy/Ph. Hoch

Monday, Sept. 10

MS2

Liquid Vapor Phase Transitions

10:30 – 12:30
Room: HS 15.02

An important issue of this minisymposium concerns the simultaneous treatment of phase transition and compressible flows. Up to now the dynamics of pure phase transition as well as the dynamics of compressible flows have been studied very extensively but seperately.

Organizer:
R. Abgrall
D. Kroener

10:30 - 10:55
The Ghostfluid Method as a Multi-Scale Method for Compressible Flow with Phase Transitions
Christian Rohde, Universität Stuttgart, Germany

11:00 - 11:25
Higher Order Methods for Simulation of Liquid-Vapor Flows with Phase Change
Dennis Diehl, University of Freiburg, Germany

11:30 - 11:55
Ghostfluid Methods for Computation of Interface Flows
Boniface Nkonga, Université Bordeaux, France

12:00 - 12:25
Numerical Simulation of Cavitation Bubbles by Compressible Two-Phase Fluids
Siegfried Müller, RWTH Aachen, Germany

Monday, Sept. 10

MS3

Geometric PDEs I

16:15 – 18:15
Room: HS 15.02

In this minisymposium computational techniques ranging from tailored finite element approaches to multiscale methods for problems on general surfaces are addressed. Additional aspects comprise global parametrizations and error analysis for curve evolution.

Organizer:
G. Dziuk,
C. Eliott

16:15 - 16:40
Computational Methods for Surface PDEs
Charlie Elliott, University of Sussex, United Kingdom

16:45 - 17:10
Computational Willmore Flow
Gerhard Dziuk, University of Freiburg, Germany

17:15 - 17:40
Multigrid methods for the discretized Laplace-Beltrami operator on arbitrary surfaces
Ralf Kornhuber, Freie Universität Berlin, Germany

17:45 - 18:10
Gloabal Parametrization of Surface Meshes
Konrad Polthier, Freie Universität Berlin, Germany

Monday, Sept. 10

MS4

Model Reduction POD I

16:15 – 18:15
Room: HS 15.03

The minisymposium addresses recent aspects in model reduction and pod. While some talks focus on passivity or strucutre preserving reduction techniques, applications in parameter id, optimal control and mathematical finance are highlighted as well.

Organizer:
P. Benner
D.C. Sorensen

16:15 - 16:40
Passivity Preserving Model Reduction
Dan Sorensen, Rice University, USA

16:45 - 17:10
Structure-Preserving Model Reduction for Resonant MEMS
David Bindel, New York University, USA

17:15 - 17:40
MOR for coupled simulations of RF systems
Wil Schilders, NXP Semiconductors, Netherlands

17:45 - 18:10
Structured perturbation theory for inexact Krylov projection methods in model reduction
Serkan Gugercin, Virginia Tech., USA

Monday, Sept. 10

CT1

Fluid-Structure Interaction

10:30 – 12:30
Room: HS 15.12

10:30 - 10:55
Splitting methods based on algebraic factorization for fluid-structure interaction
Annalisa Quaini, Ecole Polytechnique Fédérale de Lausanne, Switzerland

11:00 - 11:25
An unsteady compressible flow with very low Mach number
Petra Punčochářová, Czech Technical University in Prague, Czech Republic

11:30 - 11:55
Numerical simulations of flow induced vibrations of a profile
Radek Honzátko, Czech Technical University in Prague, Czech Republic

12:00 - 12:25
Transparent boundary conditions for elastodynamics in a VTI medium layer
Ivan L. Sofronov, Russian Academy of Sciences, Russia

Monday, Sept. 10

CT2

Inverse Problems

10:30 – 12:30
Room: HS 15.01

10:30 - 10:55
Linearized quasi inversion of seismic wave field on the base of Guassian beams decomposition
Vladimir A. Tcheverda, Novosibirsk Scientific Centre of SB RAS, Russia

11:00 - 11:25
Topological derivatives for non–homogeneous inverse problems
Maria-Luisa Rapún, Universidad Politécnica de Madrid, Spain

11:30 - 11:55
Shape optimization approach for image segmentation: Level set Formulation based on Galerkin strategy
Louis Blanchard, INRIA, France

12:00 - 12:25
An asymptotic factorization method for inverse electromagnetic scattering in a layered medium
Roland Griesmaier, Johannes Gutenberg-Universität Mainz, Germany

Monday, Sept. 10

CT3

Discontinuous Galerkin

10:30 – 12:30
Room: HS 11.01

10:30 - 10:55
Optimal error estimates in the DGFEM for nonlinear convection-diffusion problems
Miloslav Feistauer, Charles University in Prague, Czech Republic

11:00 - 11:25
***hp*-IIPG method for convection-diffusion problems: analysis and applications to fluid dynamics**
Vit Dolejší, Charles University in Prague, Czech Republic

11:30 - 11:55
Discontinuous Galerkin Method for the Numerical Solution of Inviscid and Viscous Compressible Flow
Václav Kučera, Charles University in Prague, Czech Republic

12:00 - 12:25
Is stabilization necessary for the symmetric discontinuous Galerkin method for second order elliptic problems?
Benjamin Stamm, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Monday, Sept. 10

CT4

Adaptive Methods

10:30 – 12:30
Room: HS 11.02

10:30 - 10:55
A posteriori error analysis for Kirchhoff plate elements
Jarkko Niiranen, Helsinki University of Technology, Finland

11:00 - 11:25
With discrete adjoint based optimisation towards anisotropic adaptive FEM
René Schneider, Technische Universität Chemnitz, Germany

11:30 - 11:55
Adaptive hierarchical model reduction for elliptic problems
Simona Perotto, Ecole Nationale des Ponts et Chaussées, France

12:00 - 12:25
hp-**FEM with Arbitrary Level Hanging Nodes in 3D**
Pavel Kůs, University of Texas at El Paso, USA

Monday, Sept. 10

CT5

Singular Perturbation

10:30 – 12:30
Room: LS 15.01

10:30 - 10:55
Stabilization methods for convection- diffusion problems on layer adapted meshes
Hans-G. Roos, Technische Universität Dresden, Germany

11:00 - 11:25
Superconvergence analysis of a finite element method on Shishkin mesh for two–parameter singularly perturbed problems
Helena Zarin, University of Novi Sad, Serbia

11:30 - 11:55
A finite difference method on layer-adapted meshes for an elliptic system in two dimensions
Torsten Linß, Technische Univeristät Dresden, Germany

12:00 - 12:25
A Convenient and Economical Error Control Device for Singularly Perturbed Systems
Nabendra Parumasur, University of KwaZulu-Natal, South Africa

Monday, Sept. 10

CT7

Domain Decomposition

15:00 – 16:00
Room: HS 11.02

15:00 - 15:25
Steklov–Poincare operators and domain decomposition for linear exterior boundary problems
Mauricio Barrientos, Pontificia Universidad Catolica de Valparaiso, Chile

15:30 - 15:55
BETI-DP methods for potential equations in unbounded domains
Clemens Pechstein, Universität Linz, Austria

Monday, Sept. 10

CT8

Optimal Control with Applications

15:00 – 16:00
Room: HS 15.03

15:00 - 15:25
A priori error analysis for the finite element approximation of elliptic Dirichlet boundary control problems
Rolf Rannacher, Ruprecht-Karls-Universität Heidelberg, Germany

15:30 - 15:55
An L-BFGS Method in H^1 for optimal control of a quantum system
Greg von Winckel, Karl-Franzens-Universität Graz, Austria

Monday, Sept. 10

CT9

Discontinuous Galerkin

15:00 – 16:00
Room: HS 11.01

15:00 - 15:25
A posteriori error estimates based on flux reconstruction for Discontinuous Galerkin method
Alexandre Ern, CERMICS, France

15:30 - 15:55
DGFEM for the compressible Navier-Stokes equations
Jiří Hozman, Charles University in Prague, Czech Republic

Monday, Sept. 10

CT10

Boundary Elements

15:00 – 16:00
Room: HS 15.02

15:00 - 15:25
Boundary Element Methods for the Helmholtz equation
Sarah Engleder, Technische Universität Graz, Austria

15:30 - 15:55
Boundary element methods for eigenvalue problems
Gerhard Unger, Technische Universität Graz, Austria

Monday, Sept. 10

CT11

Adaptive Methods

15:00 – 16:00
Room: HS 11.02

15:00 - 15:25
Adaptive methods for the solution of the Stokes equations by the finite element method
Martin Stiller, Charles University Prague, Czech Republic

15:30 - 15:55
Functional a posteriori error estimates for Nitsche type mortaring on non-matching grids
Satyendra K. Tomar, Austrian Academy of Sciences, Austria

Monday, Sept. 10

CT12

Fluid-Structure Interaction

16:15 – 18:15
Room: HS 15.12

16:15 - 16:40
A semi-implicit algorithm based on the Augmented Lagrangian Method for fluid-structure interaction
Cornel Murea, Université de Haute-Alsace, France

16:45 - 17:10
Numerical solution of transonic and supersonic 2D and 3D fluid–elastic structure interaction problems
Jiří Dobeš, Czech Technical University in Prague, Czech Republic

17:15 - 17:40
Numerical method for unsteady incompressible MHD boundary layer on porous surface in great accelerating fluid flow
Decan Ivanovic, University of Montenegro, Montenegro

Monday, Sept. 10

CT13

Inverse Problems

16:15 – 18:15
Room: HS 15.01

16:15 - 16:40
An inverse problem of electromagnetic shaping of liquid metals
Jean R. Roche, Université Henri Poincaré Nancy 1, France

16:45 - 17:10
Determining the threshold of compression in the wavelet transform with orthonormal wavelets
Zlatko Udovičić, University of Sarajevo, Bosnia and Herzegovina

17:15 - 17:40
Variational Formulation for Euler flow equation
Jean-Paul Zolésio, INRIA, France

Monday, Sept. 10

CT14

Waves

16:15 – 18:15
Room: LS 15.01

16:15 - 16:40
The method of freezing waves in nonlinear time-dependent PDE's
Wolf-Jürgen Beyn, Universität Bielefeld, Germany

16:45 - 17:10
Finite-Difference Modeling of Sonic Log in 3D Viscoelastic Media
Galina V. Reshetova, Novosibirsk Scientific Centre of SB RAS, Russia

17:15 - 17:40
A multigrid algorithm for the acoustic single layer equation
Nilima Nigam, McGill University, Canada

17:45 - 18:10
Numerical simulation of seismic and acousto-gravity waves in a heterogeneous Earth-Atmosphere model
Galina V. Reshetova, Novosibirsk Scientific Centre of SB RAS, Russia

Monday, Sept. 10

CT15

Discontinuous Galerkin

16:15 – 18:15
Room: HS 11.01

16:15 - 16:40
Numerical Integration in the Discontinuous Galerkin Method for Nonlinear Convection-Diffusion Problem in 3D
Veronika Sobotíková, Czech Technical University in Prague, Czech Republic

16:45 - 17:10
Discontinuous Galerkin methods based on weighted interior penalties
Paolo Zunino, Politecnico di Milano, Italy

17:15 - 17:40
A posteriori error analysis of an augmented discontinuous formulation for Darcy flow
Rommel Bustinza, Universidad de Concepción', Chile

Monday, Sept. 10

CT16

Interface Problems and Free Boundary Problems

16:15 – 18:15
Room: HS 11.02

16:15 - 16:40
Exploring mixing dynamics inside microdroplets with a Level Set method
Paul Vigneaux, Université Bordeaux, France

16:45 - 17:10
Adaptive finite element simulation of relaxed models for liquid-solid phase transition
Marcus Stiemer, Universität Dortmund, Germany

17:15 - 17:40
Adaptive Multigrid Methods for Anisotropic Allen-Cahn Equations
Uli Sack, Freie Universität Berlin, Germany

17:45 - 18:10
A free-boundary problem modelling crystal dissolution and precipitation in porous media
Tycho van Noorden, Technische Universität Eindhoven, Netherlands

Tuesday, September 11

Registration
8:00 - 16:00
Room: LS 15.03

Remarks/Changes
8:45 - 9:00
Room: HS 15.03

Reception by the Governor of Styria
19:00
Location: Old University

Schedule

Time	Talk	Room
9:00 - 10:00	**IP3**	HS 15.03
10:00 - 10:30	**Coffee Break**	
10:30 - 12:30	**MS5** **MS6** **CT17** **CT18** **CT19** **CT20** **CT21**	HS 15.03 HS 15.02 HS 11.01 HS 15.12 HS 15.01 LS 15.01 HS 11.02
12:30 - 14:00	**Lunch**	
14:00 - 15:00	**IP4**	HS 15.03
15:00 - 15:15	**Coffee Break**	
15:15 - 17:15	**MS7** **MS8** **MS9** **CT22** **CT23** **CT24** **CT25**	HS 15.02 HS 15.12 HS 15.03 HS 11.01 HS 15.01 HS 11.02 LS 15.01
17:15 - 17:30	**Coffee Break**	
17:30 - 18:30	**PL1**	HS 15.03

Tuesday, Sept. 11

IP3

Discontinuous Galerkin elements for Reissner-Mindlin plates

9:00 - 10:00
Room: HS 15.03

In a recent paper of Arnold, Brezzi, and Marini, the ideas of discontinuous Galerkin methods were used to obtain and analyze two new families of locking free finite element methods for the approximation of the Reissner-Mindlin plate problem. By following their basic approach, but making different choices of finite element spaces, we develop and analyze other families of locking-free finite elements that eliminate the need for the introduction of a reduction operator, which has been a certain feature of many locking-free methods. For $k \geq 1$, all the methods use piecewise polynomials of degree $k+1$ to approximate the transverse displacement and piecewise polynomials of degree k (or possibly subsets) to approximate both the rotation and shear stress vectors. The approximation spaces for the rotation and the shear stress are always identical. The methods vary in the amount of inter-element continuity required. In terms of smallest number of degrees of freedom, the simplest method approximates the transverse displacement with continuous, piecewise quadratics and both the rotation and shear stress with rotated linear Brezzi-Douglas-Marini elements.

Donatella Marini
University of Pavia, Italy

Tuesday, Sept. 11

IP4

Boundary and Finite Element Domain Decomposition Methods

14:00 - 15:00
Room: HS 15.03

Domain Decomposition (DD) methods are nowadays not only used for constructing highly efficient parallel solvers for Partial Differential Equations but also for coupling different physical fields, different meshes and different discretization techniques. Since Finite Element Methods and Boundary Element Methods exhibit certain complementary properties, it is sometimes very useful to couple these discretization techniques. The efficient solution of large scale systems of finite, boundary and coupled finite and boundary element DD equations is the main topic of this talk.
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For full abstract, see Abstracts Section.

Ulrich Langer
Johannes Kepler Universität Linz, Austria

Tuesday, Sept. 11

PL1

Mathematics in Facial Surgery Planning

17:30 - 18:30
Room: HS 15.03

Since 1999, the CAS group at ZIB (CAS: computer assisted surgery) has been working on operation planning for cranio-maxillofacial surgery in close cooperation with clinical surgeons, in the beginning with Zeilhofer and Sader (then TU Munich, now U Basel and U Frankfurt, respectively), today with a whole bunch of further clinics. Within the integrated software environment AMIRA the group has realized
(a) the construction of 3D virtual patients from real patients out of detailed medical imaging data (stacks of CT or MRT files), which involves the efficient generation of 3D tetrahedral grids (only few details to be given in the talk);
(b) off-line operation planning tools to be used within clinics or within teleconferences between clinics and ZIB, which involve a huge amount of software engineering (details to be skipped);
(c) preoperative prediction of the postoperative facial appearance of patients, which involves the fast numerical solution of partial differential equations for (geometrically and materially nonlinear) elasticity by an affine conjugate adaptive multilevel Newton-CCG method.
The talk will include detailed clinically relevant results for individual patients that have been operated on the basis of our plannings.

Peter Deuflhard
Zuse-Institut Berlin, Germany

Tuesday, Sept. 10

MS5

Level-set Methods, Hamilton Jacobi Equations and Applications II

10:30 – 12:30
Room: HS 15.03

The goal of this Minisymposium is to present some recent advances in this field and to show how they can be effective in several fields of application including image processing, granular materials, dislocation dynamics, homogenization and shape optimization.

Organizer:
M. Falcone

10:30 - 10:55
Finite volume level set methods for moving curves and surfaces
Karol Mikula, Slovak University of Technology in Bratislava, Slovakia

11:00 - 11:25
A dynamical versus a variational approach for the computation of the effective Hamiltonian
Marco Rorro, Universitàdi Roma "La Sapienza", Italy

11:30 - 11:55
A shape and topology optimization technique for the solution of obstacle problems
Michael Hintermüller, Karl-Franzens-Universität Graz, Austria

12:00 - 12:25
On the partially open table problem for sandpiles
Stefano Finzi Vita, Universitàdi Roma "La Sapienza", Italy

Tuesday, Sept. 10

MS6

Model Reduction-POD II

10:30 – 12:30
Room: HS 15.02

The minisymposium addresses recent aspects in model reduction and pod. While some talks focus on passivity or strucutre preserving reduction techniques, applications in parameter id, optimal control and mathematical finance are highlighted as well.

Organizer:
P. Benner
D.C. Sorensen

10:30 - 10:55
Balancing-related model reduction for parabolic control systems
Peter Benner, TU Chemnitz, Germany

11:00 - 11:25
POD Model Reduction: Parameter Estimation for nonlinear elliptic sytems and a-posteriori error estimates
Stefan Volkwein, Karl-Franzens-Universität Graz, Austria

11:30 - 11:55
Applications of Reduced Order Models in Finance
Ekkehard W. Sachs, Virginia Tech, USA

12:00 - 12:25
Reducing a Rational Eigenproblemn in Fluid-Structure Interaction by AMLS
Heinrich Voß, TU Hamburg-Harburg, Germany

Tuesday, Sept. 10

MS7

Geometric PDEs II

15:15 – 17:15
Room: HS 15.02

In this minisymposium computational techniques ranging from tailored finite element approaches to multiscale methods for problems on general surfaces are addressed. Additional aspects comprise global parametrizations and error analysis for curve evolution.

Organizer:
G. Dziuk
C. Elliott

15:15 - 15:40
ESFEM for DIGM
Vanessa Styles, University of Sussex, UK

15:45 - 16:10
Stable Finite Elements for Unfitted Meshes
Claus-Justus Heine, Albert-Ludwigs-Universität Freiburg, Germany

16:15 - 16:40
Error Analysis of a Semidiscrete Numerical Scheme for the Evolution of Elastic Curves
Klaus Deckelnick, Otto-von-Guericke-Universität Magdeburg, Germany

Tuesday, Sept. 11

MS8

Inverse Problems I

15:15 – 17:15
Room: HS 15.12

In this minisymposium lectures are presented on recent trends from various areas in the field of regularization theory for ill-posed problems.

Organizer:
A. Neubauer
O. Scherzer

15:15 - 15:40
Taut String Algorithm for High Dimensional Data
Otmar Scherzer, University of Innsbruck, Austria

15:45 - 16:10
Solution of Ill-Posed Problems via Adaptive Grid Regularization
Andreas Neubauer, Johannes Kepler Universität Linz, Austria

16:15 - 16:40
Regularization by Fractional Filter Methods and Data Smoothing
Ester Klann, Austrian Academy of Sciences, Austria

16:45 - 17:10
A multilevel regularization method for nonlinear problems with applications in hysteresis and crack identification
Barbara Kaltenbacher, Universität Stuttgart, Germany

Tuesday, Sept. 11

MS9

Modelling in Medicine I

15:15 – 17:15
Room: HS 15.03

Modelling in life sciences is a challenging task. On one hand the underlying models are komplex and typically highly nonlinear, on the other hand multiscale aspects are of importance. This minisymposium addresses recent aspects in tumor growth modelling, medical imaging as well as cancer treatment, e.g., by hyperthermia or radiation.

Organizer:
H.O. Peitgen

15:15 - 15:40
TBA
Peitgen

15:45 - 16:10
Nonparametric Deconvolution Approaches for Dynamic Contrast Enhanced Magnetic Resonance Imaging and a Proposed Theory of Tracer Transport
Stephen Keeling, Karl-Franzens-Universität Graz, Austria

16:15 - 16:45
Mathematical models and numerical simulation of drug release from stents
Paolo Zunino, MOX-Politecnico di Milano, Italy

16:45 - 17:15
Multiscale modelling of tumour growth, angiogenesis and blood flow
Markus R. Owen, University of Nottingham, UK

Tuesday, Sept. 11

CT17

Navier-Stokes

10:30 – 12:30
Room: HS 11.01

10:30 - 10:55
Functional a posteriori error estimates for viscous flow problems
Sergei Repin, V. A. Steklov Institute of Mathematics in St. Petersburg, Russia

11:00 - 11:25
Stability of Finite-Difference scheme for Stokes problem
E. Muravleva, M.V. Lomonosov Moscow State University, Russia

11:30 - 11:55
Numerical simulations of incompressible laminar flow for Newtonian and non-Newtonian fluids
Radka Keslerová, Czech Technical University in Prague, Czech Republic

Tuesday, Sept. 11

CT18

Inverse Problems

10:30 – 12:30
Room: HS 15.12

10:30 - 10:55
Inversion–based trajectory planning for the temperature distribution in a parallelepipedon
Thomas Meurer, Technische Universität Wien, Austria

11:00 - 11:25
A numerical treatment of an inverse problem to nonlinear strongly degenerate parabolic equations
Anibal Coronel, Universidad del Bío-Bío, Chile

11:30 - 11:55
Determination of a piecewise constant conductivity using boundary integral equations with application to EEG
Céline Hollandts, UTC/LMAC, France

12:00 - 12:25
Inverse Problems of Econometrics
Yuri Menshikov, Dnepropetrovsky University, Ukraine

Tuesday, Sept. 11

CT19

Optimal Control with Applications

10:30 – 12:30
Room: HS 15.01

10:30 - 10:55
Nonsmooth Newton Method for Set-Valued Saddle Point Problems
Carsten Gräser, Freie Universität Berlin, Germany

11:00 - 11:25
Regularized Hyperbolic Problems for Optimal Nodal Control of Gas Networks
Nils Bräutigam, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

11:30 - 11:55
Approximate reduced SQP methods for model-based optimization
Volker H. Schulz, Universität Trier, Germany

12:00 - 12:25
Sensitivity Analysis of Optimal Load Changes for a Fuel Cell PDAE Model
Kurt Chudej, Uiversität Bayreuth, Germany

Tuesday, Sept. 11

CT20

Multiscale Methods

10:30 – 12:30 pm
Room: LS 15.01

10:30 - 10:55
Modelling the Electrostatic Workpiece Charging during Electron Beam Lithography
Benjamin Alles, Technischen Universität München, Germany

11:00 - 11:25
Stabilized FEM for incompressible flows: Equal-order vs. inf-sup stable approximation
Gert Lube, Georg-August-Universität Göttingen, Germany

11:30 - 11:55
Local time stepping for implicit-explicit methods on the time varying grids
Marie Postel, CNRS et Université Pierre et Marie Curie, France

12:00 - 12:25
The Composite Mini Element - Coarse grid computation of Stokes flows on complicated domains
Daniel Peterseim, Universität Zürich, Switzerland

Tuesday, Sept. 11

CT21

Numerical Methods in Finance

10:30 – 12:30
Room: HS 11.02

10:30 - 10:55
Calibration of Interest Rate Volatility as a High-Dimensional PDE Problem
Christoph Reisinger, University of Oxford, United Kingdom

11:00 - 11:25
Multiscale analysis of jump processes in finance – sparse tensor product based wavelet compression
Nils Reich, ETH Zürich, Switzerland

11:30 - 11:55
Fast pricing techniques for Multi-Asset Options
Coenraad C.W. Leentvaar, Delft University of Technology, Netherlands

12:00 - 12:25
Optimal Portfolio Allocation with Quasi-Monte Carlo Methods
Mario Rometsch, Universität Ulm, Germany

Tuesday, Sept. 11

CT22

Navier-Stokes

15:15 – 17:15
Room: HS 11.01

15:15 - 15:40
Non-conforming finite elements of arbitrary order for the Stokes problem on anisotropic meshes
Thomas Apel, Universität der Bundeswehr München, Germany

15:45 - 16:10
Convergent discretizations of a Navier-Stokes-Nernst-Planck-Poisson szstem
Markus Schmuck, Universität Tübingen, Germany

16:15 - 16:40
A unified convergence analysis of local projection stabilisations applied to the Oseen problem
Gunar Matthies, Ruhr-Universität Bochum, Germany

16:45 - 17:10
Benchmark proposal for incompressible two-phase flows
Stefan Turek, Universität Dortmund, Germany

Tuesday, Sept. 11

CT23

Optimal Control with Applications

15:15 – 17:15
Room: HS 15.01

15:15 - 15:40
Fishways design: An application of optimal control theory
Miguel A. Vilar, Universidade de Santiago de Compostela, Spain

15:45 - 16:10
An Optimal Control Problem in Adoptive Cellular Immunotherapy
Gabriel Dimitriu, University of Medicine and Pharmacy Gr. T. Popa Iaşi, Romania

16:15 - 16:40
Augmented Lagrangians for Optimal Control and Topology Optimization
Dalibor Lukáš, VŠB–Technical University of Ostrava, Czech Republic

16:45 - 17:10
Discrete Gradient Flows for a Shape Optimization Problem
Marco Verani, Politecnico di Milano, Italy

Tuesday, Sept. 11

CT24

Multiscale Methods

15:15 – 17:15
Room: HS 11.02

15:15 - 15:40
A Multiscale Method for Earth Structure Determination from Normal Mode Splitting
Paula Kammann, Technische Universität Kaiserslautern, Germany

15:45 - 16:10
Multilevel Solutions of Stochastic Wick-type Heat Equations
Mohammed Seaïd, Techni sche Universität Kaiserslautern, Germany

16:15 - 16:40
Fast Approximation on the 2-Sphere by Optimally Localizing Approximate Identities
Michel Volker, Technische Universität Kaiserslautern, Germany

16:45 - 17:10
A wavelet-based dynamically adaptive scheme for viscous Burgers equation
Václav Finěk, Technical University of Liberec, Czech Republic

Tuesday, Sept. 11

CT25

Convection-Diffusion Problems

15:15 – 17:15
Room: LS 15.01

15:15 - 15:40
PSI Solution of Convection-Diffusion equation with data in L^1
Macarena Gómez Mármol, Universidad de Sevilla, Spain

15:45 - 16:10
Anisotropic space-time adaption for advection-diffusion problems
Stefano Micheletti, Politecnico di Milano, Italy

16:15 - 16:40
Analysis of an Euler implicit-mixed finite element scheme for reactive transport in porous media
Florin Adrian Radu, Max Planck Institute for Mathematics in the Sciences, Germany

16:45 - 17:10
A comparative study of mixed finite element and multipoint flux approximations of flows in porous media
Markus Bause, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Wednesday, September 12

Registration
8:15 - 13:00
Room: LS 15.03

Remarks/Changes
8:45 - 9:00
Room: HS 15.03

Reception by the Rector of the University of Graz and the Rector of the Technical University of Graz
19:00
Location: Aula - University of Graz

Schedule

Time	Talk	Room
8:30 - 9:30	**IP5**	HS 15.03
9:30 - 10:30	**IP6**	HS 15.03
10:30 - 10:45	**Coffee Break**	
10:45 - 12:45	**MS10** **MS11** **MS12** **CT26** **CT27** **CT28** **CT29**	HS 15.02 HS 15.03 HS 15.12 HS 11.01 HS 15.01 HS 11.02 LS 15.01

Wednesday, Sept. 12

IP5

On the numerical solution of higher-dimensional partial differential equations
8:30 - 9:30
Room: HS 15.03

The approximate solution of higher-dimensional partial differential equations by conventional discretization methods is in general impossible due to the so-called curse of dimensionality, i.e. the numberof degress of freedoms of a conventional discretization is of the order $O(N^d)$, where d denotes the dimension of the problem and N is the amount of degrees of freedom in one coordinate direction. We discuss under what circumstances the curse of dimensionality can be overcome, present related discretization techniques and approximation methods and give applications like the Fokker-Planck equation, the Schrödinger equation and various problems from finance.

Michael Griebel
Universität Bonn, Germany

Wednesday, Sept. 12

IP6

Open boundary conditions for wave propagation problems on unbounded domains
9:30 – 10:30
Room: HS 15.03

Whole space problems for partial differential equations appear naturally in wave propagation problems of acoustics, quantum mechanics, and fluid dynamics, e.g. For the numerical solution of such problems, the computational domain must be limited to a finite region by introducing (artificial) absorbing boundary conditions (ABCs). An appropriate ABC must lead to a well-posed (initial-) boundary value problem, yield a good approximation to the solution of the whole space problem, and allow for an efficient numerical implementation. If the ABC yields –on the truncated domain– exactly the whole space solution, it is referred to as transparent boundary condition (TBC). In this talk we shall review some recent developments in this field and focus on the following topics:

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For full abstract, see Abstracts Section.

Anton Arnold
Technische Universität Wien, Austria

Wednesday, Sept. 12

MS10

Fluid Structure Interaction I

10:45 – 12:45
Room: HS 15.02

Recent computational approaches to fluid-strucutre interaction are presented. Concerning applications, among others aeroelastic problems will be addressed.

Organizer:
J. Ballmann
S. Turek

10:45 - 11:10
Benchmarking for FSI
Josef Ballmann, RWTH Aachen, Germany
Stefan Turek, Universität Dortmund, Germany

11:15 - 11:40
About coupling issues in steady/unsteady numerical aeroelastic analyses of aircraft configurations
Lars Reimer, RWTH Aachen, Germany

11:45 - 12:10
A FEM/multigrid solver for monolithic ALE formulation of fluid-structure interaction problem
Jaroslav Hron, Charles University in Prague, Czech Republic

12:15 - 12:40
Fluid-structure interaction: ALE versus full Eulerian Formulation
Thomas Dunne, Universität Heidelberg, Germany

Wednesday, Sept. 12

MS11

Inverse Problems II

10:45 – 12:45
Room: HS 15.03

In this minisymposium lectures are presented on recent trends from various areas in the field of regularization theory for ill-posed problems.

Organizer:
A. Neubauer
O. Scherzer

10:45 - 11:10
Nonlinear Tube Methods
Markus Grasmair, Leopold Franzens Universtät Innsbruck, Austria

11:15 - 11:40
Inverse Jumps - From Asymptotics to Applications
Axel Munk, Georg-August Universität Göttingen, Germany

11:45 - 12:10
Generalized Rigid Image Registration and Interpolation by Optical Flow using Contrast Invariant Intensity Scaling
Stephen Keeling, Karl-Franzens-Universität Graz, Austria

12:15 - 12:40
Total Variation and Curves
Arne Kovac, University of Bristol, UK

Wednesday, Sept. 12

MS12

Modelling in Medicine II

10:45 – 12:45
Room: HS 15.12

Modelling in life sciences is a challenging task. On one hand the underlying models are komplex and typically highly nonlinear, on the other hand multiscale aspects are of importance. This minisymposium addresses recent aspects in tumor growth modelling, medical imaging as well as cancer treatment, e.g., by hyperthermia or radiation.

Organizer:
H.O. Peitgen

10:45 - 11:10
A multiscale model of thermoregulation in the cancer therapy regional hyperthermia
Martin Weiser, Zuse Institute Berlin, Germany

11:15 - 11:40
Cellular automaton simulation of tumour growth
Andreas Deutsch, Technische Universität Dresden, Germany

11:45 - 12:10
A multi-objective optimizer for intensity modulated radiation therapy planning
Karl-Heinz Küfer, Fraunhofer Institute for Industrial Mathematics, Germany

12:15 - 12:40
Numerical Support for Planning of Radio-Frequency Ablation
Tobias Preusser, University of Bremen, Germany

Wednesday, Sept. 12

CT26

Navier-Stokes

10:45 – 12:45
Room: LS 11.01

10:45 - 11:10
How to upgrade flow solvers to involutive and avoid LBB condition?
Bijan Mohammadi, Université Montpellier, France

11:15 - 11:40
Calibration of discretization and model parameters for turbulent channel flow
Xiaoqin Zhang, Georg-August-Universität Göttingen, Germany

11:45 - 12:10
The third order WLSQR scheme on unstructured meshes with curvilinear boundaries
Jiří Fürst, Czech Technical University in Prague, Czech Republic

12:15 - 12:40
Finite Volume Methods in Numerical Modelling of Electrochemical Flow cells
Jürgen Fuhrmann, Weierstrass Institute for Applied Analysis and Stochastics, Germany

Wednesday, Sept. 12

CT27

Hyperbolic Equations

10:45 – 12:45
Room: HS 15.01

10:45 - 11:10
A predictor-corrector approach to flux limiting for finite element discretizations of transient convection problems
Dmitri Kuzmin, Universität Dortmund, Germany

11:15 - 11:40
Numerical solution of 2D and 3D unsteady viscous flows
Petr Louda, Czech Technical University in Prague, Czech Republic

11:45 - 12:10
The coupling of two scalar conservation laws by a Dafermos regularization
Benjamin Boutin, Université Pierre et Marie Curie - Paris, France

12:15 - 12:40
Well-balanced high-order MUSTA Schemes for non-conservative hyperbolic systems
Alberto Pardo Milanés, Universidad de Málaga, Spain

Wednesday, Sept. 12

CT28

Domain Decomposition

10:45 – 12:45
Room: HS 11.02

10:45 - 11:10
New results on overlapping Schwarz methods
Olof B. Widlund, New York University, USA

11:15 - 11:40
Overlapping Additive Schwarz preconditioners for degenerated elliptic problems
Sven Beuchler, Johannes Kepler Universität Linz, Austria

11:45 - 12:10
Solution of 2D semicoercive contact problems by BETI method
Marie Sadowská, VŠB - Technical University of Ostrava, Czech Republic

12:15 - 12:40
Optimal Total FETI algorithm for contact problems in elasticity
Vít Vondrák, Technical University of Ostrava, Czech Republic

Wednesday, Sept. 12

CT29

Interface Problems and Free Boundary Problems

10:45 – 12:45
Room: LS 15.01

10:45 - 11:10
The application of complex boundary elements method to free boundary seepage problems
Adrian Carabineanu, University of Bucharest, Romania

11:15 - 11:40
PDAS-method for a hemivariational inequality
Victor A. Kovtunenko, Karl-Franzens Universität Graz, Austria

11:45 - 12:10
Advances in nonlocal electrostatics
Caroline Fasel, Universität des Saarlandes, Germany

12:15 - 12:40
Mixed fem-bem coupling for non-linear transmission problems with Signorini contact
Matthias Maischak, Brunel University, UK

Thursday, September 13

Registration

8:30 - 16:00
Room: LS 15.03

Remarks/Changes

8:45 - 9:00
Room: HS 15.03

Schedule

Time	Talk	Room
9:00 - 10:00	**IP7**	HS 15.03
10:00 - 10:30	**Coffee Break**	
10:30 - 12:30	**MS13** **MS14** **MS15** **CT30** **CT31** **CT32** **CT33**	HS 15.02 HS 15.12 HS 15.03 HS 11.01 HS 11.02 HS 15.01 LS 15.01
12:30 - 14:00	**Lunch**	
14:00 - 15:00	**IP8**	HS 15.03
15:00 - 16:00	**CT34** **CT35** **CT36** **CT37** **CT38** **CT39** **CT40**	LS 15.01 HS 11.02 HS 15.01 HS 15.12 HS 11.01 HS 15.02 HS 15.03
16:00 - 16:15	**Coffee Break**	
16:15 - 18:15	**MS16** **MS17** **MS18** **CT41** **CT42** **CT43** **CT44**	HS 15.02 HS 15.03 HS 15.12 HS 11.02 HS 15.01 LS 15.01 HS 11.01

Thursday, Sept. 13

IP7

Transparent boundary conditions, wave propogation and periodic media

9:00 - 10:00
Room: HS 15.03

Periodic media play a major role in applications, in particular in optics for micro and nano-technology or in mechanics with composite materials. One of the main interesting features is the possibility offered by such media of selecting ranges of frequencies for which waves can or can not propagate. Of course, there is a need for efficient numerical methods for computing the propagation of waves inside such structures. In a lot of applications, the media are not really periodic but differ from periodic media only in bounded regions. In such a situation, a natural idea is to reduce numerical computations to these regions which rises the question of finding a transparent boundary condition to replace the exterior medium. The question of transparent conditions for wave propagation has retained a lot of attention from applied mathematicians with the concepts of absorbing boundary conditions (of various nature) or perfectly matched layers. However most of the existing solutions concern the case where the exterior medium is homogeneous (or stratified) and exploit in some way the explicit knowledge of solutions of wave equations with constant coefficients. These solutions exploit the fact that, physically, a wave that leaves out the computational domain does not come back. This is no longer true with periodic media in which, in some sense, the waves are reflected back "up to infinity".

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For full abstract, see Abstracts Section.

Patrick Joly
INRIA, France

Thursday, Sept. 13

IP8

Geometric Integration, in particular of Euler's Rigid Body Equation

14:00 – 15:00
Room: HS 15.03

The actually very active rerearch area *Geometric Integration* studies numerical methods which preserve geometric structures of the flow, such as syplecticity, symmetry, or volume preservation. An interesting effet is that such methods also have many superiour numerical properties, e.g., for long time integrations.
The 300th anniversary of Leonhard Euler in 2007 and the 250th anniversary of the discovery of Euler's Rigid Body equations in 2008 suggest naturally a detailed study of the application of symplectic integrators to these equations.

Gerhard Wanner
Universität Genf

Thursday, Sept. 13

MS13

Fluid Structure Interaction II

10:30 – 12:30
Room: HS 15.02

Recent computational approaches to fluid-strucutre interaction are presented. Concerning applications, among others aeroelastic problems will be addressed.

Organizer:
J. Ballmann
S. Turek

10:30 - 10:55
Hybrid Discretization Methods for Aeroelastic Problems
Holger Wendland, University of Sussex, United Kingdom

11:00 - 11:25
Progress on Simulating the Transonic Aerolastic Response of Fighter Aircraft
Kenneth J. Badcock, University of Liverpool, UK

11:30 - 11:55
Reduced Order Modeling of Unsteady Aeroelastic Analysis Using the Volterra-Wiener Theory
Alexander Boucke, RWTH Aachen, Germany

Thursday, Sept. 13

MS14

Optimal Control with PDEs I

10:30 – 12:30
Room: HS 15.12

The minisymposium concentrates on computational aspects in PDE-constrained optimization. Topics ranging from numerical analysis for quasilinear problems, mesh adaptivity and mesh independence, to efficient regularization techniques for state constrained problems are considered.

Organizer:
M. Heinkenschloss
R. Hoppe

10:30 - 10:55
TBA
Matthias Heinkenschloss, Rice University, Houston, USA

11:00 - 11:25
Adaptive Finite Element Approximations of State Constrained Optimal Control Problems for Elliptic Boundary Value Problems
Ronald Hoppe, University of Huston, USA

11:30 - 11:55
A Penalization Approach for Tomographic Reconstruction of Binary Radially Symmetric Objects
Maitine Bergounioux, Universitéd'Orlns, France

12:00 - 12:25
Numerical Analysis of Some Optimal Control Problems Governed by Quasilinear Elliptic Equations
Eduardo Casas, Universidad de Cantabria, Spain

Thursday, Sept. 13

MS15

Fast Methods for Nonlocal Operators I

10:30 – 12:30
Room: HS 15.03

The minisymposium covers recent trends in preconditioning, boundary element methods, H-matrix techniques and related computational techniques.

Organizer:
M. Bebendorf
W. Hackbusch

10:30 - 10:55
Purely algebraic factorization by triangular hierchrchical matrices
Mario Bebendorf, Universität Leipzig, Germany

11:00 - 11:25
Preconditioning of Fast Boundary Element Methods
Günther Of, Technische Universität Graz, Austria

11:30 - 11:55
Sparse Second Moment Analysis for Potentials on Stochastic Domains
Helmut Harbrecht, Universität Bonn, Germany

12:00 - 12:25
Approximation of Tensor-Sums in High Dimensions with Application to Multi-Dimensional Operators
Mike Espig, Max Planck Institute for Mathematics in the Sciences, Germany

Thursday, Sept. 10

MS16

Fluid Structure Interaction III

16:15 – 18:15
Room: HS 15.02

Recent computational approaches to fluid-strucutre interaction are presented. Concerning applications, among others aeroelastic problems will be addressed.

Organizer:
J. Ballmann
S. Turek

16:15 - 16:40
Quasi-Newton algorithms for fluid-structure interaction problems
Joachim Rang, Technische Universität Braunschweig, Germany

16:45 - 17:10
Finite Element Approximation of Nonlinear Aeroelastic Problems
Petr Svacek, Czech Technical University in Prague

17:15 - 17:40
Convergence acceleration of coupled problems with partitioned solvers
Jan Vierendeels, Ghent University, Belgium

17:45 - 18:10
Interface Tracking and Mesh Update Techniques for Flow Simulation in Deforming Domains
Marek Behr, RWTH Aachen University, Germany

Thursday, Sept. 10

MS17

Optimal Control with PDEs II

16:15 – 18:15
Room: HS 15.03

The minisymposium concentrates on computational aspects in PDE-constrained optimization. Topics ranging from numerical analysis for quasilinear problems, mesh adaptivity and mesh independence, to efficient regularization techniques for state constrained problems are considered.

Organizer:
M. Heinkenschloss
R. Hoppe

16:15 - 16:40
Tailored discrete concepts for pde constrained optimization problems in the presence of control and state constraints
Michael Hinze, Universität Hamburg, Germany

16:45 - 17:10
Inexact null-space iterations in large scale optimization
Michael Hintermüller, Karl-Franzens-Universität Graz, Austria

17:15 - 17:40
Regularity and optimality conditions for state-constrained parabolic problems with time-dependent controls
Fredi Tröltzsch, Technische Universität Berlin, Germany

17:45 - 18:10
A virtual control concept for optimal control problems with pointwise state constraints
Arnd Roesch, Universität Duisburg-Essen, Germany

Thursday, Sept. 10

MS18

Fast Methods for Nonlocal Operators II

16:15 – 18:15
Room: HS 15.12

The minisymposium covers recent trends in preconditioning, boundary element methods, H-matrix techniques and related computational techniques.

Organizer:
M. Bebendorf
W. Hackbusch

16:15 - 16:40
Hierarchical Low Kronecker Rank Approximation
Lars Grasedyck, Max Planck Institute for Mathematics in the Sciences, Germany

16:45 - 17:10
An algebraic approach to preconditioning based on $\mathcal{H}-LU$ decompositions
Thomas Fischer, University of Leipzig, Germany

17:15 - 17:40
Hierarchical compression
Steffen Börm, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

17:45 - 18:10
Efficient solution of large-scale algebraic Bernoulli equations based on hierarchical matrix arithmetic
Ulrike Baur, Technische Universität Chemnitz, Germany

Thursday, Sept. 13

CT30

Hyperbolic Equations

10:30 – 12:30
Room: HS 11.01

10:30 - 10:55
A 'TVD-like' Scheme for Conservation Laws with source terms
Anna Martínez-Gavara, University of València, Spain

11:00 - 11:25
On path-conservative numerical schemes for hyperbolic systems of conservation laws with source terms
M^a Luz Muñoz-Ruiz, Universidad de Málaga, Spain

11:30 - 11:55
A WAF type method for nonhomogeneous Shallow Water Equations with pollutant
Gladys Narbona, Universidad de Sevilla, Spain

12:00 - 12:25
High order two dimensional schemes for coupled shallow water-transport systems
José Antonio García Rodríguez, Universidade da Coruña, Spain

Thursday, Sept. 13

CT31

Nonlinear PDEs

10:30 – 12:30
Room: HS 11.02

10:30 - 10:55
A domain decomposition method for second order nonlinear equations
Jean R. Roche, Université Henri Poincaré Nancy 1, France

11:00 - 11:25
Space-time higher order discretizations of non-stationary nonlinear convection-diffusion problems
Miloslav Vlasák, Charles University in Prague, Czech Republic

11:30 - 11:55
Numerical Simulation of Barium Sulphate Precipitation
Michael Roland, Universität des Saarlandes, Germany

12:00 - 12:25
Numerical Analysis of Generalized Newtonian Fluids
Michael Růžička, Albert-Ludwigs-Universität Freiburg, Germany

Thursday, Sept. 13

CT32

Domain Decomposition

10:30 – 12:30
Room: HS 15.01

10:30 - 10:55
An analysis of a FETI-DP algorithm on irregular subdomains in the plane
Axel Klawonn, Universität Duisburg-Essen, Germany

11:00 - 11:25
Pointwise constraints in space and time - on the stability and numerical robustness of pointwise constrains for stationary dynamic problems in elasticity
Rolf Krause, Universität Bonn, Germany

11:30 - 11:55
Multidimensional Coupling in a Human Knee Model
Oliver Sander, Freie Universität Berlin, Germany

12:00 - 12:25
A domain decomposition method derived from the use of Lagrange Multipliers for elliptic problems
Eliseo Chacón Vera, Universidad de Sevilla, Spain

Thursday, Sept. 13

CT33

Electromagnetism

10:30 – 12:30
Room: LS 15.01

10:30 - 10:55
Thermo-magneto-hydrodynamic simulation of melting induction furnaces with cylindrical symmetry
Dolores Gómez, Universidade de Santiago de Compostella, Spain

11:00 - 11:25
A new formulation of the eddy current problem with input current intensities as boundary data
Ana Alonso Rodríguez, Università degli Studi di Trento, Italy

11:30 - 11:55
External finite element approximations of a 2D Maxwell eigenvalue problem with curvilineair boundary
Wouter Hamelinck, Ghent University, Belgium

12:00 - 12:25
Modified boundary integral equations for electromagnetic scattering problems
Markus Windisch, Technische Universität Graz, Austria

Thursday, Sept. 13

CT34

Numerical Linear Algebra

15:00 – 16:00
Room: LS 15.01

15:00 - 15:25
On solving nonsymmetric saddle-point systems arising in FDM
Radek Kučera, VŠB-Technical University of Ostrava, Czech Republic

15:30 - 15:55
A dual dropping approximate inverse preconditioner for solving general linear systems of equations
Bruno Carpentieri, Karl-Franzens Universität Graz, Austria

Thursday, Sept. 13

CT35

Nonlinear PDEs

15:00 – 16:00
Room: HS 11.02

15:00 - 15:25
Dynamic Iteration for Transient Simulation of Shape Memory Alloys
Gunnar Teichelmann, Technische Universität München, Germany

15:30 - 15:55
A hybrid numerical scheme for aerosol dynamics
Hans Babovsky, Technische Universität Ilmenau, Germany

Thursday, Sept. 13

CT36

Domain Decomposition

15:00 – 16:00
Room: HS 15.01

15:00 - 15:25
Application of FETI method for 2D quasistatic contact problems with Coulomb friction
Oldřich Vlach, VŠB-Technical University of Ostrava, Czech Republic

15:30 - 15:55
A posteriori error analysis of penalty domain decomposition methods for linear elliptic problems
Tomás Chacón Rebollo, Universidad de Sevilla, Spain

Thursday, Sept. 13

CT37

Nonlinear Mechanics

15:00 – 16:00
Room: HS 15.12

15:00 - 15:25
Newton-like solve for elastoplastic problems with hardening and its local superlinear convergence
Jan Valdman, Universität Linz, Austria

Thursday, Sept. 13

CT38

Hyperbolic Equations

15:00 – 16:00
Room: HS 11.01

15:00 - 15:25
DAE-Index of Real Gas Flow Equations
Ayoub Hmaidi, Technische Universität München, Germany

15:30 - 15:55
A road traffic model with overtaking: Oscillatory patterns
Vladimír Janovský, Charles University in Prague, Czech Republic

Thursday, Sept. 13

CT39

Optimal Control with Applications

15:00 – 16:00
Room: HS 15.02

15:00 - 15:25
Optimal shape design of quasi-1D Euler flows with discontinuities
Antonio Baeza, Universidad Autónoma de Madrid, Spain

15:30 - 15:55
Numerical Optimization in a Real-World Application
Karsten Urban, Universität Ulm, Germany

Thursday, Sept. 13

CT40

Navier-Stokes

15:00 – 16:00
Room: HS 15.03

15:00 - 15:25
Local projection stabilization for the Oseen system on anisotropic meshes
Malte Braack, Christian-Albrechts-Universität zu Kiel, Germany

15:30 - 15:55
A comparative study of efficient iterative solvers for generalized Stokes equations
Maxim Larin, RWTH Aachen, Germany

Thursday, Sept. 13

CT41

Nonlinear PDEs

16:15 – 18:15
Room: HS 11.02

16:15 - 16:40
Computing nonclassical solutions of scalar conservation laws with a sharp interface and fully conservative scheme
Christophe Chalons, Université Paris-Diderot Paris 7, France

16:45 - 17:10
Convergence of Adaptive Finite Element Methods for the p-Laplace Equation
Lars Diening, Albert-Ludwigs Universität Freiburg, Germany

17:15 - 17:40
Finite elements for spatially correlated stochastically perturbed parabolic equations
Omar Lakkis, University of Sussex, UK

17:45 - 18:10
Exact Stekhlov-Poincaré maps for planar stress in general domains
Nilima Nigam, McGill University, Canada

Thursday, Sept. 13

CT42

Numerical Linear Algebra

16:15 – 18:15
Room: HS 15.01

16:15 - 16:40
Stabilization and Acceleration of Iterative Solvers for Linear Systems of Equations: Exploiting Recursive Properties of Fixed Point Algorithms
Aleksandar Jemcov, ANSYS/Fluent Inc., USA

16:45 - 17:10
Special iterative method for solution of transport-dominated convection-diffusion problems
Lev A. Krukier, Southern Federal University, Russia

17:15 - 17:40
Fractional Step Runge-Kutta-Nyström methods and order reduction
M[a] Jesus Moreta, Universidad Complutense de Madrid, Spain

17:45 - 18:10
A High Performance Parallel Linear Algebra Toolbox: Building Blocks for a Parallel Algebraic Multigrid Solver
Manfred Liebmann, Karl-Franzens-Universität Graz, Austria

Thursday, Sept. 13

CT43

hp-Finite Elements

16:15 – 18:15
Room: LS 15.01

16:15 - 16:40
Local Projection Stabilizations for Inf-sup Stable Finite Elements applied to the Oseen Problem
Gerd Rapin, Georg-August-Universität Göttingen, Germany

16:45 - 17:10
Higher order finite elements on pyramids
Joel Phillips, McGill University, Canada

17:15 - 17:40
Bilinear shell elements and boundary layers
Antti H. Niemi, Helsinki University of Technology, Finland

17:45 - 18:10
On efficient solution of linear systems arising in *hp*-FEM
Tomáš Vejchodský, Czech Academy of Sciences, Czech Republic

Thursday, Sept. 13

CT44

Electromagnetism

16:15 – 18:15
Room: HS 11.01

16:15 - 16:40
Schwarz domain-decomposition for an external magnetostatic problem
Aleš Janka, Université de Fribourg, Switzerland

16:45 - 17:10
Mixed Conforming Elements for the Large-Body Limit in Micromagnetics
Markus Aurada, Technische Universität Wien, Austria

17:15 - 17:40
Analysis of a Centered Flux Discontinuous Galerkin Method for Maxwell's Equations on Cartesian Grids
Thomas Lau, Technische Universität Darmstadt, Germany

17:45 - 18:10
Functional type a posteriori error estimates for Maxwell's equations
Antti Hannukainen, Helsinke University of Technology, Finland

Friday, September 14

Registration

8:00 - 14:30
Room: LS 15.03

Remarks/Changes

8:45 - 9:00
Room: HS 15.03

Schedule

Time	Talk	Room
8:30 - 9:30	**IP9**	HS 15.03
9:30 - 10:30	**IP10**	HS 15.03
10:30 - 10:45	**Coffee Break**	
10:45 - 12:45	**MS19** **CT45** **CT46** **CT47** **CT48** **CT49** **CT50**	HS 15.03 HS 15.02 HS 15.12 HS 15.01 HS 11.01 HS 11.02 LS 15.01
12:45 - 13:00	**Coffee Break**	
13:00 - 15:00	**CT53** **CT54**	HS 15.02 HS 15.12

Friday, Sept. 14

IP9

Robust Interactive Methods for PDEs with Rough Coefficients

8:30 - 9:30
Room: HS 15.03

In this talk, we will present a number of results on discretization, adaptive and iterative methods for systems of partial differential equations with coefficients that are highly oscillatory, or strongly discontinuous, or degenerating. We will first show how a diffusion equation with highly oscillatory coefficients can be solved by simple preconditioning and multigrid methods. We will then demonstrate how these simple methods would deteriorate if the coefficients have large discontinuous jumps and how these methods can be made more robust. We will continue the talks with new techniques for several other equations including Maxwell equations, Stokes equations and its coupling with Darcy's law.

Jinchao Xu
PennState University, USA

Friday, Sept. 14

IP10

The worst scenario method: a red thread running through various approaches to problems with uncertain input data

9:30 – 10:30
Room: HS 15.03

Uncertain inputs appear in many, if not all, industrial problems; methods to tackle uncertainties are numerous as well. Among them, the worst scenario method plays a significant role as either a self-contained method or a fundamental sub-method of other methods.
The method has three main ingredients: $\mathcal{U}_{\mathrm{ad}}$, a set of admissible data; $A(a)u = f(a)$, a state problem dependent on $a \in \mathcal{U}_{\mathrm{ad}}$; and $\Phi(a, u)$, a criterion functional evaluating a quantity of interest that directly depends on u and, possibly, on a; take local stress, temperature, or velocity, for example. The worst scenario problem lies in finding a^0 that maximizes $\Phi(a, u(a))$, where $u(a)$ solves the state problem and $a \in \mathcal{U}_{\mathrm{ad}}$. If $\Phi(a, u(a))$ is continuous with respect to a and $\mathcal{U}_{\mathrm{ad}}$ is compact, a^0 exists. Then $\Phi(a^0, u(a^0))$ maximizes the quantity of interest.
If a_0, the minimizer of $\Phi(a, u(a))$ over $\mathcal{U}_{\mathrm{ad}}$ (the best scenario), is obtained, then the range of $\Phi(a, u(a))$ over $\mathcal{U}_{\mathrm{ad}}$ is defined by the interval $[\Phi(a_0, u(a_0)), \Phi(a^0, u(a^0))]$.
...
For full abstract, see Abstracts Section.

Jan Chleboun
Academy of Sciences, Prag, Czech Republic

Friday, Sept. 14

MS19

Optimal Control with PDEs III

10:45 – 12:45
Room: HS 15.03

The minisymposium concentrates on computational aspects in PDE-constrained optimization. Topics ranging from numerical analysis for quasilinear problems, mesh adaptivity and mesh independence, to efficient regularization techniques for state constrained problems are considered.

Organizer:
M. Heinkenschloss
R. Hoppe

10:45 - 11:10
A new mesh independence result for semismooth Newton methods
Michael Ulbrich, Technische Universität München, Germany

11:15 - 11:40
An SQP method for semi-linear optimal control problems with mixed constraints
Roland Griesse, Johann Radon Institute for Computational and Applied Mathematics (RICIAM), Austria

11:45 - 12:10
Adaptive Multilevel Methods for PDE-Constrained Optimization
Stefan Ulbrich, Technische Universität Darmstadt, Germany

12:15 - 12:40
A priori error analysis for space-time finite element discretization of parabolic optimal control problems
Boris Vexler, Johann Radon Institute for Computational and Applied Mathematics (RICIAM), Austria

Friday, Sept. 14

CT45

Navier-Stokes

10:45 – 12:45
Room: HS 15.02

10:45 - 11:10
An augmented Lagrangian approach to linearized problems in hydrodynamic stability
Maxim A. Olshanskii, M.V. Lomonosov Moscow State University, Russia

11:15 - 11:40
On Some Uniqueness results of Incompressible Flow through Cascade of Profiles
Tomáš Neustupa, Czech Technical University in Prague, Czech Republic

11:45 - 12:10
Justification of the splitting scheme for the large-scale ocean circulation problem
Georgy M. Kobelkov, M.V. Lomonosov Moscow State University, Russia

12:15 - 12:40
Numerical and analytical research of multimode solutions of the Jeffery-Hamel problem
Dimitri V. Georgievskii, M.V. Lomonosov Moscow State University, Russia

Friday, Sept. 14

CT46

Convection-Diffusion Problems

10:45 – 12:45
Room: HS 15.12

10:45 - 11:10
Numerical solution of singularly perturbed systems of convection-diffusion equations
Martin Stynes, National University of Ireland, Cork

11:15 - 11:40
Edge stabilization of higher order elements for convection diffusion equations
Friedhelm Schieweck, Otto-von-Guericke-Universität Magdeburg, Germany

11:45 - 12:10
On the choice of parameters in stabilization methods for convection–diffusion equations
Petr Knobloch, Charles University in Prague, Czech Republic

12:15 - 12:40
Mixed hybrid DG methods for convection-diffusion problems
Herbert Egger, RWTH Aachen, Germany

Friday, Sept. 14

CT47

hp-Finite Elements

10:45 – 12:45
Room: HS 15.01

10:45 - 11:10
Integrodifferential approach in the linear theory of elasticity
Vasily V. Saurin, Russian Academy of Sciences, Russia

11:15 - 11:40
FEM realization based on integral strain-stress relations
Georgy V. Kostin, Russian Academy of Sciences, Russia

11:45 - 12:10
Constraints Coefficients in ***hp*****-FEM**
Andreas Schröder, Universität Dortmund, Germany

12:15 - 12:40
p**-Sparse BEM for weakly singular integral equation on a random surface**
Alexey Chernov, ETH Zürich, Switzerland

Friday, Sept. 14

CT48

ODEs and Fractional Step Methods

10:45 – 12:45 pm
Room: HS 11.01

10:45 - 11:10
Rosenbrock methods for Large-Scale Differential Riccati Equations
Hermann Mena, Technische Universität Chemnitz, Germany

11:15 - 11:40
A second order scheme for solving optimization-constrained differential equations with dicontinuities
Chantal Landry, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Friday, Sept. 14

CT49

Electromagnetism

10:45 – 12:45
Room: HS 11.02

10:45 - 11:10
Space-and-Time Adaptive Calculation of Transient 3D Magnetic Fields
Markus Clemens, Helmut-Schmidt-Universität - Universität der Bundeswehr Hamburg, Germany

11:15 - 11:40
***hp*-FEM and High-Order BIE Method for Efficient Modelling of Photonic Crystal Materials with Negative Refraction**
Kersten Schmidt, ETH Zürich, Switzerland

11:45 - 12:10
An efficient iterative method for finite element discretizations, with application to 3D electromagnetic problems
Alexander Bespalov, Baker Huges Inc., USA

Friday, Sept. 14

CT50

Modelling in Medicine

10:45 – 12:45
Room: LS 15.01

10:45 - 11:10
Numerical modelling of epidermal wound healing
Etelvina Javierre, Delft University of Technology, Netherlands

11:15 - 11:40
Numerical Simulation and Optimization of Fracture Healing
Daniel Nolte, Universität Ulm, Germany

11:45 - 12:10
Special efficient solutions for multicriterial transport problems
Liana Lupşa, Babeş-Bolyai University, Romania

12:15 - 12:40
Multiple Dynamic Programming Applied in Cervical Cancer Screening
Luciana Neamţiu, Oncological Institute "Prof. Dr. Ion Chiricuţă" of Cluj-Napoca, Romania

Friday, Sept. 14

CT53

Optimal Control with Applications

13:00 – 15:00
Room: HS 15.02

13:00 - 13:25
An optimal control problem for stochastic elliptic PDEs
Hassan Manouzi, Laval University, Canada

13:30 - 13:55
Optimal Shape Design Subject to Variational Inequalities
Antoine Laurain, Karl-Franzens-Universität Graz, Austria

14:00 - 14:25
Optimal Control of Complementarity Problems
Ian Kopacka, Karl-Franzens-Universität Graz, Austria

14:30 - 14:55
Multigrid Methods for Distributed Elliptic Optimal Control Problems
Michelle C. Vallejos, Karl-Franzens-Universität Graz, Austria

Friday, Sept. 14

CT54

Convection-Diffusion Problems

13:00 – 15:00
Room: HS 15.12

13:00 - 13:25
A finite element model for bone ingrowth into a prosthesis
Fred J. Vermolen, Technische Universiteit Delft, Netherlands

13:30 - 13:55
A third order method for Convection Diffusion Equations with Delay
Jörg Frochte, Universität Duisburg Essen, Germany

14:00 - 14:25
Asymptotic behavior of solution of elliptic pseudodifferential equation near cone
Vladimir B. Vasilyev, Bryansk State University, Russia

Abstracts

IP 1
Imaging in Random Media

I will present an overview of some recently developed methods for imaging with array and distributed sensors when the environment between the objects to be imaged and the sensors is complex and only partially known to the imager. This requires modeling and analysis in random media, and the use of statistical algorithms which increase the overall computational complexity. Imaging is done by backpropagating local correlations rather than traces (interferometry). I will illustrate the theory with applications from non-destructive testing and from other areas.

George Papanicolaou[1]
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IP 2
Parametric Approximation of Geometric Evolution Equations

Geometric flows, in which hypersurfaces move such that an energy, involving surface and bending terms, decreases appear in many situations in the natural sciences and in geometry. Classic examples are mean curvature, surface diffusion and Willmore flows. Computational methods to approximate such flows are based on one of three approaches (i) parametric methods, (ii) phase field methods or (iii) level set methods. The first tracks the hypersurface, whilst the other two implicitly capture the hypersurface; see the review article [6]. A key problem with the first approach, apart from the fact that it is does not naturally deal with changes of topology, is that in many cases the mesh has to be redistributed after every few time steps to avoid coalescence of mesh points.
In this talk we present a new variational formulation of the parametric approach, which leads to an unconditionally stable, fully discrete finite element approximation. In addition, the scheme has very good properties with respect to the distribution of mesh points, and if applicable volume conservation. We illustrate this for (anisotropic) mean curvature and (anisotropic) surface diffusion flows of closed curves in $\mathbb{R}^2$. We extend these flows to curve networks in $\mathbb{R}^2$. Here the triple junction conditions, that have to hold where three curves meet at a point, are naturally approximated in the discretization of our variational formulation; see [1], [2] and [3]. Moreover, we extend this approximation to flows on closed hypersurfaces in $\mathbb{R}^3$; see [4] and [5].

[1] J. W. Barrett, H. Garcke, R. Nürnberg, "A parametric finite element method for fourth order geometric evolution equations", *J. Comput. Phys.*, Vol. 222, pp. 441–467, (2007).

[2] J. W. Barrett, H. Garcke, R. Nürnberg "On the variational approximation of combined second and fourth order geometric evolution equations", *SIAM J. Sci. Comput.*, Vol. 29, pp. 1006–1041, (2007).

[3] J. W. Barrett, H. Garcke, R. Nürnberg "Numerical approximation of anisotropic geometric evolution equations in the plane", *IMA J. Numer. Anal.*, (to appear).

[4] J. W. Barrett, H. Garcke, R. Nürnberg "On the parametric finite element approximation of evolving hypersurfaces in $\mathbb{R}^3$ ", Preprint No. 18/2006, University of Regensburg, Germany.

[5] J. W. Barrett, H. Garcke, R. Nürnberg " A variational formulation of anisotropic geometric evolution equations in higher dimensions", Preprint No. 7/2007, University of Regensburg, Germany.

[6] K. Deckelnick, G. Dziuk, C. M. Elliott "Computation of geometric partial differential equations and mean curvature flow", *Acta Numerica*, Vol. 14, pp.139–232, (2005).

John W. Barrett[1]
Harald Garcke[2]
Robert Nürnberg[1]
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IP 3
Discontinuous Galerkin elements for Reissner-Mindlin plates

In a recent paper of Arnold, Brezzi, and Marini [1], the ideas of discontinuous Galerkin methods were used to obtain and analyze two new families of locking free finite element methods for the approximation of the Reissner-Mindlin plate problem. By following their basic approach, but making different choices of finite element spaces, we develop and analyze other families of locking-free finite elements that eliminate the need for the introduction of a reduction operator, which has been a certain feature of many locking-free methods. For $k \geq 1$, all the methods use piecewise polynomials of degree $k+1$ to approximate the transverse displacement and piecewise polynomials of degree k (or possibly subsets) to approximate both the rotation and shear stress vectors. The approximation spaces for the rotation and the shear stress are always identical. The methods vary in the amount of inter-element continuity required. In terms of smallest number of degrees of freedom, the simplest method approximates the transverse displacement with continuous, piecewise quadratics and both the rotation and shear stress with rotated linear Brezzi-Douglas-Marini elements.

[1] D.N. Arnold, F. Brezzi, and L.D. Marini, "A Family of Discontinuous Galerkin Finite Elements for the Reissner-Mindlin plate", *J. Scientific Computing*, Vol. 22(1), pp. 25–45 (2005).

D.N. Arnold[1]
F. Brezzi[2]
R.S. Falk[3]
L.D. Marini[4]
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IP 4
Boundary and Finite Element Domain Decomposition Methods

Domain Decomposition (DD) methods are nowadays not only used for constructing highly efficient parallel solvers for Partial Differential Equations but also for coupling different physical fields, different meshes and different discretization techniques. Since Finite Element Methods and Boundary Element Methods exhibit certain complementary properties, it is sometimes very useful to couple these discretization techniques. The efficient solution of large scale systems of finite, boundary and coupled finite and boundary element DD equations is the main topic of this talk.

We give a short introduction to primal, dual and dual-primal iterative substructuring methods. The finite element versions of these non-overlapping DD methods and their analysis can be find in the monograph [2]. The boundary element and the coupled versions are discussed in [1]. In this talk, we discuss some special features connected with the coupling of linear and non-linear problems in bounded and unbounded regions. In particular, Boundary and Finite Element Tearing and Interconnecting methods lead to very robust DD solvers. The boundary and interface concentrated finite element methods have some common features with data-sparse boundary element methods, but their applicability is by far wider. We present primal and dual iterative substructuring solvers which exhibit the same complexity as the corresponding data-sparse boundary element solvers, i.e. the arithmetical cost and the memory demand are basically proportional to the degrees of freedoms living on the skeleton of domain decomposition given. Finally, we use the boundary element DD technology in order to construct finite element approximations on polygonal and polyhedral meshes, or even more general meshes. Fast solvers based on multigrid and DD techniques are also provided. The talk is based on joint work with S. Beuchler (Linz), T. Eibner (Chemnitz), G. Of (Graz), C. Pechstein (Linz), D. Pusch (Linz), O. Steinbach (Graz) and W. Zulehner (Linz). This work has been supported by the Austrian Science Fund 'Fonds zur Förderung der wissenschaftlichen Forschung (FWF)' under the grants P19255 and SFB F013 'Numerical and Symbolic Scientific Computing', and by the Johann Radon Institute for Computational and Applied Mathematics (RICAM) of the Austrian Academy of Sciences.

[1] U. Langer , O. Steinbach "Coupled Finite and Boundary Domain Decomposition Methods", In "Boundary Element Analysis" ed. by M. Schanz and O. Steinbach, Lecture Notes in Applied and Computational Mechanics, Vol. 29, pp. 61–96, (2007).

[2] A. Toselli, A. Widlund "Domain Decomposition Methods - Algorithms and Theory", Springer Series in Computational Mathematics, Vol. 34, (2005).

Ulrich Langer[1]
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PL 1
Mathematics in Facial Surgery Planning

Since 1999, the CAS group at ZIB (CAS: computer assisted surgery) has been working on operation planning for cranio-maxillofacial surgery in close cooperation with clinical surgeons, in the beginning with Zeilhofer and Sader (then TU Munich, now U Basel and U Frankfurt, respectively), today with a whole bunch of further clinics. Within the integrated software environment AMIRA the group has realized
(a) the construction of 3D virtual patients from real patients out of detailed medical imaging data (stacks of CT or MRT files), which involves the efficient generation of 3D tetrahedral grids (only few details to be given in the talk);
(b) off-line operation planning tools to be used within clinics or within teleconferences between clinics and ZIB, which involve a huge amount of software engineering (details to be skipped);
(c) preoperative prediction of the postoperative facial appearance of patients, which involves the fast numerical solution of partial differential equations for (geometrically and materially nonlinear) elasticity by an affine conjugate adaptive multilevel Newton-CCG method.
The talk will include detailed clinically relevant results for individual patients that have been operated on the basis of our plannings.

[1] P. Deuflhard, M. Weiser, S. Zachow "Mathematics in Facial Surgery", *Notices of the AMS*, Vol. 53, pp. 2-6 (2006).

[2] S. Zachow, H.-C. Hege, P. Deuflhard, "Computer Assisted Planning in Cranio-Maxillofacial Surgery", *Journal of Computing and Information Technology (CIT)*, Vol. 14, pp. 53-64 (2006).

Peter Deuflhard[1]
[1] Zuse Institute Berlin (ZIB) and Freie Universität Berlin, Dept. Mathematics / Computer Science and DFG Research Center Matheon, "Mathematics for Key Technologies, Berlin, Germany
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IP 5
On the numerical solution of higher-dimensional partial differential equations

The approximate solution of higher-dimensional partial differential equations by conventional discretization methods is in general impossible due to the so-called curse of dimensionality, i.e. the numberof degress of freedoms of a conventional discretization is of the order $O(N^d)$, where d denotes the dimension of the problem and N is the amount of degrees of freedom in one coordinate direction.
We discuss under what circumstances the curse of dimensionality can be overcome, present related discretization techniques and approximation methods and give applications like the Fokker-Planck equation, the Schr"odinger equation and various problems from finance.

Michael Griebel[1]
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IP 6
Open boundary conditions for wave propagation problems on unbounded domains

Whole space problems for partial differential equations appear naturally in wave propagation problems of acoustics, quantum mechanics, and fluid dynamics, e.g. For the numerical solution of such problems, the computational domain must be limited to a finite region by introducing (artificial) absorbing boundary conditions (ABCs). An appropriate ABC must lead to a well-posed (initial-) boundary value problem, yield a good approximation to the solution of the whole space problem, and allow for an efficient numerical implementation. If the ABC yields –on the truncated domain– exactly the whole space solution, it is referred to as transparent boundary condition (TBC). In this talk we shall review some recent developments in this field [1] and focus on the following topics:
The *TBC for the time dependent Schrödinger equation* is a Dirichlet-to-Neumann map, represented by a pseudo-differential operator that is nonlocal both in time and in the boundary manifold. The numerical discretizations of this TBC is far from trivial, as it may easily render the initial-boundary value problem unstable. Based on a regular discretization in the exterior domain (Crank-Nicolson finite difference scheme, e.g.) we shall construct for the 1D and 2D Schrödinger equation a *dicrete TBC*, which makes the overall scheme unconditionally stable [3, 5]. Efficient implementations of the TBC are based on approximating the involved discrete convolutions by exponential sums the resulting numerical scheme [6]. The derived boundary conditions are illustrated with applications to a quantum waveguide [2] and from underwater acoustics [4].
TBCs for nonlinear equations were only found very recently. As they are based on inverse scattering theory, that approach is limited to fully integrable systems (e.g. sine-Gordon or nonlinear Schrödinger equations [7]). For *semilinear Klein-Gordon equations* we shall hence discuss an alternative approach based on the *perfectly match layer* (PML). The construction is based on a reformulation of the PDE as a semilinear hyperbolic system with an exponential damping of outgo-

ing waves in the PML-zone. Well-posedness of the resulting system and large-time stability are crucial aspects in the PML-design. 1D and 2D simulations reveal the advantage over conventional linearization approaches to such open boundary conditions [8].

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IP 7

Transparent boundary conditions, wave propagation and periodic media

Periodic media play a major role in applications, in particular in optics for micro and nano-technology or in mechanics with composite materials. One of the main interesting features is the possibility offered by such media of selecting ranges of frequencies for which waves can or can not propagate. Of course, there is a need for efficient numerical methods for computing the propagation of waves inside such structures. In a lot of applications, the media are not really periodic but differ from periodic media only in bounded regions. In such a situation, a natural idea is to reduce numerical computations to these regions which rises the question of finding a transparent boundary condition to replace the exterior medium.
The question of transparent conditions for wave propagation has retained a lot of attention from applied mathematicians with the concepts of absorbing boundary conditions (of various nature) or perfectly matched layers. However most of the existing solutions concern the case where the exterior medium is homogeneous (or stratified) and exploit in some way the explicit knowledge of solutions of wave equations with constant coefficients. These solutions exploit the fact that, physically, a wave that leaves out the computational domain does not come back. This is no longer true with periodic media in which, in some sense, the waves are reflected back "up to infinity".
In this talk, I will present a strategy developed at INRIA for the last past 3 years, jointly with J. R. Li and S. Fliss for handling 2D time-harmonic wave propagation in locally perturbed periodic media. The general idea is to take advantage of the periodic structure of the problem to design a method for the construction of exact DtN conditions

$$\frac{\partial u}{\partial n} + \Lambda u = 0, \tag{1}$$

by solving only problems posed on one periodicity cell. I will consider successively three particular situations of increasing complexity, each case using the solution for the previous one.
Periodic waveguides. The domain of propagation in of the form $\mathbb{R}^+ \times \,]0,1[$ and the problem is periodic in the x direction. The operator Λ^W appearing in (1) is constructed from the sollution of an operator valued Ricatti equation whose coefficients are determined by solving local cell problems. This Ricatti equation is constructed by revisiting the well known Floquet theory.
Periodic half-space. One constructs the operator Λ^H associated with a periodic half-space by using the partial Floquet-Bloch transform in the direction parallel to the boundary of the halfspace. One obtains

$$\Lambda = \int_0^{2\pi} \Lambda^W(k)\, dk = 0, \tag{2}$$

where k in the Floquet-Bloch wave number and $\Lambda^W(k)$ is the operator associated to a (k-dependent) waveguide problem.
The general case For simplicity, we shall restrict ourselves to the case where the periodicity cell is a square and presents at least two symmetries, which is often the case in the applications. We want to restrict the computations to a square whose side is a multiple of the size of the periodicity cell. The key point of the method relies on the factorization of the DtN operator as:

$$\Lambda = \Lambda^H \circ D, \tag{3}$$

where the first operator Λ^H is the DtN operator corresponding to a periodic half space problem and the second one, D is the solution of a new affine operator valued equation.
The theoretical aspects of the problem and corresponding numerical issues will be addressed in the talk. Preliminary numerical results will be presented.

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IP 8

Geometric Integration, in Particular of Euler's Rigid Body Equations

The actually very active rerearch area *Geometric Integration* studies numerical methods which preserve geometric structures of the flow, such as syplecticity, symmetry, or volume preservation. An interesting effet is that such methods also have many superiour numerical properties, e.g., for long time integrations.
The 300th anniversary of Leonhard Euler in 2007 and the 250th anniversary of the discovery of Euler's Rigid Body equations in 2008 suggest naturally a detailed study of the application of symplectic integrators to these equations.

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IP 9

Robust Iterative Methods for PDEs with Rough Coefficients

In this talk, we will present a number of results on discretization, adaptive and iterative methods for systems of partial differential equations with coefficients that are highly oscillatory, or strongly discontinuous, or degenerating. We will first show how a diffusion equation with highly oscillatory coefficients can be solved by simple preconditioning and multigrid methods. We will then demonstrate how these simple methods would deteriorate if the coefficients have large discontinuous jumps and how these methods can be made more robust. We will continue the talks with new techniques for several other equations including Maxwell equations, Stokes equations and its coupling with Darcy's law.

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IP 10
The worst scenario method: a red thread running through various approaches to problems with uncertain input data

Uncertain inputs appear in many, if not all, industrial problems; methods to tackle uncertainties are numerous as well. Among them, the worst scenario method plays a significant role as either a self-contained method or a fundamental sub-method of other methods.
The method has three main ingredients: $\mathcal{U}_{\text{ad}}$, a set of admissible data; $A(a)u = f(a)$, a state problem dependent on $a \in \mathcal{U}_{\text{ad}}$; and $\Phi(a, u)$, a criterion functional evaluating a quantity of interest that directly depends on u and, possibly, on a; take local stress, temperature, or velocity, for example. The worst scenario problem lies in finding a^0 that maximizes $\Phi(a, u(a))$, where $u(a)$ solves the state problem and $a \in \mathcal{U}_{\text{ad}}$. If $\Phi(a, u(a))$ is continuous with respect to a and $\mathcal{U}_{\text{ad}}$ is compact, a^0 exists. Then $\Phi(a^0, u(a^0))$ maximizes the quantity of interest.
If a_0, the minimizer of $\Phi(a, u(a))$ over $\mathcal{U}_{\text{ad}}$ (the best scenario), is obtained, then the range of $\Phi(a, u(a))$ over $\mathcal{U}_{\text{ad}}$ is defined by the interval $[\Phi(a_0, u(a_0)), \Phi(a^0, u(a^0))]$.
Although the knowledge of the range of Φ is useful in modeling with uncertainty, a potential weakness is that a not only belongs to $\mathcal{U}_{\text{ad}}$, but is also often weighted in some sense. In fuzzy set theory, the weight is represented by a membership function $\mu_{\mathcal{U}_{\text{ad}}} : \mathcal{U}_{\text{ad}} \to [0, 1]$, and the goal of computation is to infer the membership function for $\Phi(a, u(a))$. This goal can be achieved by finding the ranges of Φ over $\{\mathcal{U}_{\text{ad}}^{\alpha}\}$, an α-controlled sequence of embedded subsets of $\mathcal{U}_{\text{ad}}$ (known as α-cuts in fuzzy set theory). That is, an α-dependent sequence of the worst and the best scenarios is to be found.
A similar sequence appears in information-gap theory, where α is interpreted as a parameter controlling the acceptable amount of uncertainty in inputs.
In evidence theory applied to models with uncertainty, subsets of the admissible set are weighted, or even different admissible sets can be considered, each with its own weight (called basic probability assignment in this theory). To construct two key functions, namely the belief function and the plausibility function, the weights have to be transferred from the input data set to the output quantity of interest. In other words, the relevant ranges of Φ have to be inferred, that is, again, the worst and the best scenarios have to be found.
It is not uncommon to deal with uncertain scalar parameters. In models based on differential equations, however, uncertain functions appear as coefficient functions or right-hand sides, for instance. Consequently, the focus will be on the worst (best) scenario in admissible sets of functions.
Some theoretical results of the worst scenario method will be presented. These include the existence of both the worst scenario (WS) and an approximate worst scenario (AWS) as well as the convergence of the AWS to the WS. The continuous dependence of $u(a)$ on $a \in \mathcal{U}_{\text{ad}}$ is fundamental to the worst scenario method; the continuity (in a proper function space) has been proved for a number of nonlinear state problems used in the mechanics of deformable solids, heat conduction, etc.
Special attention will be given to fuzzy sets of input functions. Although various concepts of fuzzy state solutions have been proposed, the above-mentioned approach based on crisp state solutions and the α-cut technique is ready for applications.

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MS1
Fast Marching Semi-Lagrangian Methods for Hamilton-Jacobi Equations

The development of fast methods for partial differential equations related to the level-set method has attracted several researchers in the last few years (see e.g. [4] for the origins of these methods, [3] for a recent sweeping method and [5] for the ordered upwind method). We introduce two fast marching methods which are extensions of the semi-Lagrangian FM (FM-SL) method presented in [1]. The first extension is a tentative to accelerate convergence using the informations driven by the characteristics and looks like a clever group marching method. The second extends the original scheme in order to deal with anisotropic front propagation and non convex Hamiltonian (e.g. the Isaacs equation related to differential games)

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MS1
Discretization of Hamilton-Jacobi Equations on Unstructured Triangulations

We discuss a piecewise linear discretization of Dirichlet problems for static Hamilton-Jacobi equations on unstructured triangulations. The discretization is based on simplified localized Dirichlet problems that are solved by a type of Hopf-Lax formulas. This idea generalizes several approaches known in the literature and allows for a simple and transparent convergence theory. We present recent results on convergence rates, error propagation, and the complexity of discrete solvers.

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MS1
Recent advances on large time-step schemes for degenerate second-order equations and Mean Curvature Motion

In this talk we present a review of some recent works on the application of Semi-Lagrangian (SL) techniques to second-order, possibly degenerate, parabolic equations. Most of the emphasis will be given to the model problem of the Mean Curvature Motion, which leads, in the framework of level set techniques and restricting to the codimension-1 case, to the equation

$$\begin{cases} v_t(x,t) = \operatorname{div}\left(\frac{Dv(x,t)}{|Dv(x,t)|}\right) \ |Dv(x,t)| \quad \text{in } R^N \times (0,T) \\ v(x,0) = v_0(x). \end{cases} \tag{1}$$

A basic SL scheme for (1) has been proposed in [4]. In subsequent works, this idea has been extended to treat the codimension-2 case in [1] and the stationary version of (1) in [3]; moreover, a first study of adaptivity has been performed in [2].

In the talk, we will present the main ideas underlying this approach, show how such ideas can be applied to the various situations and try to compare SL schemes with more conventional methods.

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MS1
A Generalized Fast Marching method applied to dislocations dynamics

We study dislocation dynamics with a level set point of view.
The model represents a dislocation in a 2D plane by the zero level set of the solution of a non local and non convex eikonal equation. We first present a new Fast Marching algorithm for a non-convex eikonal equation modeling front evolutions in the normal direction [1]. The algorithm is a generalization of the Fast Marching Method [3] since the new scheme can deal with a *time-dependent* velocity without *any restriction on its sign.* We prove its convergence in the class of discontinuous viscosity solutions [2]. We then extend the algorithm to evolutions with non local speed and we present some numerical simulations of fronts propagating in $\mathbb{R}^2$ applied to dislocations dynamics.

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MS2
The Ghostfluid Method as a Multi-Scale Method for Compressible Flow with Phase Transitions

The dynamics of a compressible fluid which occurs in a liquid and a vapour phase can be described on the continuum mechanical level as a free boundary problem where the bulk phases are governed by the Euler equations (or the Navier-Stokes equations in viscous media). Close to phase changes additional informations which can be obtained by solving micro-scale problems are important to guarentee the wellposedness of the overall model. These additional informations can be computed by e.g. construction of so-called kinetic relations or solving locally more accurate models like phase field models. We propose a heterogenous multiscale method that provides the possibility to use both micro-scale models mentioned before and present a number of numerical examples. The core tool is a generalization of the ghostfluid approach that has been developed originally to resolve contact discontinuities.

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MS2
Higher Order Methods for Simulation of Liquid-Vapor Flows with Phase Change

We consider a fluid of Korteweg type that can undergo liquid-vapor phase transitions, i.e. a fluid that can be modelled by the Navier-Stokes-Korteweg equations.

$$\begin{aligned}
&\rho_t + \nabla\cdot(\rho\mathbf{u}) = 0,\\
&(\rho\mathbf{u})_t + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p(\rho,\theta) = \nabla\cdot(\tau + K),\\
&E_t + \nabla\cdot\big((E+p(\rho,\theta))\mathbf{u}\big) + \lambda\nabla\cdot\big(\rho(\nabla\cdot\mathbf{u})\nabla\rho\big)\\
&= \nabla\cdot\big((\tau+K)\mathbf{u}\big) + \kappa\Delta\theta,\\
&\qquad \rho(\cdot,0)=\rho_0,\quad \mathbf{u}(\cdot,0)=\mathbf{u}_0,\quad \theta(\cdot,0)=\theta_0.
\end{aligned}$$

This system belongs to the class of Diffuse-Interface models where the liquid and vapor phases are characterized by the value of the density. The unknowns are the density $\rho > 0$, the velocity $\mathbf{u}$ and the temperature $\theta > 0$. The function p is given by a van-der-Waals equation of state, τ is the usual Navier-Stokes tensor, $E = E(\rho, \mathbf{u}, \theta, |\nabla\rho|)$ the total energy of the system and K the Korteweg tensor

$$K = \lambda\left[\left(\rho\Delta\rho + \frac{1}{2}|\nabla\rho|^2\right)I - \nabla\rho\nabla\rho^T\right], \quad \lambda > 0.$$

The system is known to cause problems on the discrete level when nontrivial static equilibrium configurations are present. To avoid numerical artefacts we have developed (well balanced) higher order methods based on a non conservative reformulation of the system. In order to resolve the diffuse interface (for real world applications very small) techniques like local mesh adaption and parallelization have to be applied.
I will present higher order methods based on the Discontinuous Galerkin approach for the numerical treatment of the isothermal and temperature dependent Navier-Stokes-Korteweg system in multiple space dimensions.

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MS2
Ghost fluid methods for computations of interfaces flows

We consider the numerical computation of an interfaces flow with compressibles fluids. Therefore, we focus on numerical strategies based on the Ghost Fluid Method (GFM) formulation. In this context, the position of the interface is defined as the zero of a level set function. The evolution of the level set function, governed by a transport equation related to the fluid velocity, will define the location of the interface where some transmission conditions are needed. For conservative fluid models and finites volumes approximations, this can be resumed to a flux evaluation between two states associated to different equations of states (EOS). The main principle of the Ghost Fluid Method is to project the different states around the interface using the other EOS. The projection are Ghost fluids that are implicitly used for flux computation and thereby for wave transmition. The original GFM method considers a projection where pressure, normal velocity and entropy in a cell are preserved in the associated Ghost cell. To prevent overheating errors, the densities are fixed from appropriated neighbour cells. However, this method have some inconsistency that makes it unefficient when the fluids are very different. The modified GFM and single fluid (SFM) methods seems to overcome this problem by defining a projection based on the solution of a suitable approximated Riemann problem. We will investigate these approches for multi dimensional flow and propose numerical strategies on unstructured mesches. In particular, the transport of the level set function will be approximated by a high order discontinu Galerkin method.

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MS2
Numerical Simulation of Cavitation Bubbles by Compressible Two-Phase Fluids

The present work deals with the numerical investigation of collapsing cavitation bubbles in compressible fluids. Here the fluid of a two-phase vapor-liquid mixture is modeled by a single compressible medium. This is characterized by the stiffened gas law using different material parameters for the two phases.
For the discretization of the stiffened gas model the approach of Saurel and Abgrall [1] is employed where the flow equations, here the Euler equations, for the conserved quantities are approximated by a finite volume scheme and an upwind discretization is used for the non-conservative transport equations of the gas fraction by which the different phases are indicated. The original 1st order discretization is extended to higher order applying 2nd order ENO reconstruction to the primitive variables. The derivation of the non-conservative upwind discretization for the gas fraction is presented for arbitrary unstructured grids. The efficiency of the numerical scheme is significantly improved by employing local grid adaptation. For this purpose multiscale-based grid adaptation [2,3] is used in combination with a multilevel time stepping strategy [4] to avoid small time steps for coarse cells. The resulting numerical scheme is then applied to the numerical investigation of the collapse of a vapor bubble near to a rigid wall [5]. These computations reveal new insight to the mechanism of the bubble collapse and the formation of a liquid jet penetrating the bubble and hitting the wall. The impact of the jet causes a high pressure load to the wall that can cause severe material damage.

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MS3
Computational methods for surface PDEs

Partial differential equations on evolving surfaces occur in many applications. For example, traditionally they arise naturally in fluid dynamics and materials science and more recently in the mathematics of images. In this talk we describe computational approaches to the formulation and approximation of transport and diffusion of a material quantity on an evolving surface in $\mathbb{R}^{n+1}$ (n=1,2). We have in mind a surface which not only evolves in the normal direction so as to define the surface evolution but also has a tangential velocity associated with the motion of material points in the surface which advects material quantities such as heat or mass. For our purposes here we assume that the surface evolution is prescribed. We describe the evolving surface finite element method (ESFEM) based on triangulated surfaces and an Eulerian approach in which surface PDEs are solved on all level surfaces of a prescribed level set function. This is joint work with G. Dziuk.

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[3] G. Dziuk and C. M. Elliott *Eulerian finite element method for parabolic equations on implicit surfaces* Interfaces and Free Boundaries (submitted)

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MS3
Computational Willmore Flow

We discuss discretization techniques for the elastic flow of parametric surfaces. Willmore flow is the L^2-gradient flow of the classical bending energy

$$W(\Gamma) = \frac{1}{2}\int_\Gamma H^2$$

where H is the mean curvature of the surface Γ. We derive a new finite element algorithm for the system of nonlinear PDEs, which describes Willmore flow. This algorithm is easy to implement and it is stable in adequate norms. We also show how the algorithm can be generalized to anisotropic Willmore flow.

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MS3
Multigrid methods for the discretized Beltrami operator on arbitrary surfaces

We present a multigrid approach to finite element dicretizations of the Laplace–Beltrami operator as introduced in [1]. In contrast to existing algorithms as considered, e.g. in [2], our approach does not make any use of a parametrization of the underlying surface Γ. Assuming that the approximating piecewise triangular surface Γ_h has a logical refinement structure, we prove polylogarithmic bounds that rely only on the ellipticity of the operator and on the shape regularity of the (planar) triangles. Full mesh independence can be shown under additional assumptions. Numerical experiments illustrate our theoretical findings. A brief outlook on the treatment of discretized phase field equations on manifolds will conclude the talk.

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MS3
Global Parametrization of Surface Meshes

We introduce an algorithm for the automatic computation of a global parameterization of arbitrary simplicial 2-manifolds. The parameter lines are guided by a given frame field, for example, by principal curvature frames. The parametrization is globally continuous and allows a remeshing of the surface into quadrilaterals.
The algorithm converts a given frame field into a single vector field on a branched covering of the 2-manifold, and then generates an integrable vector field by a Hodge decomposition on the covering space. Except an optional smoothing and alignment of the initial frame field, the algorithm is fully automatic and generates high quality quadrilateral meshes.

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MS4
Passivity Preserving Model Reduction

Preservation of passivity is an important aspect of model order reduction. This is particularly important in circuit simulation applications. This talk will present a methodology for passivity preserving model reduction based upon approximate computation of a basis for a selected invariant subspace of a block structured skew-symmetric/symmetric matrix pencil. This pencil is constructed so that its eigenvalues are the spectral zeros of the transfer function of a related linear time invariant system. It is shown how to construct low rank approximate solutions to Algebraic Riccati Equations (ARE) , in particular to the maximal and minimal symmetric solutions.
Approximate passive balancing is obtained via approximate low rank factored form solutions of ARE that are minimal for reachability and observability Riccati equations respectively. Balanced reduction is derived from the minimal passive low rank factors. This leads to approximation results that guarantee stability, passivity and balancing for every truncation obtained from the balanced Riccati equations.

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MS4
Structure-Preserving Model Reduction for Resonant MEMS

In the design of resonant micro-electro-mechanical systems (MEMS), controlling the amount of damping is critical. These simulations lead to non-Hermitian problems which depend nonlinearly on a frequency parameter. In this talk, we discuss model reduction methods which use two types of structure present in the full discrete model: algebraic structure, such as complex symmetry of the system matrices, that is inherited from the underlying PDEs; and geometric structure, such as the presence of beam-like or plate-like components. We illustrate our methods with models of anchor loss and thermoelastic damping in a variety of resonant microstructures.

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MS4
MOR for coupled simulations of RF systems

In this presentation, we will address the problem of simulating complete RF blocks. As it is not possible to simulate such blocks as one entity, a divide and conquer approach needs to be used. A complicating issue is the fact that a combination of circuit, device and electromagnetic simulations is needed to adequately address the behaviour of such systems. After having simulated the different parts of the RF block, model order reduction techniques are used to reduce the size of the systems to be coupled. The coupling of the blocks provides an additional problem, as straightforward coupling may lead to loss of passivity and other important properties. Several methods have been suggested. These will be discussed, as well as some recent new developments by our research group.

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MS4
Structured perturbation theory for inexact Krylov projection methods in model reduction

In this talk, we introduce the use of inexact solves in a Krylov-based model reduction setting and present the resulting structured perturbation effects on the underlying model reduction problem. For a selection of interpolation points that satisfy first-order necessary H_2-optimality conditions, a primitive basis remains remarkably well-conditioned and errors due to inexact solves do not tend to degrade the reduced order models. Conversely, for poorly selected interpolation points, errors can be greatly magnified through the model reduction process.
When inexact solves are performed within a Petrov-Galerkin framework, the resulting reduced order models are backward stable with respect to the approximating transfer function. As a consequence, Krylov-based model reduction with well chosen interpolation points is robust with respect to the structured perturbations due to inexact solves. General bounds on the H_2 system error associated with an inexact reduced order model are introduced that provide a new tool to understand the structured backward error and stopping criteria.

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MS5
Finite volume level set methods for moving curves and surfaces

We present finite volume computational schemes for solving level set formulations of curve and surface evolution driven by advection, (weighted) mean curvature and laplacian of curvature. First order advective part represents externally given velocity field or motion of an interface in normal direction, the higher order curvature terms express dependence of the flow on surface and elastic energies. Particular attention will be given to image processing applications.

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MS5
A dynamical versus a variational approach for the computation of the effective Hamiltonian

We introduce two discretizations for two different approaches for the computation of the effective Hamiltonian. In both cases, for each value of the effective Hamiltonian, we deal with a PDE on a periodical domain. A semi-Lagrangian method is applied to compute a viscosity solution of the originally convex Hamiltonian, and a finite difference scheme is applied for the discretization of the Eulero-Lagrange equation related to the variational formulation. Both solutions are further exploited to give some approximation of the so called Aubry-Mather set.

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MS5
A shape and topology optimization technique for the solution of obstacle problems

In this talk a new numerical approach for solving a class of state constrained minimization problems in function space is presented. The aim is to develop a method which exhibits a mesh independent behavior. The key ingradients in the development are a reformulation of the original problem as a shape resp. topology optimization problem. Then tools from topological and shape sensitivity are employed for computing descent flows for minimizing the objective. The numerical realization is based on level set framework. The talk ends by a report on numerical results including a comparision of the new technique with a primal-dual active set solver, which is considered to be highly efficient for the underlying problem class.

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MS5
On the partially open table problem for sandpiles

We study the mathematical characterization and the numerical approximation of stationary solutions for the growing sandpile model on a partially open flat support under the influence of a vertical source. We are able to extend a previous result of [1] for the completely open table case. The presence of walls on a subset of the boundary strongly affects the regularity of such solutions, since the tangential component of the surface sand flux can now be discontinuous. At a numerical level suitable techniques have to be employed for a good resolution of solutions across such discontinuity region. We discuss the results of some simulations on different test problems. [Work in collaboration with G. Crasta and M. Falcone]

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MS6
Balancing-Related Model Reduction for Parabolic Control Systems

We will discuss model reduction techniques for (optimal) control of dynamical processes described by parabolic partial differential equations from a system-theoretic point of view. The methods considered here are based on spatial semi-discretization of the PDE followed by balanced truncation techniques applied to the resulting large-scale system of ordinary differential equations. Several choices of the system Gramians that are used for balancing will be presented. We will discuss open-loop and closed-loop techniques that allow to preserve system properties important for controller design as shown in [3]. Furthermore we will discuss an error estimate based on a combination of FEM and model reduction error bounds. We will also discuss how the state of the full-order system can be recovered from the reduced-order model. We will survey different implementation approaches for sparse and data-sparse systems following ideas given in [1,2,4]. Several numerical examples will be used to demonstrate the proposed model reduction techniques.

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MS6
POD Model Reduction: Parameter Estimation for nonlinear elliptic sytems and a-posteriori error estimates

Proper orthogonal decomposition (POD) is a powerful technique for model reduction of linear and nonlinear systems. It is based on a Galerkin type discretization with basis elements created from the system itself. In this talk POD is applied to estimate parameters in nonlinear elliptic partial differential equations (PDEs). The parameter estimation is formulated in terms of an optimal control problem that is solved by an augmented Lagrangian method combined with a sequential quadratic programming (SQP) algorithm. Numerical examples illustrate the efficiency of the proposed approach. In the second part of the talk, a-posteriori error analysis is carried out to estimate the distance between the computed suboptimal control and the unknown optimal control. From this information, one can determine the number of POD basis functions that are applied in the Galerkin projection of a linear-quadratic optimal control problem in such a way that the error between the suboptimal control and the optimal control is less than a given tolerance.

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MS6
Applications of Reduced Order Models in Finance

Pricing of derivatives can be carried out either by a solution formula in several instances or in the more general case by solving a system of stochastic ordinary differential equations numerically or by solving a partial differential equation. If one considers model calibration, it is necessary to solve these many times in the course of the optimization. In this talk, we explore the possibility to use reduced order models for the partial differential equation in particular and discuss the feasibility of this approach.

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MS6

Reducing a Rational Eigenproblemn in Fluid-Structure Interaction by AMLS

Over the last few years, a new method for huge eigenvalue problems, known as *Automated Multi–Level Substructuring (AMLS)*, has been developed by Bennighof and co-authors [1], and has been applied to frequency response analysis of complex structures. Here the large finite element model is recursively divided into very many substructures on several levels based on the sparsity structure of the system matrices. Assuming that the interior degrees of freedom of substructures depend quasistatically on the interface degrees of freedom, and modeling the deviation from quasistatic dependence in terms of a small number of selected substructure eigenmodes, the size of the finite element model is reduced substantially yet yielding satisfactory accuracy over a wide frequency range of interest.
Recent studies in vibro-acoustic analysis of passenger car bodies where huge FE models with more than six million degrees of freedom appear and several hundreds of eigenfrequencies and eigenmodes are needed have shown that AMLS is considerably faster than Lanczos type approaches for this sort of problems [3].
In this presentation we discuss the application of AMLS to a rational eigenvalue problem governing free vibrations of a fluid–solid structure [2].

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MS7
ESFEM for DIGM

We apply the new evolving surface finite element method (ESFEM) of Dziuk and Elliott [2] coupled with the parametric finite element approximation of evolving hypersurfaces presented in [1] to the following model for diffusion induced grain boundary motion (DIGM), see [3]

$$V = \kappa + f(c) \tag{2}$$

$$\dot{c} = \Delta_\Gamma c - V\kappa c - Vc \quad \text{on } \Gamma(t). \tag{3}$$

Here $\Gamma(t)$ is an evolving hypersurface in $\mathbb{R}^3$ with normal velocity V and mean curvature κ. Furthermore Δ_Γ denotes the Laplace - Beltrami operator and $\dot{c}$ denotes the material derivative of the scalar function c.
We use the techniques presented in [1] to derive a parametric finite element approximation for the forced mean curvature evolution law (2) and combine this with an ESFEM scheme for (3) that is obtained using techniques from [2]. We then present some numerical results.

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MS7
Stable Finite Elements for Unfitted Meshes.

One example of a mesh-less method for the discretisation of partial differential equations are *unfitted finite elements* [1] where the computational domain $\Omega \subset G$ is a subset of a large container G which is triangulated by a fixed finite element mesh $\mathcal{T}_h$. In this setting the triangulation $\mathcal{T}_h$ is not fitted to the boundary of the computational domain Ω; instead, the domain of integration is restricted to Ω during the assembling of the discrete system of equations. Typically, one loops over all elements $T \in \mathcal{T}_h$ but the actual per-element contributions are computed by integration only with respect to $T \cap \Omega$. The use of unfitted finite elements can be beneficial, for example, in the context of transient free boundary problems where the use of a moving mesh method can lead quickly to mesh-degeneration, or when tracking of topological changes is desired, or when the computational domain becomes very complicated. For geometric problems unfitted finite elements come into play in the context of an unaligned narrow band method recently proposed by C.M. Elliott.
The direct application of unfitted finite elements, however, leads to a loss of control over the spectral condition number of all involved discrete linear systems. This is clear because $\inf_{T\cap\Omega\neq\emptyset} |T \cap \Omega|$ can be uncontrollably small and thus the associated stiffness matrices may have rows which are almost zero. In this sense the direct application of the unfitted finite element method leads to a discretisation which is unstable. Luckily it is possible to overcome this problem by carrying over techniques developed in [2] for the context of B-Splines on Cartesian grids to standard Lagrangian finite elements. The result are stable finite elements for unfitted meshes which still possess the same asymptotic approximation properties as the unmodified finite element spaces.

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MS7
Error Analysis of a Semidiscrete Numerical Scheme for the Evolution of Elastic Curves

The gradient flow for the elastic energy of curves in $\mathbb{R}^n$ leads to the fourth order parabolic PDE

$$f_t = -\partial_s^2\vec{\kappa} - \frac{1}{2}|\vec{\kappa}|^2\vec{\kappa} + \lambda\vec{\kappa} \quad \text{in } [0,1]\times(0,\infty) \qquad (4)$$

$$f(0) = f_0 \quad \text{in } [0,1]. \qquad (5)$$

Here, $f : [0,1]\times(0,\infty) \to \mathbb{R}^n$ is periodic in space, $\vec{\kappa} = \partial_s^2 f$ is the curvature vector and ∂_s denotes differentiation with respect to arclength. Furthermore, $\lambda > 0$ and $f_0 : [0,1] \to \mathbb{R}^n$ are given. Based on a suitable weak formulation of (4) which uses the parametrization f and the curvature vector $\vec{\kappa}$ as variables we suggest a numerical scheme in order to approximate solutions of (4), (5). We present error estimates for the relevant geometric quantities and show examples of test calculations.
Global existence of smooth solutions of (4), (5) has been obtained in [3]. Other numerical schemes which are equally based on a variational formulation and also employ a splitting idea but are different from ours were suggested in [1] and [2].

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MS8
Taut String Algorithm for High Dimensional Data

We study the problem of density estimation with total variation minimization. the basic ingredient is an equivalence relation between the taut-string algorithm and total variation minimization. Moreover, we show scale-space properties of total variation minimization which allows to explain the taut-string algorithm as a two-step algorithm. This explanation allows to generalize the algorithm to higher dimension, using Voronoi-Diagrams and filtering of pre-processed data. Moreover, we discuss various other filtering techniques.

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MS8
Solution of Ill-Posed Problems via Adaptive Grid Regularization

When studying (linear or nonlinear) ill-posed problems

$$F(x) = y, \quad F : \mathcal{D}(F)(\subset \mathcal{X}) \to \mathcal{Y},$$

where usually only noisy measurements y^δ of y with $\|y^\delta - y\| \le \delta$ are given, $\mathcal{Y}$ is a Hilbert space and $\mathcal{X}$ is a Banach space, it is well known by now that standard regularization methods are not appropriate for ill-posed problems with discontinuous solutions, since they have a smoothing effect on regularized solutions.
If one expect discontinuous solutions, special care has to be taken in choosing the regularization method. Bounded variation regularization has turned out to be an efficient method when dealing with such problems. An other approach is regularization for graph and surface representations. Based on these ideas, the author recently developed a new method, namely *adaptive grid regularization*, an iterative method, where local grid refinement techniques are combined with adaption of the regularizing norm after each iteration. The method has already been successfully applied to linear integral equations and nonlinear parameter estimation problems in 1D and 2D. Thenumerical results show that this method is an efficient and fast tool to identify discontinuities of solutions of ill-posed problems. Numerical results and convergence results are presented.

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MS8
Regularization by Fractional Filter Methods and Data Smoothing

We aim at the regularization of linear ill-posed problems by a combination of a data-smoothing operator and a so-called *fractional filter operator*. Given an operator equation

$$Kf = g$$

with linear, compact operator K and noisy data $g^\delta = g + \delta \mathrm{d}W$ with additive white noise of known error level δ, we construct an approximation $f_{\alpha,\lambda}$ as follows: First we apply a smoothing operator S_λ to g^δ to gain a data estimate $\tilde{g}$ and second we apply a reconstruction operator R_α to $\tilde{g}$,

$$f_{\alpha,\lambda} := R_\alpha S_\lambda g^\delta \ .$$

For the data smoothing we use wavelet shrinkage denoising whereas for the reconstruction we use *fractional filter methods*. These fractional filter methods are based on the standard Tikhonov (or Landweber) filter function but use only a certain fraction of the filter. By that, the fractional methods avoid at least partially the well-known effect of oversmoothing. This is demonstrated by the simple numerical example of reconstructing a function with a discontinuity, e.g. the step function, from its integral.
We prove order-optimality of the fractional methods and convergence rates for the combined method of wavelet shrinkage and fractional methods.

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MS8
A multilevel regularization method for nonlinear problems with applications in hysteresis and crack identification

Combining the idea of regularization by discretization with an iterative solution aspect, we propose a multilevel regularization method for nonlinear ill-posed operator equations

$$F(x) = y$$

as follows: Considering a sequence of projections Q_l onto finite dimensional subspaces $(Y_l)_{l\in\mathbf{N}}$ of data space Y, we minimize the distance of x to an initial guess under a constraint on the norm of the projected residual

$$\min \|x - x_0\|^2 \ \text{ s.t. } \ \|Q_l(F(x) - y^\delta)\|^2 \le \eta_l^2 \,, \qquad (PI_l)$$

where η_l is a sequence of tolerances tending to zero with

$$\eta_l \ge \delta \ ,$$

for all discretization levels under consideration. (In here δ dentotes the data noise level, hence there is a correspondence to the well-known discrepancy principle.) Using a solution of (PI_l) as a starting guess for the iterative minimization of (PI_{l+1}), one arrives at a multilevel method.
Advantages of this approach are the following:
By the use of information on coarser levels of discretization, one gains efficiency especially for large scale or nonlinear problems.
Restrictions on the nonlinearity of the forward operator as typically required for a convergence (rate) analysis in the context of nonlinear ill-posed problems can be considerably relaxed.
A start on a very coarse discretization as well as appropriate continuation between sucessive levels enable to define a globally convergent iterative method.
Convergence rates under source conditions can be established.
Finite dimensional projection in data space naturally arises in several applications.
After a derivation of the method and a short discussion of each of the points above, we will especially focus on the last one in this talk. For this purpose, we will show two application examples, namely the identification of hysteresis operators for material characterization and the nondestructive detection of cracks. Numerical results will illustrate the theoretical findings.

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MS9
Nonparametric Deconvolution Approaches for Dynamic Contrast Enhanced Magnetic Resonance Imaging and a Proposed Theory of Tracer Transport.

Efforts to perform nonparametric deconvolution for the determination of tissue transport properties led to a proposed revision of the theory of tracer transport. Counterexamples are used to motivate the revision of the established theory. Then dynamic contrast enhanced magnetic resonance imaging in particular is conceptualized in terms of a fully distributed convection-diffusion model from which a widely used convolution model is derived using, alternatively, compartmental discretizations or semigroup theory. On this basis, applications and limitations of the convolution model are identified. For instance, it is proved that perfusion and tissue exchange states cannot be identified on the basis of a single convolution equation alone. Yet under certain assumptions, particularly that flux is purely convective at the boundary of a tissue region, physiological parameters such as mean transit time, effective volume fraction, and volumetric flow rate per unit tissue volume can be deduced from the kernel. On this basis, a deconvolution framework is developed which constrains the convolution kernel to be non-increasing. Under this constraint it is proved that kernel estimates have bounded variation and thus readily manifest a well known staircasing effect. Further regularization is implemented by the choice of a function basis. Both spline bases and exponential bases are investigated. For exponential bases a condition for monotonicity is derived which is a considerable generalization over a previous condition implying complete monotonicity. Spline bases are found to be better suited for reconstructing kernels corresponding to plug flow, but exponential bases are found to be better suited to typical physiological data. Therefore the exponential approach is applied to dynamic contrast enhanced magnetic resonance imaging data to determine physiological parameters pixelwise to visualize a cerebral tumor, and the results are compared favorably with those of the standard Truncated Singular Value Decomposition approach.

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MS9

Mathematical models and numerical simulation of drug release from stents

Drug eluting stents (DES) are apparently simple medical implanted devices used to restore blood flow perfusion into stenotic arteries. However, the design of such devices is a very complex task because their performance in widening the arterial lumen and preventing further restenosis is influenced by many factors such as the geometrical design of the stent, the mechanical properties of the material and the chemical properties of the drug that is released.

In this framework, numerical simulation techniques play a relevant role in understanding what are the most appropriate choices for the optimal design of DES. The main computational difficulties arise from the need to deal with phenomena that take place on multiple scales in space and time. Concerning the space scales, we remind that DES for cardiovascular applications are miniaturized metal structures that are coated with a micro-film containing the drug that will be locally released into the arterial walls for healing purposes. The thickness of this film generally lays within the range of microns. As regards the time scales, we observe that the release of drug is deliberately very slow. In general, it persists until a few weeks after the stent implantation.

To address these topics, we start from a general model for mass transfer through heterogeneous media, consisting on an advection-diffusion-reaction equation for each different layer of material or tissue into the stent and the arterial walls, see for instance [1]. Such model has already been applied in [2] for computational studies about drug release from stents. However, we point out that simulation studies based on this model involve extremely high computational costs and by consequence, to our knowledge, only studies concerning simplified stent geometries have been pursued so far. Starting from this point, we propose a reduced model for mass transfer from a thin layer, which significantly cuts down the computational cost for the simulation of the drug release from stents. Another difficulty arise from the fact that the release of the drug represents a stiff problem, whose numerical approximation requires the application of an adaptive stepping strategy. Combining these techniques it is possible to obtain simulations involving realistic expanded stent geometries, obtained in [3], and long time scales. The efficacy of our approach is demonstrated by means of numerical results concerning realistic situations.

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MS9

Multiscale modelling of tumour growth, angiogenesis and blood flow

A multiscale model for vascular tumour growth is presented which includes subcellular and tissue levels within an individual-based framework for cancerous and normal cells, with blood flow through an embedded vascular network. The vascular network is dynamically remodelled in response to environmental stimuli (such as flow rates and oxygen levels) via the growth of new vessels and the death of collapsed vessels. Interactions between the spatial scales are mediated in part by reaction-diffusion equations for the spatio-temporal dynamics of nutrient and key signalling chemicals, which couple to systems of ordinary differential equations for the cell cycle and apoptosis (programmed cell death) in individual cells. We present studies of the invasive behaviour of tumour cells and the tumour's response to chemotherapy. In particular, we find that enhanced cell movement increases the rate of tumour growth and expansion, but that increasing the tumour cell carrying capacity leads to the formation of less invasive dense hypoxic tumours containing a smaller total number of tumour cells. For many parameter regimes, the model sustains large spatio-temporal fluctuations in oxygenation, and hence in the numbers of cells of different types. Such fluctuations can dramatically affect drug delivery and the efficacy of chemotherapy. With regard to angiogenesis and vascular remodelling, we find that the average vascular density in normal tissue can adapt to the metabolic demands of the healthy tissue that it perfuses. When cancer cells are added, they can cause collapse of existing vessels, regions of oxygen deprivation, and hence significant new vessel growth.

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MS10
Benchmarking for FSI

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MS10
About coupling issues in steady/unsteady numerical aeroelastic analyses of aircraft configurations

Experimental aeroelastic testing can be costly, time consuming and in some cases even unfeasible. Consequently, there is a growing demand for accurate and efficient numerical methods, which reliably predict the aeroelastic behaviour of present-days aircrafts at early design stages regarding flight performance and static/dynamic flight stability margins.
Following these needs the numerical aeroelastic method SOFIA is progressively developed within the Collaborative Research Center (SFB) 401 "Flow Modulation and Fluid-Structure Interaction at Airplane Wings" at RWTH Aachen University [1]. Due to missing monolithic solution methods SOFIA couples well-established and validated numerical solution methods for compressible fluid flow and structural deformation in terms of a partitioned method. In SOFIA the 3D time-dependent compressible RANS equations are solved using currently either the FLOWer or TAU code. The elastic structure of wing or aircraft configurations is modeled in SOFIA preferably by quasi-1D multi-axial Timoshenko beams, but detailed structural representations using shell or solid elements are supplementally available in the in-house FE solver FEAFA, which is used to compute the time-dependent structural deformation.
The transfer of aerodynamic loads and structural deformations between both partitions is controlled via the in-house Aeroelastic Coupling Module (ACM) in a discrete conservative manner over generally non-matching interface meshes [2,3]. Moreover, the temporal synchronisation of flow and structural solvers is provided by the ACM in a manner which follows the classifications given in [4,5,6]. Accordingly for unsteady aeroelastic problems different loose coupling schemes are available including extrapolation techniques for flow and structural deformation states as well as an imperative tight coupling scheme. For steady aeroelastic problems an under-relaxed block Gauss-Seidel scheme is used.
The presentation will focus on spatial coupling concepts realised in the ACM with emphasis on aspects of applications to elastic complex complete aircraft configurations. A second focus will be on the temporal coupling used in the ACM regarding stability, accuracy and efficiency properties during applications to elastic wing configurations.

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MS10
A FEM/multigrid solver for monolithic ALE formulation of fluid-structure interaction problem.

We investigate a monolithic algorithm for solving the time dependent interaction between an incompressible, possibly non-newtonian, viscous fluid and an elastic solid. The continuous formulation of the problem and its discretization is done in a monolithic way, treating the problem as one continuum and discretized by the Q2/P1 finite elements. The resulting set of nonlinear algebraic system of equations is solved by an approximate Newton method with coupled geometric multigrid linear solver for solving the linear subproblems. We discuss possible efficient strategies of setting up the resulting system and its solution. A 2-dimensional configurations is presented and compared to experimental data to test the developed method. It is based on the DFG benchmark *flow around cylinder* for incompressible laminar fluid flow and extended to fluid-structure interaction in [1].

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MS10
Fluid-structure interaction: ALE versus full Eulerian Formulation

When using an 'arbitrary Lagrangian-Eulerian' (ALE) framework, large deformations are known to lead to a breakdown of the solver. Well-known approaches to circumventing this are either a 'remeshing' of the problem or a 'fixed grid' approach. In the 'fixed grid' approach a combination of overlapping domain decomposition and chimera-like formulations are used. These approaches though entail an additional amount of data management, that would otherwise not occur 'out of the box'.
As an alternative we propose an Eulerian framework for the finite element approximation of fluid-structure interaction problems. The modeling is based on an Eulerian description of the (incompressible) fluid as well as the (elastic) structure. Thus an Eulerian framework does not encounter the same problems as the ALE approach, since the deformation data is stored in the spatial Eulerian reference frame and no transformation of the fluid domain onto a reference domain is needed. This is achieved by tracking the movement of the initial positions of all 'material' points. In this approach the displacement

appears as a primary variable in the Eulerian framework. Our approach uses a technique which is similar to the 'Level Set' method in so far that it also tracks initial data, in our case the movement of the 'Initial Position' (IP) set, and from this determines to which 'phase' a point belongs. To avoid the need for reinitialization of the IP set in the fluid domain, we employ the biharmonic continuation of the structural displacement field into the fluid domain. Results from [1] and further examples based on large deformations are presented.

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MS11
Nonlinear Tube Methods.

It is well known that onedimensional total variation regularization, that is, minimization of the functional

$$\mathcal{T}_\alpha(u) := \frac{1}{2}\int_a^b (u-u^\delta)^2 + \alpha|Du|(a,b)\,,$$

for given noisy data $u^\delta \in L^\infty(a,b)$, and $\alpha > 0$, is equivalent to the so called taut string algorithm (see [1,2,3]). The first step in this algorithm is the integration of the data: instead of u^δ one considers $U^\delta(x) := \int_a^x u^\delta(y)\,dy$. Now, one constructs a tube around U^δ consisting of all functions U such that $U(a) = U^\delta(a)$, $U(b) = U^\delta(b)$, and $|U(y) - U^\delta(y)| \le \alpha$ on (a,b). Within this tube the function U_α of minimal graph length is computed. The derivative of U_α then coincides with the minimizer of $\mathcal{T}_\alpha$.
In this talk a generalization of this method to more general onedimensional regularization functionals of the form

$$\mathcal{T}_{\Phi,\alpha,l}(u) = \int_a^b \Phi(u-u^\delta) + \alpha|D^l u|(a,b)$$

is discussed. Here, Φ is a strictly convex function attaining its minimum at zero, and $D^l u$ denotes the l-th order total variation of u.

It is shown that minimization of $\mathcal{T}_{\Phi,\alpha,l}$ again is equivalent to a higher order nonlinear tube method, where the tube consists of all those functions u such that the l-th primitive of the function $\Phi'(u-u^\delta)$ is smaller or equal than α and satisfies homogeneous boundary conditions up to order $l-1$. We show that the formulation as tube method immediately implies some properties of the minimizer u_α. Additionally, a unique characterization of u_α is provided.

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MS11
Inverse Jumps - From Asymptotic to Applications

Initially, the use of piecewise constant functions for regression has been proposed by [4], who called the corresponding reconstruction the regressogram. [4] proposed it as a simple explanatory tool. For a given set of jump locations, the regressogram simply averages the data between two successive jumps. A difficult issue, however, is a proper selection of the location of jumps and its convergence analysis. In this work we formalize this concept and investigate an l^0 penalized least square estimator which penalizes the complexity of the reconstruction by the number of intervals where the reconstruction is locally constant, or equivalently by the number of of jumps of the reconstruction. Compared to the total variation approach obviously, this method more easily captures extreme plateaus, but is less robust to outliers. This might be of interest in applications where extreme plateaus are informative, like for example in mass spectroscopy.
Moreover, we address the problem of estimating a jump function in the context of an inverse regression equation $Y_i = Kf(x_i) + \epsilon_i$, $i = 1, \ldots, n$, where K is a known (linear) integral operator and $f : [0,1] \to \mathbb{R}$ is the unknown function to be estimated. The x_i are (regular, possibly random) design points. It turns out that here a $\sqrt{n}$-rate of convergence is generic and and minimax, provided the kernel of K is bounded and continuous. In fact, the jump locations together with the jump sizes are asymptotically multivariate normal. To this end we require an identifiability condition related to the theory of radial basis functions on the kernel K, which turns out to be crucial for recovering jump functions in noisy inverse problems.
Asymptotic normality can be used to construct confidence bands for jump functions or for a piecewise linear regression function in multiphase regression.

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MS11
Generalized Rigid Image Registration and Interpolation by Optical Flow using Contrast Invariant Intensity Scaling.

A generalization of rigid image registration and interpolation is achieved variationally by penalizing a departure from rigidity of an optical flow. The image similarity measure is based upon the difference between scaled intensities. This similarity measure achieves contrast invariance purely by composition with scaling functions, while other contrast invariant measures are based upon differential formulations. Such rescaling is additionally found to have a smoothing effect on noisy images. Results obtained by Tikhonov regularization of scaling functions are superior to those obtained by a restricted set of basis functions. It is found that the computational cost for the implementation of scaling functions is very small, and yet the resulting image similarity can provide a match between images which is closer than that obtained by a sum of squared differences alone. The optical flow approach is investigated theoretically and numerically as well as with respect to a geometric multigrid solution process. For computations, a lumped finite element Eulerian discretization is used to solve the optimality system for the optical flow under natural boundary conditions. Also, a Lagrangian integration of the intensity along optical flow trajectories has the advantage of prohibiting diffusion among trajectories which would otherwise blur interpolated images. For the solution of the optimality system determining the optical flow, it is shown that the Hackbusch convergence criteria are met. Specifically, the Galerkin formalism is used together with a multi-colored ordering of unknowns to permit vectorization of a symmetric successive over-relaxation on image processing systems. The procedure is shown to be independent of image order. Also, it is shown that non-autonomous optical flows are theoretically possible, but that autonomous flows may be used in practice to achieve a great computational savings. This work is motivated by applications in histological reconstruction and in dynamic medical imaging, and results are shown for such realistic examples.

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MS11
Total Variation and Curves

We consider the approximation of data using total variation-based techniques. A multiresolution analysis of the residuals of an approximating function f provides a criterion to decide whether the function f is sufficiently close to the data or not. The idea is that for an adequate function the residuals should look like noise. Our aim will be to minimise complexity among all adequate functions. We use the model

$$y_i = Kf(t_i) + \varepsilon_i \qquad i = 1, \ldots, n,$$

where K is a linear operator and ε_i is white noise. We show how the idea can be combined with various forms of regularization to provide an adequate approximating function. One example is the minimization of the total variation which results in a function f with a small number of extreme values such that Kf_n gives a good approximation to the data.

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MS12
A multiscale model of thermoregulation in the cancer therapy regional hyperthermia.

Regional hyperthermia with microwave radiation is a cancer therapy aiming at heating deeply seated tumors in order to make them more susceptible to an accompanying radio- or chemotherapy. In the standard case, diffusion and cooling by perfusion of arterial blood dominate the temperature distribution. The talk presents a multiscale perfusion model that introduces a hierarchical coupling between vessels of different size as well as a regional coupling between tissue areas (steal effect). This multiscale model is able to reproduce effects observed in clinical practice and offers new possibilities for optimizing individual treatment plans. Numerical results for clinical data are presented.

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MS12
Cellular automaton simulation of tumour growth.

Deciphering the principles of tumour growth is crucial for the development of new therapy concepts. Besides increasingly complex molecular investigations, mathematical modelling and computer simulation of selected aspects of tumour growth have become attractive within the last few years (mathematical oncology). We are focusing on glioblastoma multiforme (GBM) which is the most frequent and most malignant primary brain tumour. A lattice-gas cellular automaton model allows for a straightforward integration of the anatomical brain structure. Sophisticated neuroimaging determines the spatial and temporal distribution of the proliferating and infiltrating tumour with respect to the brain parenchyma. In the talk, preliminary simulation results will be presented. In the future, we attempt to test by means of simulations different therapeutic scenarios (different degrees of resection, different time points for radiation and chemotherapy) for a given GBM patient. This requires development of 3D and multiscale models. Obviously, our approach can also be applied to other tumours. This project is conducted in close cooperation with other partners within the EU-Marie-Curie Network "Modeling, Mathematical Methods and Computer Simulation of Tumour Growth and Therapy".

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MS12
A multi-objective optimiser for intensity modulated radiation therapy planning.

Clinical radiation therapy is a tight rope walk between underdosing cancer tissue and overdosing critical structures. Ideal planning goals are given in terms of lower bounds for the curative dose in the target volume and tolerance doses for critical structures nearby. Typically, these ideal objectives are conflicting and there is a natural need to compromise between them. Therefore, it is natural to model optimisation of radiotherapy planning as a multi-criteria optimisation problem. The problem is to find good physical parameters that guarantee pareto optimal approximations of these ideal goals. Mathematically, this inverse problem can be formulated as a large scale convex multi-criteria program. In order to compute an approximation of a clinically relevant subset of the pareto solutions in reasonable computation time there is need for the definition of an appropriate numerical environment that allows numerous inverse calculation in short time.
In most planning systems optimization of IMRT is modelled as a large scale convex or non-convex nonlinear mathematical program, where typically the single objective funtion forms a weighted sum of costlets reflecting underdose or overdose measures with respect to ideal planning goals. Even in this environment a single run of such a mathematical program will take between half a minute and several minutes depending on the particular problem size.
We model the radiotherapy optimisation problem as a generic multicriteria problem. Our goal is to find a reasonable continuous (non-discrete) approximation of a clinically meaningful subset of the pareto set, which can be searched in real time by an intuitive navigation tool.
The talk will introduce mathematical models and numerical techniques for tackling these problems and will provide possible extensions and generalizations.

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MS12
Numerical Support for the Planning of Radio-Frequency Ablation.

The radio-frequency (RF) ablation is a promising minimally invasive treatment for lesions in the human liver: A probe containing electrodes is placed in the tumor and connected to a generator. Consequently an electric current flows through the tissue and heats it up to temperatures of more than 60 degrees Celsius. This leads to a coagulation of the cell's proteins and thus a destruction of the malignant tissue.
The success of the treatment heavily depends on a variety of patient-individual quantities, e.g. the local structure of the vascular system and material parameters like the water content of the tissue, its heat-capacity, its heat- and electric-conductivity, etc. So in the interest of the patient a thorough planning of the therapy must be made yielding an optimal position and orientation of the probe, and taking these important patient-individual properties into account.
The talk focusses on various aspects of a numerical support for the planning of an RF-Ablation. A balance between the rigorous mathematical modeling and applicability in the clinical practice is shown. On the one hand the talk presents the modeling of RF ablation. This leads to a system of partial differential equations for the forward simulation as well as an optimal control problem for the RF-probe. On the other hand robust heuristics based on the mathematical model are presented, which are specifically tailored to support certain aspects of the therapy planning process for RF ablation.

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MS13
Hybrid Discretization Methods for Aeroelastic Problems.

The radio-frequency (RF) ablation is a promising minimally invasive treatment for lesions in the human liver: A probe containing electrodes is placed in the tumor and connected to a generator. Consequently an electric current flows through the tissue and heats it up to temperatures of more than 60 degrees Celsius. This leads to a coagulation of the cell's proteins and thus a destruction of the malignant tissue.
The success of the treatment heavily depends on a variety of patient-individual quantities, e.g. the local structure of the vascular system and material parameters like the water content of the tissue, its heat-capacity, its heat- and electric-conductivity, etc. So in the interest of the patient a thorough planning of the therapy must be made yielding an optimal position and orientation of the probe, and taking these important patient-individual properties into account.
The talk focusses on various aspects of a numerical support for the planning of an RF-Ablation. A balance between the rigorous mathematical modeling and applicability in the clinical practice is shown. On the one hand the talk presents the modeling of RF ablation. This leads to a system of partial differential equations for the forward simulation as well as an optimal control problem for the RF-probe. On the other hand robust heuristics based on the mathematical model are presented, which are specifically tailored to support certain aspects of the therapy planning process for RF ablation.

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MS13
Progress on simulating the transonic aerolastic response of fighter aircraft

There is a continuing interest in CFD based aeroelasticity for several reasons. Behaviour observed in flight (F-16 LCOs, B2 residual pitch oscillations) probably requires more than linear potential aerodynamics. This has lead to simulation methods being developed which can calculate an aeroelastic response in the time domain by coupling CFD with an FEM code. The problem with this approach is practical the computational cost can be high. This has encouraged efforts to produce reduced order models of the aerodynamics which retain the fidelity of the full order system, but at a reduced cost.
The talk will describe efforts to make CFD based aeroelastic simulations routine for industrial collaborators. This has involved investigating various aspects of the time domain simulation, culminating in a number of demonstrations for real aircraft. Building on the time domain simulations, methods have been developed to investigate stability and system behaviour based on the eigenspectrum and associated eigenvectors. The aim of these methods is to represent the system behaviour at a cost comparable to steady state CFD simulations. Results will be presented for various model wings to illustrate the performance of these methods.

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MS13
Reduced Order Modeling of Unsteady Aeroelastic Analysis Using the Volterra-Wiener Theory

Direct numerical simulation of fluid structure interaction is a very important tool to fully understand the effects of wing elasticity on the efficiency and stability of a flight vehicle. Recent years have seen a lot of research and interest in this subject. The biggest drawback of the direct simulation of aeroelastic problems is the amount of computational time needed. This results in the research for reduced order modeling to be able to avoid large sets of direct simulations as needed during aircraft development.
During the 1930s Volterra developed a theory based on functionals that formulates the response of a nonlinear time-invariant system as an infinite sum of convolution integrals of increasing order. In the case of a weakly nonlinear system, such as most aeroelastic systems can be assumed, the magnitude of the higher order terms decreases rapidly, so that these can be neglected.
Be $y(t, x(t))$ the response of the aeroelastic system to an arbitrary input $x(t)$ then the matching volterra series is of the form

$$\begin{aligned} y(t,x(t)) &= \int_0^t h_1(t-\tau)\dot{x}(\tau)d\tau \\ &+ \int_0^t \int_0^t h_2(t-\tau_1, t-\tau_2)\dot{x}(\tau_1)\dot{x}(\tau_2)d\tau_1 d\tau_2 + \ldots \end{aligned}$$

where h_1 is the first order kernel, h_2 the second order kernel. The elastic body will be represented within $x(t)$ using the degrees of freedom of rigid body motion and natural modes of deformation vibration.
The Volterra-kernels need to be identified through direct aeroelastic simulation using pulse repsonses for every degree of freedom. In the linear range a single simulation run is needed for every degree of freedom. If non-linear dependence need to be modeled, then Volterra kernels of 2nd or even 3rd order will be needed. The price is a very high computational effort because of the multidimensional character of the convolution integral domains. But the result is a system description in its entirety. This is not self-evident for non-linear systems.
First applications in comparison with simulations as well as experimental measurements on the HIRENASD wing using only the first order kernel give very good results for lift and elastic deflection of the wing. Determining the Volterra-kernels has proven reliable and quick in comparison to the traditional method of using derivative-based reduced modeling.

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MS14
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MS14
Adaptive Finite Element Approximations of State Constrained Optimal Control Problems for Elliptic Boundary Value Problems

We develop, analyze, and implement adaptive finite element approximations of state constrained distributed optimal control problems for linear second order elliptic boundary value problems. In particular, we derive a residual-type a posteriori error estimator and prove its efficiency and reliability up to oscillations in the data of the problem and a consistency error term. In contrast to the case of control constraints, the analysis is more complicated, since the multipliers associated with the state constraints live in measure spaces. The analysis essentially makes use of appropriate regularizations of the multipliers both in the continuous and in the discrete regime. Numerical examples are given to illustrate the performance of the error estimator.
We will also address Lavrentiev regularizations in terms of mixed control-state constraints and a goal-oriented dual weighted approach. The results are based on joint work with Michael Hintermüller and Michael Kieweg.

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MS14
A penalization approach for tomographic reconstruction of binary radially symmetric objects.

We investigate a monolithic algorithm for solving the time dependent interaction between an incompressible, possibly non-newtonian, viscous fluid and an elastic solid. The continuous formulation of the problem and its discretization is done in a monolithic way, treating the problem as one continuum and discretized by the Q2/P1 finite elements. The resulting set of nonlinear algebraic system of equations is solved by an approximate Newton method with coupled geometric multigrid linear solver for solving the linear subproblems. We discuss possible efficient strategies of setting up the resulting system and its solution. A 2-dimensional configurations is presented and compared to experimental data to test the developed method. It is based on the DFG benchmark *flow around cylinder* for incompressible laminar fluid flow and extended to fluid-structure interaction in [1].

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MS14
Numerical Analysis of Some Optimal Control Problems Governed by Quasilinear Elliptic Equations.

In this talk we consider some optimal control problems governed by quasilinear elliptic equations of type

$$\begin{cases} -\text{div}[a(x,y(x))\nabla y(x)] + f(x,y(x)) = u(x) \text{ in } \Omega, \\ y(x) = 0 \quad \text{on } \Gamma. \end{cases}$$

The goal is to carry out the numerical analysis of the control problem providing some error estimates of the approximations. The main difficulty of this analysis comes from the possible lack of uniqueness of the state equation as well as from the possible nonexistence of a solution of the adjoint state equation. In order to overcome these difficulties we make a regularity assumption on the optimal pair (control,state) which is the key for the analysis of the control problem.
Before the numerical analysis we have to obtain the first and second order optimality conditions. The first order conditions allow us to deduce the regularity of the optimal controls necessary to derive the error estimates of the approximations. The sufficient second order conditions are an essential tool in the proof of these estimates.

Our results extend some previous works devoted to the study of optimal control problems governed by semilinear elliptic equations; see the references below.

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MS15

Purely algebraic factorization by triangular hierarchical matrices.

Although the asymptotic complexity of direct methods for the solution of large sparse finite element systems arising from second-order elliptic partial differential operators is far from being optimal, these methods are often preferred over modern iterative methods. This is mainly due to their robustness. In this talk it is shown that an (approximate) LU decomposition can be computed in the algebra of hierarchical matrices with logarithmic-linear complexity and with the same robustness as the classical LU decomposition.
An important application of low-precision approximants are preconditioners. It will be seen from both, analysis and numerical experiments, that a problem independent number of iterations can be guaranteed.
The approximation by hierarchical matrices relies on a so-called admissibility condition which is a geometric condition on the localisation of the degrees of freedoms associated with the rows and columns of each subblock. Since this condition is only sufficient, we will generalize it to a purely algebraic condition and prove existence of approximants.

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MS15

Preconditioning of fast boundary element methods

Several preconditioning techniques for the iterative solution of boundary element methods are described. The Laplace equation and the system of linear elastostatics are considered as model problems. The boundary element method is based on the symmetric boundary integral formulation and a Galerkin discretization. The fast multipole method is used as a fast and data-sparse realization of all discrete boundary integral operators. Boundary integral operators of opposite order are used as preconditioners. The algebraic multigrid method is based on an artificial hierarchy created by the clustering techniques and is optimized for the fast multipole method. Further, preconditioners using BPX techniques and artificial hierarchies of nested trial spaces are described. Numerical examples show the efficiency of the preconditioners as well as the applicability to industrial problems.

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MS15

Sparse Second Moment Analysis for Potentials on Stochastic Domains.

This talk is concerned with the numerical solution of Dirichlet problems in domains $D \in \mathbb{R}^d$ with random boundary perturbations. Assuming normal perturbations with small amplitude and known mean field and two-point correlation function, we derive, using a second order shape calculus, deterministic equations for the mean field and the two-point correlation function of the random solution for the Dirichlet problem in the stochastic domain.
The two-point correlation of the random solution satisfies a boundary value problem on the tensor product domain $D \times D$. It can be approximated in sparse tensor product spaces. This yields densely populated system matrices, independently of using the finite element method in $D \times D$ or the boundary element method on $\partial D \times \partial D$.
We present and analyze algorithms to approximate the random solution's two-point correlation function in essentially $\mathcal{O}(N)$ work and memory, where N denotes the number of unknowns required for consistent discretization of the domain (in case of finite element methods) or its boundary (in case of boundary element methods). Here “essentially” means up to powers of $\log N$.

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MS15

Approximation of Tensor-Sums in High Dimensions with Application to Multi-Dimensional Operators.

When an algorithm in dimension one is extended to dimension d, in almost every case its computational cost grows to the power of d. Tensor-sums (TS) are promising objects for multi-dimensional operators. Linear algebra operations can be performed in this representation using only d times one-dimensional operations. In iterative methods with tensor-sums it is important to solve the following prob-

lem.
For a given Tensor-Sum $A = \sum_{i=1}^{R} \otimes_{\mu=1}^{d} A_{i\mu} \in \mathrm{TS}(R)$ and $\varepsilon \in \mathbb{R}_+$, find $X^* = \sum_{i=1}^{r_\varepsilon} \otimes_{\mu=1}^{d} X^*_{i\mu} \in \mathrm{TS}(r_\varepsilon)$ such that:

$$\begin{aligned} \|A - X^*\| &\leq \varepsilon, \\ \|A - X^*\| &= \min_{X \in \mathrm{TS}_c(r_\varepsilon)} \|A - X\|. \end{aligned}$$

We will introduce a numerical approach that solves this approximation problem and present numerical results in high dimensions.

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MS16
Quasi-Newton algorithms for fluid-structure interaction problems.

Problems of fluid-structure interaction contain of a fluid and a structure part. Both problems are coupled by the boundary conditions on a common interface. In the simulation of fluid-structure interaction often so-called partioned methods are used, i.e. both problems are solved by different software packages [1]. In our case the fluid-solver OpenFOAM and the structure-code ParaFep are used.
Partioned methods allow the so-called weak coupling which is not sufficient for some problems. Therefore in this talk the so-called strong coupling is considered. These idea requires iteration in each time step.
We compare the usual block-Gauss-Seidel iteration with the block-Newton and the block-quasi-Newton-method. The Newton- and the quasi-Newton-method are implicit and have the advantage that they have better convergence properties as the block-Gauss-Seidel iteration [2].
Some practical examples from the ship building industry show the interaction of the software and that our approach gives good and fast results.

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MS16
Finite element approximation of nonlinear aeroelastic problems.

Problems of fluid-structure interaction contain of a fluid and a structure part. Both problems are coupled by the boundary conditions on a common interface. In the simulation of fluid-structure interaction often so-called partioned methods are used, i.e. both problems are solved by different software packages [1]. In our case the fluid-solver OpenFOAM and the structure-code ParaFep are used. Partioned methods allow the so-called weak coupling which is not sufficient for some problems. Therefore in this talk the so-called strong coupling is considered. These idea requires iteration in each time step. We compare the usual block-Gauss-Seidel iteration with the block-Newton and the block-quasi-Newton-method. The Newton- and the quasi-Newton-method are implicit and have the advantage that they have better convergence properties as the block-Gauss-Seidel iteration [2]. Some practical examples from the ship building industry show the interaction of the software and that our approach gives good and fast results. In this paper the numerical approximation of a two dimensional aeroelastic problem is addressed. The mutual interaction of fluids and structure can be met in many different situations, cf. [1]. The main objectives of the engineering problems is to determine the critical velocity for loose of the system stability. In many cases simplifications of the aeroelastic model are used, e.g. linearized models, etc. Here, the fully coupled formulation of incompressible viscous fluid flow over a structure is used. For the flow model we use the incompressible system of Navier-Stokes equations with large values of the Reynolds number $10^4 - 10^6$. The Navier-Stokes equations are spatially discretized by the FE method and stabilized with a modification of the Galerkin Least Squares (GLS) method; cf. [3]. The motion of the computational domain is treated with the aid of Arbitrary Lagrangian Eulerian(ALE) method, cf. [2]. The GLS stabilizing terms are modified in a consistent way with the weak formulation of the ALE method. The structure model is considered as a solid body with two/three degrees of freedom (bending, torsion and torsion of the control section). The motion is described with the aid of a system of nonlinear differential equations. The construction of the ALE mapping is based on the solution of an elastic problem. The method is applied onto several benchmark problems, where several technical parameters are compared with reference values. Also the comparison for different fluid models (e.g. Navier-Stokes, Reynolds Averaged Navier-Stokes equations) is presented. The nonlinear behaviour of the coupled system is shown for the nearby critical velocity.
Acknowledgment This research was supported under the project of the Grant Agency of the Academy of Science of the Czech Republic No IAA200760613 " and under Research Plan MSM 6840770003 of the Ministry of Education of the Czech Republic.

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MS16
Convergence acceleration of coupled problems with partitioned solvers based on model order reduction.

A method is presented that allows for the implicit coupling of black box partitioned solvers. The method will be explained for fluid-structure interaction applications. During a fluid-structure interaction (FSI) calculation the fluid solver is called with a position of the interface and returns a load distribution on that interface. On the other hand the structural solver is called with a load distribution on the interface and returns an updated position of that interface. We assume that the fluid solver software and the structural solver software are not accessible so that we can not obtain information for the

construction of a Jacobian matrix, which is needed if we want to use Newton iterations to obtain the coupled solution for each time step. However, if we would be able to construct approximate Jacobians for the fluid and the structural solver we can use the approximate Newton method to compute the coupled solution for each time step. During the calculation, we store the interface positions applied to the fluid solver and the corresponding computed load distributions and also the load distributions applied to the structural solver and the corresponding computed interface positions. With these input and output information of the solvers we construct reduced order models for both solvers. The Jacobians of these reduced order models can then be used as approximate Jacobians for the real solvers. These approximate Jacobians for the interface position related to the load distribution on that interface and vice versa are then used to accelerate the convergence of the coupling iterations.
The method is applied to the unsteady blood flow in a straight artery and it is verified whether the computed wave speed corresponds with the analytical wave speed given by the Bramwell-Hill equation.
A second application is the simulation of the dynamics of a gas bubble in a liquid. The interface position determines the curvature and the pressure difference across the interface is related to this curvature and the surface tension coefficient. An interface solver is constructed with as input the pressure coming from the fluid side computed with a fluid solver and as output the corresponding interface position is returned. This solver can be seen as a 'strucural' solver. When computing for this interface position a reduced order model for the fluid solver is used in order to obtain an approximate Newton method when solving for the interface position. In the latter application the 'structural' solver software for the interface position is accessible, so here a second reduced order model for this solver is not needed. The rising of an air bubble submerged in a liquid is simulated and verified with experiments from the literature.

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MS16
Interface Tracking and Mesh Update Techniques for Flow Simulation in Deforming Domains

Moving-boundary flow simulations are an important design and analysis tool in many areas of engineering, including civil engineering, marine and coating industries, and off-shore exploration. Two alternative computational approaches - interface-tracking and interface-capturing - are commonly considered. While interface-capturing offers unmatched flexibility for complex free-surface motion, the interface-tracking approach is very attractive due to its better mass conservation properties at low resolution. This provides motivation for expanding the reach of the interface-tracking methods.
The fundamentals of interface-tracking moving-boundary flow simulations - stabilized discretizations of Navier-Stokes equations, ALE and space-time formulations on moving grids, general mesh update mechanisms based on solid mechanics - are widely known and adopted. Challenges still exist, and we discuss some of the issues that are limiting the success of interface-tracking approach.
The generalized form of the kinematic condition, in the form of an elevation equation, as well as its stabilized GLS formulation, has been derived for cases where surface nodes move along prescribed straight lines. This method was then used to simulate water motion in trapezoidal tanks and channels. A further generalization is proposed for cases where surface nodes move along prescribed curvilinear spines. This allows for robust representation of the kinematic condition in an even wider set geometries, such as cylindrical vessels and channels.
Combination of large regular displacements and smaller general displacements often calls for a mixture of mesh update methods to be employed. Such is the case in the case of variable-pitch propellers, such as Voith-Schneider Propeller, where small movements of individual blades are superimposed on rapid rotation of the entire propeller. Simulation of such systems call for combination of the shear-slip mesh update method and the elasticity-based mesh update method.

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MS17
Tailored discrete concepts for pde constrained optimization problems in the presence control of and state constraints

We discuss tailored discretization concepts for optimal control problems with elliptic and parabolic pdes in the presence of constraints. In particular we consider

- control constraints combined with state constraints [3,4], and
- control constraints combined with constraints on the gradient of the state [1].

We consider distributed control as well as Neumann and Dirichlet boundary control and prove optimal error bounds on the primal optimization variables. Furthermore, we present an extension of the DWR concept to control and/or state constrained optimal control problems which among other things avoids the numerical evaluation of differences formed by multipliers [2]. Finally we present numerical examples which confirm our analytical findings.

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MS17
Inexact null-space iterations in large scale optimization

For a class of PDE-constrained optimization problems it is assumed that the following building blocks for a solver of the KKT-system are available: an iterative procedure for the forward as well as the adjoint equation and a (simple) preconditioner for the KKT-system, which itself has the flavor of an iterative procedure. In fact, the overall method defines an inexact null space iteration (within an SQP framework). Therefore, in general it cannot be guaranteed that a search direction provides sufficient progress toward optimality. In this talk, under suitable conditions, a convergence analysis of such inexact null space iterations is provided and a report on numerical tests is given.

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MS17
Regularity and optimality conditions for state-constrained parabolic problems with time-dependent controls

In many applications of PDE constrained optimization, pointwise inequalitites must be imposed on the state of the controlled system. Lagrange multipliers associated with such state constraints are in general measures. To show their existence, a standard assumption is the continuity of the state function. Then, the interior of the cone of nonnegative functions is non-empty so that multiplier rules of Fritz John type can be proven and, under a Slater type constraint qualification, they hold in qualified form. The desire to have continuous state functions implies some consequences for the analysis of state-constrained problems. Different regularization concepts were suggested. In the talk, some of these methods are discussed in parallel to the analysis of the regularity of state functions in different settings and for different types of controls. We concentrate on problems with linear elliptic and parabolic equations. Special emphasis is laid on the application of Lavrentiev type regularization to elliptic and parabolic boundary control problems.

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MS17
A virtual control concept for optimal control problems with pointwise state constraints

A linear elliptic control problem with pointwise state constraints is considered. These constraints are given in the domain. In contrast to this, the control acts only at the boundary. Consequently, a direct application of a Lavrentiev regularization (see [1],[3]) is not possible. We propose a new virtual control concept in this talk. The virtual control is introduced in objective, state equation, and constraints. Moreover, additional control constraints for the virtual control are investigated. An error estimate for the regularization error will be presented. The theory is illustrated by numerical tests. A detailed presentation of all results is contained in [2].

[1] S. Cherednichenko, and A. Rösch “Error estimates for the regularization of optimal control problems with pointwise control and state constraints.“ Accepted for publication in Journal for Analysis and its Applications.

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MS18
Hierarchical Low Kronecker Rank Approximation

A linear elliptic control problem with pointwise state constraints is considered. These constraints are given in the domain. In contrast to this, the control acts only at the boundary. Consequently, a direct application of a Lavrentiev regularization (see [1],[3]) is not possible. We propose a new virtual control concept in this talk. The virtual control is introduced in objective, state equation, and constraints. Moreover, additional control constraints for the virtual control are investigated. An error estimate for the regularization error will be presented. The theory is illustrated by numerical tests. A detailed presentation of all results is contained in [2].

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MS18
An algebraic approach to preconditioning based on $\mathcal{H} - LU$ decompositions

In this talk we introduce a method for preconditioning finite element systems with an approximate $\mathcal{H} - LU$ decomposition. To this end we use a nested dissection scheme.
In contrast to the usual way of clustering, which requires geometric information, we present an algebraic clustering method. In this approach we divide the cluster into three parts, two of approximatly the same size and a relatively small interface. The subdivision algorithm uses the matrix graph. It divides this graph using a multilevel graph decomposition algorithm whose principles are coarsing the graph, using spectral bisection in the lowest level and uncoarsening the graph. The algebraic approach requires to compute the nearfield / farfield of a cluster in an algebraic manner in order to determine admissibility of a block in a $\mathcal{H}$-matrix. This setup does not take more than $\mathcal{O}(n \log n)$ operations. We show first numeric results.

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MS18
Hierarchical compression

Treating non-local operators by standard discretization schemes usually leads to large dense matrices. Storing these matrices in the standard representation, i.e., as a two-dimensional array, would require far more storage than is available on most of today's computers. Fortunately, most of the matrices appearing in practical applcations have special properties that can be exploited in order to handle them more efficiently: for integral operators, the local analyticity of the kernel function can be used to replace it by a short sum of tensor products, which leads to a mosaic low-rank approximation. For the solution operators of elliptic partial differential equations, separable, possibly non-smooth, expansions can be used in a similar fashion and lead to similar results.
The standard schemes for the construction of low-rank approximations split the matrix into a number of blocks and treat each block separately. While this approach leads to simple and efficient algorithms, it cannot take advantage of connections between the blocks to reduce the storage requirements even further. In this talk, I present a technique for recovering these connections and using them to reduce storage requirements by representing the dense matrix by an $\mathcal{H}^2$-matrix. The recovery algorithm adds only a small computational overhead, and experiments show that it halves the storage requirements even for moderate problem dimensions and becomes more efficient for larger problems.
The basic idea of the algorithm is to convert submatrices into $\mathcal{H}^2$-matrices and then merge these submatrices to form larger submatrices until the entire matrix has been approximated. The merging process is carried out by computing the singular value decompositions of small matrices, and the singular values provide enough information to guarantee that the approximation error can be closely controlled.
In practical applications, the hardware is given, therefore the fixed amount of available storage is the limiting factor for large-scale computations. Since the new algorithm is more storage-efficient than its predecessors, it allows us to treat much larger problems on the same somputers.

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MS18
Efficient solution of large-scale algebraic Bernoulli equations based on hierarchical matrix arithmetic

We consider the algebraic Bernoulli equation (ABE)

$$A^T X + XA - XBB^T X = 0,$$

where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, and $X \in \mathbb{R}^{n\times n}$ is the matrix of unknowns.

The ABE has several applications in control and system theory as in stabilization problems of linear dynamical systems,

$$\dot{x}(t) = Ax(t) + Bu(t), \quad x(0) = x^0 \in \mathbb{R}^n,$$

and model reduction of unstable systems arising, e.g., from the discretization and linearization of parabolic PDEs.
As standard methods for the solution of ABEs are of limited use for large-scale systems, we investigate approaches based on the matrix sign function method. To make this iterative method applicable in the large-scale setting, we incorporate structural information from the underlying PDE model into the approach. By using data-sparse matrix approximations, hierarchical matrix formats, and the corresponding formatted arithmetic we obtain an efficient solver having linear-polylogarithmic complexity.

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MS19
A new mesh independence result for semismooth Newton methods

Mesh independence is a very desirable property for numerical methods that involve discretizations of an underlying infinite dimensional problem like those arising in optimal control with PDEs. Roughly, mesh independence ensures that for sufficiently fine discretizations the convergence behavior of the numerical algorithm is very much like that of the abstract counterpart of the algorithm for the infinite dimensional problem. The derivation of such results for semismooth Newton methods, which are very well suited for constrained optimal control problems, turns out to be quite involved [1]. The aim of this talk is to point out the intrinsic difficulties, to discuss possibilities for establishing mesh independence results, and to present new results.

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MS19
An SQP Method for Semilinear Optimal Control Problems with Mixed Constraints

In this talk we consider a class of optimal control problems with semilinear state equation. Mixed inequality constraints involving both the control and state variables are also present. Such problems arise as regularizations of purely state-constrained problems, but they are also of independent interest. We present a recent local quadratic convergence result in suitable function spaces for an SQP (sequential quadratic programming) method, in the context of semilinear optimal control problems with mixed and additional pure control constraints. Numerical examples illustrate and confirm the predicted behavior.

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MS19
Adaptive Multilevel Methods for PDE-Constrained Optimization

We present a class of inexact adaptive multilevel SQP-methods for the efficient solution of PDE-constrained optimization problems. The algorithm starts with a coarse discretization of the underlying optimization problem and provides

1. implementable criteria for an adaptive refinement strategy of the current discretization based on local error estimators and
2. implementable accuracy requirements for iterative solvers of the PDE and adjoint PDE on the current grid

such that global convergence to the solution of the infinite-dimensional problem is ensured.
We illustrate how the adaptive refinement strategy of the multilevel SQP-method can be implemented by using existing reliable a posteriori error estimators for the state and the adjoint equation.
Numerical results are presented that illustrate the potential of the approach.

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MS19
A priori error analysis for space-time finite element discretization of parabolic optimal control problems

In this talk we discuss a priori error analysis for Galerkin finite element discretization of optimal control problems governed by linear parabolic equations and subject to inequality control constraints. The space discretization of the state variable is done using usual conforming finite elements, whereas the time discretization is based on discontinuous Galerkin methods. For different types of control discretization we provide error estimates of optimal order with respect to both space and time discretization parameters taking into account the spacial and the temporal regularity of the optimal solution. For the treatment of the control discretization we discuss different approaches extending techniques known from the elliptic case. Numerical results illustrate theoretical investigations.

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CT1
Splitting methods based on algebraic factorization for fluid-structure interaction.

We address the numerical simulation of fluid-structure interaction (FSI) problems characterized by a strong added-mass effect. We propose semi-implicit algorithms based on inexact block-LU factorization of the linear system obtained after the space-time discretization and linearization of the FSI problem.
The basic idea of a semi-implicit scheme [1] consists in coupling implicitly the pressure stress to the structure, while the other terms (dissipation, convection and geometrical non-linearities) are treated explicitly. To achieve this explicit-implicit splitting the convective velocity and fluid domain are evaluated using information from previous steps. Consequently these methods show low computational costs (in comparison to fully implicit coupling algorithms) and good stability properties.
We investigate explicit-implicit decomposition through algebraic splitting techniques originally designed for the FSI problem. This algebraic splitting is superior to the classical semi-discrete splitting, because consistent boundary conditions are applied on the interface and do not exhibit an inaccurate pressure boundary layer. We have considered two different families of methods which extend to FSI the algebraic pressure correction method and the Yosida method, two schemes that were previously adopted for pure fluid problems [2]. In both cases the perturbation error has been analyzed and the convergence properties of the methods have been checked through numerical experiments. Improved incremental versions are also used. Furthermore, we propose predictor-corrector methods that use inexact factors as preconditioners. The best feature of these procedures is that the predictor-corrector iterations are insensitive to the added-mass effect.
The numerical properties of these methods have been tested on a model problem representing blood-flow in a compliant vessel.

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CT1
An unsteady compressible flow with very low Mach number

This work presents an unsteady numerical solution of the system of Navier-Stokes equations for compressible laminar flow in a two-dimensional channel. The unsteady flow is forced by a prescribed time periodical motion of a part of the channel wall. The numerical solution is realized by finite volume method and the explicit predictor-corrector MacCormack scheme with Jameson artificial viscosity using a grid of quadrilateral cells. The moved grid of quadrilateral cells is considered in the form of conservation laws using Arbitrary Lagrangian-Eulerian method.
It is well known that using the compressible system of Euler equations one has to modify a numerical method when very small Mach numbers are computed. The viscous compressible numerical method presented here has been developed to show, that also for flows with very low Mach numbers we can achieve successful results without any modification of the method.
Some numerical results of unsteady flows in the symmetrical and unsymmetrical channel are presented for inlet Mach number $M_\infty \in (0.01 - 0.02)$, Reynolds number $Re \approx 10^4$ and for frequency of the wall motions 20-100 Hz. As a real simulation, the authors present the numerical solution of flows in a human vocal tract with two different geometries.
The numerical results were obtained using special software developed by our group.

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CT1
Numerical simulations of flow induced vibrations of a profile

The work deals with a numerical solution of the interaction of two-dimensional inviscid incompressible flow and a vibrating profile with two degrees of freedom. The profile can oscillate around an elastic axis and in the vertical direction. The mathematical model is represented by the system of incompressible unsteady Euler equations. Numerical schemes in the finite volume method are applied. Two strategies, an artificial compressibility approach [1] and a dual-time stepping method [2, 3], are employed for numerical solution of governing equations. The motion of the profile is described by a system of two non-linear ordinary differential equations [4]. This system is transformed to the system of first order ordinary differential equations and solved numerically using four-order Runge-Kutta method. Deformations of the computational domain due to the profile motion are treated using arbitrary Lagrangian-Eulerian method. Numerical schemes applied respect the geometric conservation law [5]. Numerical simulations of flow-induced vibrations are performed for different upstream velocities for the profile NACA 0012. The results are presented for translation and rotation of the profile in time domain. Also pressure and veocity fields around the profile are shown at several time instants. The two numerical strategies are compared.

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CT1
Transparent boundary conditions for elastodynamics in a VTI medium layer

The model of Vertical Transverse Isotropy medium, a special case of anisotropy, has wide application in seismoelasticity. The problem of the construction of non-reflecting boundary conditions on the open boundaries of computational domains for such media is crucial both for practical simulations of the propagation of waves and for the methods of computational mathematics, since the known analytical approaches no longer work. Also the popular PML approach can fail in anisotropic media, see [1].

In order to provide non-reflecting and stable conditions for long-time simulations, we develop the concept of *transparent boundary conditions* (TBCs) that are based on the Green's function of governing equations in the external unbounded domain. Recently the advantages of the method have been demonstrated for the case of azimuthal anisotropy [2].

Here we develop the approach for generating *quasi-analytic* TBCs on the side surface of a cylinder $r \leq R_0$ for the equations of the transverse-isotropic medium:

$$\begin{cases} \rho\dfrac{\partial^2 u}{\partial t^2} = & A_{11}\frac{\partial}{\partial r}\left(\frac{1}{r}\left(\frac{\partial(ru)}{\partial r}\right)\right) + \frac{\partial}{\partial z}\left(A_{44}\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial r}\right)\right) \\ & +A_{13}\frac{\partial^2 w}{\partial r\partial z} \\ \rho\dfrac{\partial^2 w}{\partial t^2} = & \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(A_{44}\left(\frac{\partial w}{\partial r}+\frac{\partial u}{\partial z}\right)+\frac{\partial}{\partial z}\left(A_{13}u\right)\right)\right) \\ & +\frac{\partial}{\partial z}(A_{33}\frac{\partial w}{\partial z}), \end{cases}$$

u, w are radial and axial displacements in $(r, z)-$geometry; $A_{11}(z)$, ..., $A_{44}(z)$ are the elastic parameters of VTI medium that may depend on z.

The generic scheme of obtaining TBCs for anisotropic media in polar coordinates (r, θ) is described in [2]. The required Green's function of the exterior domain is obtained numerically: firstly, the Laplace transform reduces the task from time-domain to set of auxiliary elliptic tasks; then the correspondent Green's functions are calculated from well-posed exterior Dirichlet problems. Numerical algorithm solving the elliptic problems finds the functions with a maximally possible accuracy in order to provide the numerically stable inverse Laplace transformation afterwards. In particular, for the VTI case we develop a highly-accurate elliptic solver using the Galerkin method with basis functions in $z-$direction.

Accuracy and stability of the proposed transparent boundary conditions are demonstrated on several numerical tests.

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CT2
Linearized quasi inversion of seismic wave field on the base of Guassian beams decomposition.

1. Presented inversion procedure is destined for imaging of rapid variations of the earth velocities embedded within background with *a priori* known macrovelocity model. It should be noted that besides necessity to recover proper geometry of these structures it is very important to provide their ”true amplitude” imaging. As true amplitude imaging we mean images being free from influence of geometrical spreading produced by macro-velocity background.

2. Let us suppose that a medium we are dealing with possesses *a priori* known macrovelocity $c_0(x,z)$ and we are searching for its rapid perturbation $c_1(x,z)$. Under some reasonable assumptions scattered/reflected waves on the free surface (input multishot/multioffset data) can be represented as the following (linear or Born's approximation):

$$2\omega^2 \int\int_X \frac{1}{c_0^2(\xi,\eta)} \frac{c_1(\xi,\eta)}{c_0(\xi,\eta)} G_0(\xi,\eta;x_s,0;\omega)G_0(x_r,0;\xi,\eta;\omega)d\xi\eta = \phi(x_r,x_s;\omega). \quad (1)$$

Here $(x_r,0)$, $(x_s,0)$ are receiver and source positions respectively and $G_0(\xi,\eta;x,z;\omega)$ is Green's function for macro-velocity model. The problem is to resolve linear integral equation (30) with respect to function $\frac{c_1}{c_0}$ for given macro-velocity model c_0.

3. Green's function can be represented as superposition of Gaussian beams. Gaussian beam is some special kind of waves which propagates along specific ray and mainly concentrated in the rather close vicinity of this ray. Moreover, these Gaussian beams possess something like "orthogonality". At least we can use them in order to split integral equation (30) to a family of ones with kernels made of a product of Gaussian beams. Gaussian beam is concentrated within rather small vicinity of a ray, so their product is concentrated within cross-section of these vicinities, that is within vicinity of some interior point where these Gaussian beams were shoot from. Within this vicinity we can apply Taylor expansion and to use explicit formulaes for Gaussian beam. Really, we suppose macrovelocity model is rather smooth so it can be treated as homogeneous within mentioned above area of integration, but for homogeneous media Gaussian beam can be represented in explicit manner.

Finally, after some additional weighting and integration the initial linear integral equation transforms to the following one:

$$M < \frac{c_1}{c_0} > \equiv (T_0 + T_1 + \ldots) < \frac{c_1}{c_0} > = K < \phi(x_r,x_s,\omega) > \quad (2)$$

Here linear integral operator $T_k : C \to C^k$ and is pseudodifferential one. The most important property of this representation is the fact that T_0 is "almost" identity operator. It would be exactly identity if source function would be Dirac δ-function in time, while sources and receivers envelop a target area $suppc_1 \neq 0$. Otherwise it is identical with respect to some constituent of the spatial spectrum of rapid perturbation c_1.

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CT2
An inverse problem of electromagnetic shaping of liquid metals.

Electromagnetic forces allow contactless heating, shaping and controlling of chemical aggressive hot metals. Applications of this industrial technique are electromagnetic shaping of aluminium ingots using soft-contact confinement of liquid metal, electromagnetic shaping of superalloy material (Ni,Ti,....) in aeronautical engines and control metals solidification.

The principal objective of this work is to give an algorithm to solve a shape optimization inverse problem. The studied model concerns a vertically falling molten metal column shaped by an externally applied magnetic field created by currents in givens inductors. Under suitable assumptions, the equilibrium liquid metal configurations are described by a set of equations containing an equilibrium relation at the boundary between electromagnetic, surface tension forces and gravity. It involves the curvature of the boundary and an elliptic exterior boundary value problem. This equilibrium shape is shown to be the stationary state of the total energy under the constraint that the volume is prescribed.

The goal is to give a algorithm to place suitable inductors and currents around the molten metal so that the equilibrium shape be as near as possible to the given one. Two different approaches are introduced, in the first one, we seek for a set of inductors such that the equilibrium shape minimize the distance with a given target shape. In the second approach we look for a set of inductors such that they minimize the equilibrium relation in the boundary of the target shape.

A SAND, Simultaneous Analysis and Design, mathematical programming method is stated in both cases and solved with FAIPA, the feasible arc interior point algorithm. In this method, not only the position of the inductors, but also the shape and the state variables are considered as unknowns.

Numerical examples are presented and commented.

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CT2
Shape optimization approach for image segmentation: Level set Formulation based on Galerkin strategy

In this paper, we present a new variational formulation for image segmentation problem that forces the level set function to be expend in a finite vector space through Galerkin expansion. The proposed Galerkin strategy for level set formulation has two main advantages over the traditional level set formulation. First of this concerns the standard partial differential equation (PDE) evolution for the level set function that, in the Galerkin expansion turns into a ordinary differential equation system. Second, in our formulation the level set function can be initialized with several function through the choice of the Galerkin expansion parameters, and doesn't need to be re-initialized during the evolution process. However, according to the level set decomposition in a vector space of a finite dimension, our motivation is more focused on topology than on high accuracy for the boundary approximation. Furthermore, We discuss accuracy following the choice of different basis concerning the Galerkin expansion of the level ser function. Finally, the proposed Galerkin strategy for level set formulation is validated by various numerical experiments in 2D and 3D.

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CT2
An asymptotic factorization method for inverse electromagnetic scattering in a layered medium

We consider a simple but fully three dimensional model for the electromagnetic exploration of finitely many small perfectly conducting objects buried within the lower half space of an unbounded two-layered background medium. In possible applications the two layers would e.g. correspond to air (upper layer) and soil (lower layer). Moving a set of electric devices parallel to the surface of ground at constant height in order to generate a (time-harmonic) electromagnetic field, we measure the induced magnetic field within the devices. From these data we want to reconstruct the number and the positions of the unknown small scatterers.

We first investigate the corresponding direct scattering problem in detail and explain how to derive an asymptotic expansion of the scattered field in terms of the incident field, the centers of the scatterers and their geometry, as the size of the scatterers tends to zero. Our proof of this asymptotic formula is based on integral equation methods and generalizes the approach we used in [1] for a boundary value problem in electrostatics and in [4] for the scattering problem as described above but in a homogeneous background medium. Similar formulas have recently been derived formally in [2] and [5] and they have subsequently been successfully applied in MUSIC-type algorithms.

Using the asymptotic expansion we then study the inverse problem of recovering the number and the positions of the small scatterers from magnetic near-field scattering data as described above. Inspired by [3] we design a direct reconstruction algorithm that is closely related to factorization methods and also to MUSIC-type methods. This leads to a simple, robust, and efficient visualization method for the solution of our inverse problem. The viability of this method is documented by numerical examples.

A complete derivation of these results for homogeneous background medium including numerical reconstructions can be found in [4]. A corresponding work for two-layered medium is in preparation.

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CT3
Optimal error estimates in the DGFEM for nonlinear convection-diffusion problems

In this paper we shall be concerned with error estimates for the DGFEM applied to nonstationary nonlinear convection-diffusion problems. The DGFEM is based on a piecewise polynomial approximation of the sought solution without any requirement on the continuity on interfaces between neighbouring elements. It is particularly convenient for the solution of conservation laws with discontinuous solutions or singularly perturbed convection-diffusion problems with dominating convection, when solutions contain very steep gradients. The main attention will be paid to the analysis of optimal error estimates in the optimal $L^2(H^1)$- and $L^\infty(L^2)$-norms for the DG space semidiscretization and to the DG space discretization combined with backward difference formulas used for the time stepping. We shall also mention the effect of numerical integration for the evaluation of integrals in the formulation of the discrete problem. The theoretical results will be illustrated by numerical experiments.

In the second part of the paper we shall show some applications of the DGFEM to the numerical simulation of compressible flow in order to manifest the robustness of the method with respect to the Mach number.

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CT3
hp-IIPG method for convection-diffusion problems: analysis and applications to fluid dynamics

Our aim is to develop a sufficiently robust, accurate and efficient numerical scheme for the solution of the system of the compressible Navier-Stokes equations which describes a motion of viscous compressible flows. For simplicity, we study a model problem represented by a scalar nonlinear non-stationary convection-diffusion equation. In contrast with our recent papers (e.g., [4], [5]), we consider a general nonlinear diffusion term in the form $\nabla \cdot \vec{R}(u, \nabla u)$, where $\vec{R} : \mathbb{R}^{d+1} \to \mathbb{R}^d$ and $d = 2, 3$ is the dimension of the computational domain.
We discretize this equation with the aid of the *discontinuous Galerkin method* (DGM) which is based on a piecewise polynomial but discontinuous approximation, for a DGM survey see, e.g., [1], [2]. Among several types of discontinuous Galerkin methods, we prefer the schemes based on a primal formulation as SIPG, NIPG, Baumann - Oden schemes, see [1]. These schemes do not increase the number of unknowns in contrast to scheme based on a mixed formulation. However, the mentioned method can not be easily applied to the considered convection-diffusion equation with a general nonlinear diffusion term. So that we used the so-called *incomplete interior penalty Galerkin* (IIPG) variant of DGM ([3]) which has no favourable properties as coercivity or optimal order of convergence in the L^2-norm but allows to avoid troubles arising in the discretization of the nonlinear diffusion.
Within this presentation, we discretize the nonlinear convection - diffusion equation with the aid of the $hp-$variant of the IIPG method and derive a priori error estimates in the L^2-norm and the energy norm. We show numerical experiments verifying the theoretical results, discuss an extension of this approach to the system of the Navier-Stokes equations and present several preliminary numerical examples.

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CT3
Discontinuous Galerkin Method for the Numerical Solution of Inviscid and Viscous Compressible Flow.

In this work we are concerned with the numerical solution of a viscous compressible gas flow (compressible Navier-Stokes equations) with the aid of the discontinuous Galerkin finite element method (DGFEM). Our goal is to incorporate viscous terms into existing semi-implicit DGFEM scheme for the Euler equations, which is capable of solving flows with a wide range of Mach numbers [1]. The incomplete interior penalty Galerkin method (IIPG, [2]) is used for it's simple formulation among other DGFEM formulations [2]. The resulting nonlinear viscous terms are linearized in a similar manner as nonlinear convective terms in the original scheme, thus enabling semi-implicit time stepping. The resulting scheme is practically unconditionally stable and requires the solution of one sparse linear system per time level. Special attention is paid to the treatment of boundary conditions and to the stabilization of the method in the vicinity of discontinuities avoiding the Gibbs phenomenon. We present results for standard inviscid and viscous test cases, involving both transonic and low-Mach flows.

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CT3
Is stabilization necessary for the symmetric discontinuous Galerkin method for second order elliptic problems?

In this talk we analyze the necessity of stabilization operators for the symmetric discontinuous Galerkin (DG) method for second order elliptic problems depending on the space dimension and the polynomial approximation.
In a recent paper [1] we prove that in one space dimension, the symmetric DG method is stable for polynomial orders $p \geq 2$ without using any stabilization parameter. The method yields optimal convergence rates in both the broken energy norm and the L^2 -norm and can be written in conservative form with fluxes independent of any stabilization parameter.
Then we will give special focus on the particular case of affine approximation spaces in two or three space dimensions. We give a precise characterization on how much stabilization is needed to obtain well-posedness and optimal convergence. Surprisingly well-posedness requires no stabilization on internal faces. Optimal convergence on

the other hand may be perturbed by checkerboard modes for nonregular data. Finally we show how to recover optimal convergence with reduced stabilization, by enriching the approximation space with quadratic bubbles.

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CT4
A posteriori error analysis for Kirchhoff plate elements

We present a posteriori error analysis for two finite element methods for the Kirchhoff plate bending model. The first method is a family of finite elements introduced in [1] which uses C^0-continuous basis functions for the deflection and the rotation, i.e., the same approach as typically used for the Reissner–Mindlin model. The second method is the classical nonconforming Morley element which approximates the deflection by second order piecewise polynomial basis functions [2].
For both methods, we present an a posteriori error estimator for adaptive mesh refinements. First, we recall the main results of the error analysis accomplished in [1,3] and show that the esimators are both reliable and efficient. Second, by benchmark computations, we illustrate and compare the robustness of the a posteriori error estimators in various types of problems with different kinds of boundary conditions.

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CT4
With discrete adjoint based optimisation towards anisotropic adaptive FEM

Efficient numerical approximation of solution features like boundary or interior layers by means of the finite element method requires the use of layer adapted meshes. Anisotropic meshes, like for example Shishkin meshes, allow the most efficient approximation of these highly anisotropic solution features. However, application of this approach relies on *a priori* analysis on the thickness, position and stretching direction of the layers. If it is impossible to obtain this information *a priori*, as it is often the case for problems with interior layers of unknown position for example, automatic mesh adaption based on *a posteriori* error estimates or error indicators is essential in order to obtain efficient numerical approximations.
Historically the majority of work on automatic mesh adaption used locally uniform refinement, splitting each element into smaller elements of similar shape. This procedure is clearly not suitable to produce anisotropically refined meshes. The resulting meshes are over-refined in at least one spatial direction, rendering the approach far less efficient than that of the anisotropic meshes based on *a priori* analysis.
Automatic anisotropic mesh adaption is an area of active research. Here we present a new approach to this problem, based upon using not only an *a posteriori* error estimate to guide the mesh refinement, but its sensitivities with respect to the positions of the nodes in the mesh as well. Once this sensitivity information is available, techniques from mathematical optimisation can be used to minimise the estimated error by moving the positions of the nodes in the mesh appropriately.
The basic idea of minimising an error estimate is of course not new, but the approach taken to realise it is. The discrete adjoint technique is utilised to evaluate the sensitivities of an error estimate, reducing the cost of this evaluation to solving one additional equation system. This approach is crucial to make gradient based optimisation techniques, such as BFGS-type schemes, applicable. For more details, see [1,2]

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CT4
Adaptive hierarchical model reduction for elliptic problems

Most engineering problems exhibit a spatial dimension predominant over the others. This is the case, for instance, of river dynamics, blood flow problems or internal combustion engines. In these cases a good compromise between the need of reliable results and low computational costs is to resort to 1D models. On the other hand the simplifying assumptions at the basis of these models can fail to be verified locally, for instance in correspondence with the junction of two rivers, or with an aneurysm in haemodynamics. In the presence of these configurations one ideally would like to enrich locally the 1D model via a proper higher-dimensional one, for instance 2D or 3D. In this paper we propose a mathematical tool able to automatically select the space dimension of the models to be used. We move from a different representation of the main space variable with respect to the other ones. The former is spanned by a classical piecewise polynomial basis. The latter is expanded according to a set of functions identifying a *modal basis*. Thus we end up with a real hierarchy of simplified models, distinguishing one another for the different number of activated modal functions, i.e. for the different dimension. Then moving from this setting, we derive a proper *a posteriori modeling error estimator* able to identify the number of modes to be switched on, over the different parts of the domain, so that the corresponding modeling error (defined as the difference between the full higher-dimensional solution and the simplified one) is guaranteed within a desired tolerance. This estimator represents the desired automatic tool.

The presentation particularizes this approach to a steady diffusion - advection - reaction problem. The theoretical framework as well as some numerical test-cases are addressed.

This work combines model adaption with coupling of dimensionally - heterogeneous models (see, for instance, [1,2,3]).

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CT4
hp-FEM with Arbitrary Level Hanging Nodes in 3D

We present a new algorithmic technology for adaptive higher-order finite element methods (*hp*-FEM) in three spatial dimensions which is based on arbitrary-level hanging nodes. One of the most difficult aspects of computer implementation of adaptive hp-FEM is the element refinement. This operation is simple in traditional FEM where typically one has less than five refinement candidates. However, in the hp-FEM this number is much higher: around 100 in 2D and 1000 in 3D. In [2] we have shown that this step can be simplified substantially by introducing arbitrary-level hanging nodes. Then, the hp refinement can be done fully locally in elements. In other words, when refining an element, adjacent elements never have to be refined. Such additional refinements which are needed to satisfy mesh regularity rules are called forced refinements. These unwanted refinements slow down the convergence and their algorithmic treatment is problematic because of their recursive nature. We describe the treatment of arbitrary-level hanging nodes on 3D elements.

Compared to the two-dimensional case, the 3D setting is much more complicated and a number of interesting new problems appear. Not only one has more situations to take into account, but also some qualitatively new phenomena appear. For example, in 3D one has more types of hierarchic basis functions with a more complicated structure than in 2D. Higher-order numerical quadrature is more difficult in 3D and less results are available than in 2D. In 3D it is more difficult to handle correctly geometrical aspects such as orientation of faces and edges, and element refinements. Also when implementing arbitrary level hanging nodes, mamy technical new technical problems appear. We have to take into account more types of constrains (for example faces constrain not only faces, but also edges and vertices, etc.). Probably the most problematic is correct handling of indirecty constrained edges (in 2D, only vertices are subjects to indirect constrains).

In this talk we present the hp-FEM in 3D, mention differences with respect to the 2D setting, and show some numerical results to verify its efficiency.

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CT5
Stabilization methods for convection - diffusion problems on layer adapted meshes

Stabilized finite element methods are formed by adding to the standard Galerkin method terms that are mesh-dependent, in many cases (but not necessary) consistent and numerically stabilizing. Starting with the streamline upwind Petrov-Galerkin (SUPG) or streamline fiffusion finite element method (SDFEM) today there exist many different stabilization techniques.

In a survey published 2006 Franca, Hauke and Masud discuss SUPG and its variants GLS and USFEM, the variational multiscale method and bubble enriched methods. But they do not mention subgrid modelling, the continuous interior penalty method, discontinuous Galerkin and local projection stabilizations.

In this paper we first discuss the relation between different stabilization techniques, with special emphasis on properties of difference schemes generated by these methods on uniform meshes.

If layer adapted meshes are used in the discretization so far there exist only few results for all these stabilization techniques which prove robustness with respect to the singular perturbation parameter. Often only problems with exponential layers are studied, but it is very important as well to consider problems with characteristic layers.

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CT5
Superconvergence analysis of a finite element method on Shishkin mesh for two - parameter singularly perturbed problems

We consider the following singularly perturbed problem with two small independent parameters

$$\begin{aligned} -\varepsilon_1\Delta u + \varepsilon_2 b(x)u_x + c(x)u &= f(x,y), \quad \text{in } \Omega = (0,1)\times(0,1),\\ u &= 0, \quad \text{on } \partial\Omega, \end{aligned} \tag{3}$$

where $0 < \varepsilon_1, \varepsilon_2 \ll 1$. The functions b, c and f are sufficiently smooth, $b(x) \geq \beta > 0$, $c(x) \geq \gamma > 0$, $x \in [0,1]$, and f satisfies the compatibility conditions $f(0,0) = f(0,1) = f(1,0) = f(1,1) = 0$. The solution of the problem (3) is characterized by exponential layers at $x = 0$ and $x = 1$, parabolic layers at characteristic boundaries $y = 0$ and $y = 1$, and corner layers at four corners of the domain. The width of exponential layers depends on the relation between the parameters ε_1 and ε_2.
In [2], under certain assumptions a solution decomposition of (3) has been proved, while in [3], the authors consider numerical solving of the same problem using standard Galerkin method with linear/bilinear elements on Shishkin mesh. In an energy norm, they have proved a robust error estimate

$$\|u - u^N\|_E \leq C(N^{-2} + (\varepsilon_2 + \varepsilon_1^{1/2})^{1/2} N^{-1} \ln N), \tag{4}$$

where u and u^N are the exact and the discrete solution, respectively. Here we show that for the same discretization mesh and finite element method with bilinear elements, a better estimate than (4) for $\|u^I - u^N\|_E$ is possible, where u^I is a nodal interpolant of u. We have proved

$$\|u^I - u^N\|_E \leq C(N^{-2} + (\varepsilon_2 + \varepsilon_1^{1/2})^{1/2} N^{-2} \ln^2 N),$$

indicating the superconvergence property of the method. We have also applied a simple postprocessing technique from [1] which yields more accurate discrete solution. Numerical tests confirm our theoretical results.

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CT5
A finite difference method on layer-adapted meshes for an elliptic system in two dimensions

We consider a system of $M \geq 2$ coupled singularly perturbed linear reaction-diffusion equations:

$$\boldsymbol{\mathcal{L}u} := -\varepsilon^2\Delta\boldsymbol{u} + \boldsymbol{Au} = \boldsymbol{f} \quad \text{in } \Omega = (0,1)^2, \quad \boldsymbol{u}|_{\partial\Omega} = \boldsymbol{g}, \tag{5}$$

where the parameter ε satisfies $0 < \varepsilon \ll 1$. Systems of this type are relevant, for example, to the investigation of diffusion processes in electro-analytical chemistry in the presence of chemical reactions. The coupling matrix is assumed to satisfy

$$\boldsymbol{v}^T\boldsymbol{Av} \geq \gamma^2 \boldsymbol{v}^T\boldsymbol{v} \text{ in } \Omega \quad \text{for all } \boldsymbol{v} \in \mathbb{R}^m \tag{6}$$

with a positive constant γ.
The operator $\boldsymbol{\mathcal{L}}$ is shown to be maximum-norm stable although it does not obey a maximum principle. We derive bounds on the derivatives of $\boldsymbol{u}$ that are sharper then those previously found in the literature [3].
Then (5) is discretized using central differencing on arbitrary tensor-product meshes. This discretization too is shown to be maximum-norm stable. Based on the a priori derive bounds layer-adapted meshes can be constructed the yield uniform 2nd convergence no matter how small the perturbation parameter ε. In [2] we prove that the nodal error satisfies

$$\left\|\boldsymbol{u} - \boldsymbol{u}^N\right\|_{\omega,\infty} \leq \begin{cases} CN^{-2} & \text{on Bakhvalov meshes,}\\ CN^{-2}\ln^2 N & \text{on Shishkin meshes,} \end{cases}$$

where $\boldsymbol{u}^N$ is the numerical solution on a mesh with N mesh intervals in each coordinate direction.
Numerical experiments complement our theoretical findings.

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CT5
A Convenient and Economical Error Control Device for Singularly Perturbed Systems.

We present an algorithm, proposed in [1], for solving the initial value problem

$$\varepsilon \frac{d^2x}{dt^2} + A\frac{dx}{dt} + f(x) = 0, \quad x(0) = \alpha, \quad \frac{dx}{dt}(0) = \beta, \qquad (7)$$

where $t \in [0, t_1]$, $t_1 > 0$, $x(t), f(x)$, $\alpha, \beta \in \mathbf{R}^n$, $n \geq 1$ and ε is a small positive parameter. The eigenvalues of the matrix A have all positive real parts, hence A is invertible. Following the approach given in [2], we truncate the expansions to first order in ε in order to derive the first order version of the steady state approximation. The main feature of the algorithm lies in the use of the error estimate derived in the asymptotic analysis as a practical means of accessing the error. This maybe very useful, especially in experiments in chemical and nuclear reactors. We demonstrate the effectiveness of the method on various cases arising in applications.

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CT8
A priori error analysis for the finite element approximation of elliptic Dirichlet boundary control problems

The talk presents recent results of an a priori error analysis for the finite element approximation of Dirichlet boundary control problems governed by elliptic partial differenial equations. For a model problem of the form

$$\begin{aligned} &J(u,q) = \tfrac{1}{2}\|u-\bar{u}\|^2_{\Omega} + \tfrac{1}{2}\alpha\|q\|^2_{\partial\Omega} \to \min, \\ &-\Delta u = f \ \text{ in } \Omega, \quad u = q \ \text{ on } \partial\Omega, \end{aligned}$$

error estimates are proven for the primal variable u, the control q, and the associated adjoint variable λ. These estimates are of optimal order with respect to the solution's regularity to be expected on polygonal domains. The finite element discretization considered is based on variational formulations of the control problem differing in the way the Dirichlet boundary control is incorporated in the problem. The proofs rely on the Euler-Lagrange formulation of the optimal control problem and employ standard duality techniques and optimal-order L^p error estimates for the finite element Ritz projection. These estimates improve corresponding results in the literature and are supported by computational experiments.

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CT8
An L-BFGS Method in H^1 for optimal control of a quantum system

The choice of function space and the accuracy of numerical solution of the governing equations is important to the convergence of PDE-constrained optimization problems. In particular, defining the gradient of the cost function in H^1 leads to a significantly improved performance over the L^2 gradient.
The control equations for the transport of Bose–Einstein condensates in magnetic microtraps is formulated in the optimal control framework and solved using a function space L-BFGS and nonlinear conjugate gradient methods.
The time evolution of the wavefunction of the Gross–Pitaevskii and Schrödinger equations and can be controlled through modulating the confining potential. In order to define an optimal control strategy an appropriate cost functional is introduced that must be minimized under the constraint of satisfying the evolution equation. The resulting optimality system consists of two Schrödinger-type equations with opposite time orientation coupled with an third equation for the control. These equations are descritized using split-operator time-stepping and pseudospectral methods.

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CT9
A posteriori error estimates based on flux reconstruction for Discontinuous Galerkin methods

We investigate a new approach to derive residual a posteriori error estimates for Discontinuous Galerkin (DG) approximations of convection–diffusion–reaction equations. The main idea, which generalizes previous work for finite volume schemes [1], consists of reconstructing an $H(\mathrm{div})$-conforming diffusive flux. Most of the a posteriori error estimates previously derived in the literature for DG approximations contain three contributions, the two usual ones found in a posteriori error estimates for continuous finite element methods (namely the element-wise residual and a measure of non-conformity of diffusive fluxes based on normal gradient jumps), plus a measure of the non-conformity of the actual discrete solution based on its jumps. The present methodology allows to transform the element-wise residual contribution into a higher order term, thus fully taking advantage of the spectral degrees of freedom within each element available in the DG method. Simultaneously, the estimator of normal gradient jumps is replaced by a comparison of the original and reconstructed diffusive fluxes, which is proved to be a lower bound for the former classical estimator. Moreover, the upper bound is sharp since it is established for arbitrary conforming reconstructions of the discrete solution itself and of its diffusive flux. The estimator also yields a guaranteed upper bound since all constants are carefully evaluated. In practice, the conforming reconstruction can be achieved using the so-called Oswald interpolation operator for the discrete solution and Raviart–Thomas finite elements for the diffusive flux. Finally, numerical examples are presented to illustrate the theoretical results.

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CT9
DGFEM for the compressible Navier-Stokes equations

A specific wide class of problems of fluid mechanics is formed of viscous compressible flow, which is described by the system of the compressible Navier–Stokes equations. To solve these problems, the discontinuous Galerkin finite element method (DGFEM) is used in view of its simplicity and ease of implementation. With this method, the semi–discrete system is obtained from the continuous weak formulation by selecting the finite dimensional subspaces for the piecewise polynomial but discontinuous test functions, for a DGFEM survey see, e.g., [1]. The following time discretization with the aid of a backward difference formula (BDF) leads to the full discrete system, see [2]. Moreover, using a linearization of inviscid as well as viscous fluxes and applying a suitable explicit extrapolation for nonlinear terms presented in [3], we have to solve only a linear algebraic problem at each time step. Then we obtain an efficient numerical scheme which is almost unconditionally stable and has a higher degree of approximation with respect to the space and time coordinates.
In this contribution, we present several variants of DGFEM, namely NIPG, SIPG and IIPG types of stabilizations of viscous terms. We compare this techniques from the point of view of their accuracy, efficiency and applicability to the system of the compressible Navier-Stokes equation. We mention several implementation aspects and the following problems. We show several numerical results reflecting the potency of semi–implicit approach and discuss another possible extensions of this approach.

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CT10
Boundary Element Methods for the Helmholtz equation

Although the exterior boundary value problems for the Helmholtz equation with either Dirichlet or Neumann boundary conditions are unique solvable, related boundary integral equations may not be solvable, or the solutions are not unique. In particular, the boundary integral operators are not injective when the wave number κ^2 is an eigenvalue of the interior Dirichlet or Neumann eigenvalue problem, respectively. Considering linear combinations of different boundary integral formulations this results in combined boundary integral equations, which are unique solvable for all wave numbers. The most known formulations are those of Brakhage–Werner and Burton–Miller. However, since the combined boundary integral equation involves boundary integral operators of both first and second kind, the analytical framework offers different settings. The classical combined boundary integral equations are considered in $L_2(\Gamma)$, where the uniqueness results are based on Gårdings inequality and Fredholm's alternative. To ensure the compactness of certain boundary integral operators, sufficient smoothness of the surface Γ is required. Recently, different regularized formulations are discussed, which ensure the unique solvability even for Lipschitz surfaces Γ.
Here we will analyse modified boundary element methods for the Helmholtz equation with either Dirichlet or Neumann boundary conditions and give estimates for their stability and convergence. Moreover we will look at the condition number of the linear system corresponding to the boundary element method and discuss possibilities for preconditioners. Finally we will give numerical results to verify the theoretical estimates.

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CT10
Boundary element methods for eigenvalue problems

The solution of Laplace eigenvalue problems by using boundary integral equation methods usually involves some Newton potentials which may be resolved by using a multiple reciprocity approach. Here we propose an alternative approach which is in some sense equivalent to the above. Instead of a linear eigenvalue problem for the partial differential operator we consider a nonlinear eigenvalue problem for a boundary integral operator. This nonlinear eigenvalue problem can be solved by using some approriate iterative scheme, i.e. a Newton scheme. We will discuss the convergence and the boundary element discretization of this algorithm, and give numerical results. Moreover we will discuss alternative solution strategies and more efficient discretization techniques.

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CT11
Adaptive methods for the solution of the Stokes equations by the finite element method

In many cases, the solution to a differential equation is rapidly varying only in restricted regions. For such problems, it makes sense to adapt the mesh to match the variation in the solution. The difference in approximation power between a mesh chosen to solve general problems versus one adapted to a particular one can be substantial. In current computer simulations, meshes are often adapted to the solution either using a priori information regarding the problem being solved or a posteriori after an initial attempt at solution.
In this contribution, we consider Stokes equations as a model problem and, following the work [1], we focus on an easily computable upper bound for the error, which is in fact the difference between the exact solution of the model and its approximation measured in the corresponding energy norm. The estimate obtained is completely independent of the numerical technique used to compute approximate solutions and can be made as close as resources of concrete computer used allow. Reliability and efficiency of the estimate is tested on numerical examples and compared with several other estimators.

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CT11
Functional a posteriori error estimates for Nitsche type mortaring on non-matching grids

We shall present a posteriori error estimates for Nitsche type approximations of self-adjoint second order elliptic boundary value problems on non-matching grids. In this work, following the lines of our work on functional a posteriori error estimates for discontinuous Galerkin approximations [3], we first project the approximate solution onto the energy space and then apply the functional a posteriori estimates [1,2] to this projected solution. Computable upper bounds for the errors in a suitable norm are derived. Several numerical examples, which support the theoretical analysis and confirm the efficiency of the approach, will be presented.

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CT12
A semi-implicit algorithm based on the Augmented Lagrangian Method for fluid-structure interaction

The paper presents a semi-implicit algorithm based on the Augmented Lagrangian Method for solving an unsteady fluid-structure interaction.
The fluid is governed by the Navier-Stokes equations written in the Arbitrary Lagrangian Eulerian framework. The structure verifies the linear elasticity equations using the Lagrangian coordinates.
The algorithm for solving numerically the fluid-structure interaction was obtained by combining the backward Euler scheme with a semi-implicit treatment of the convection term for the fluid and Newmark scheme for the structure equations.
At each time step, the position of the interface is determined in a explicit way. Then, the Augmented Lagrangian Method is employed for solving a fluid-structure coupled problem, such that the continuity of the velocity as well as the continuity of the stress hold on the interface. During the Augmented Lagrangian iterations, the fluid mesh does not move, which reduces the computational effort. The term "semi-implicit" used for the fully algorithm means that the interface position is computed explicitly, while the displacement of the structure, velocity and the pressure of the fluid are computed implicitly. This kind of algorithm was introduced in [1].
Numerical results are presented.

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CT12
Numerical solution of transonic and supersonic 2D and 3D fluid–elastic structure interaction problems

We solve a system of compressible Navier-Stokes equations in conservative ALE formulation, supplemented by a suitable turbulence model. The structural dynamic is described by the equations of anisotropic elastic continuum with large or small displacements. The problem is closed by the interface conditions. In some cases, we consider a set of Euler equations as the simplification of the flow dynamics.
We present several numerical methods for fluid dynamic problems:

1. A cell centered finite volume method with linear least square reconstruction with nonlinear WENO type weights. This method uses the Kok's k–ω TNT model.

2. Cell centered finite volume method with linear reconstruction and Barth's limiter.

3. Multidimensional upwind residual distribution scheme.

The second and third methods are presented for inviscid flows only. To allow a large time steps, all the considered methods uses implicit time stepping formulated in dual time.
The elastic problem is solved by a simple finite element method with quadratic elements and Newmark time integration scheme.
The mesh motion is given either by a simple algebraic procedure or computed by a finite element method. The whole problem is formulated in dual time and solved by a simple sub-iteration procedure.
We present several numerical tests documenting the behavior of the method. Namely, 2D transonic turbulent flows past forced oscillatory pitching NACA0012 airfoil, 2D inviscid supersonic panel flutter case and 3D inviscid flow past the elastic AGARD 445.6 wing.

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CT12
Numerical method for unsteady incompressible MHD boundary layer on porous surface in great accelerating fluid flow

The MHD boundary layer theory has a significant place in the development of the magnetic hydrodynamics. The results of this theory have a wide application in tehnical practice, especially in nuclear reactors, MHD-generators, as well as in different devices in chemical technology etc. The behaviour of a boundary layer in the presence of a positive or negative pressure gradient along the surface, is particularly important for the calculation of the drag as well as for the understanding of the processes which take in a diffuser, because there is transition from laminar to turbulent flow which determines the dividing line between a region with low drag and one where drag is dramatically increased. So one can control laminar-turbulent transition by fluid which has been injected or ejected through the porous contour or by use the magnetic field. Apart from skin friction we are interested in knowing whether the boundary layer will separate under given circumstances and if so, we shall wish to determine the point of separation. So the unsteady plane MHD boundary layer on a porous surface, has been stidied. The fluid, flowing past the surface, is incompressible and its electro-conductivity is constant. The present magnetic field is homogenous and perpendicular to the surface and through the porous contour also in perpendicular direction, the fluid of the same properties as incompressible fluid in basic flow, has been injected or ejected with velocity who is a function of the contour longitudinal coordinate and time. In order to study this problem, a polyparametric method known as generalized similarity method has been established. The corresponding equations of this unsteady boundary layer, by introducing the appropriate variable transformations, momentum and energy equations and three similarity parameters sets, being transformed into so-called universal, i.e. generalized form. These parameters are expressing the influence of the outer flow velocity, the injection or ejection velocity, magnetic induction and the flow history in boundary layer, on the boundary layer characteristics. The numerical integration of the universal equation with boundary conditions has been performed by means of the difference schemes and by using Tridiagonal Algorithm Method with iterations in the four parametric and twice localized approximation, where the first unsteady, dynamic, magnetic and porous parameters will remaine, while all others will be let to be equal to zero, and where the derivatives with respect to the first porous and magnetic parameters will be considered equal to zero. The obtained results can be used in the withdrawing of general conclusions on the development of boundary layer model and in the calculation of particular problems, as there is a problem with great accelerating fluid flow over past porous aerofoil when its center velocity changes in time as a degree function and when potential external velocity on aerofoil is measured in free flight. A part of the obtained results is given in the form of diagrams from which one can see that the unsteady parameter has a significant influence on the friction distribution and especially on the location of seperation point, ie. laminar-turbulent transition, of the MHD boundary layer. When this parameter is increasing the friction magnitude is incresing and the separation point location is removing toward the greater absolute values of the negative dynamic parameter. It means, that the positive local acceleration leads to the postponing of the separation of the MHD boundary layer in the diffuser region. Also, for both in confuser and in diffuser regions as well as for both the accelerating and decelerating flows, the ejection of fluid increases the friction and postpones the separation of boundary layer, and vice versa the injection of fluid reduces the friction and favours the separation of flow. Magnetic field, for both acceleration and deceleration of flow, and for both injection and ejection of the fluid , increases the friction and postpones the separation of boundary layer.

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CT13
Topological derivatives for non–homogeneous inverse problems

Nondestructive testing is an important field that has grown considerably in recent times. The range of applications is huge: tomography and magnetic resonance in medicine, earthquake location in geophysics, reservoir characterization in oil industry. These lead to inverse scattering problems, usually posed as optimization problems with constraints given by partial differential equations. In electromagnetic, thermal or acoustic scattering, the constraints are often transmission problems for Helmholtz equations. While level-set-based optimization strategies are slow, iterative methods using topological derivatives provide an efficient alternative. Recent work on topological derivatives analyzes homogeneous problems with different boundary conditions [1–4]. We address here non–homogeneous materials, giving expressions for the topological derivatives by first finding the shape derivative of the associated cost functional and then carrying out asymptotic expansions of the solutions of Helmholtz transmission problems in domains with vanishing holes. An efficient numerical scheme to compute topological derivatives is presented. We test its accuracy for different two dimensional geometries. The simple calculation of the topological derivative provides good initial guesses of the number of obstacles and their size. For a better description of their shape, we propose a topological derivative based iterative scheme. A few iterations suffice to find the correct shapes.

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CT13
Determining the Threshold of Compression in the Wavelet Transform with Orthonormal Wavelets

We described one nonstandard way for determining the threshold of compression in dependance of the allowed relative error of reconstruction. By using the same technique we determined the optimal threshold of compression. The basic characteristic of the presented idea is that we used geometrical interpretation of the pyramidal algorithm together with the basic definitions of the theory of probability.

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CT13
Variational Formulation for Euler flow equation.

Maquing use of the transverse field equation (governed by Lie brackets of the two vector fields) we characterize the necessary optimality condition associated to a vatiational problem leading to the usual Euler equation for non viscous filed. INdeed the variational principle can be rather looked as an optimal control problem as it is constrainted by a "state equation" such as the density convection and the final solution is then claissequely obtained through an adjoint problem.

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CT14
The method of freezing waves in nonlinear time-dependent PDE's.

We consider nonlinear time dependent PDE's on unbounded domains, the solutions of which show specific spatio-temporal patterns. Examples are provided by nonlinear reaction diffusion systems on $\mathbb{R}^d$, such as

$$u_t = \Delta u + f(u),\ u(x,0) = u_0(x), \quad x \in \mathbb{R}^d, t \geq 0, u(x,t) \in \mathbb{R}^m. \quad (8)$$

If the nonlinearity f is of the so called excitable type (e.g. a bimodal cubic in case $m = 1$) such systems exhibit travelling or rotating waves for $d = 1$, rigidly rotating or meandering spiral waves for $d = 2$, and scroll waves for $d = 3$.
The *method of freezing*, introduced in [1] (for a related approach see [4]) transforms the Cauchy problem (8) into a partial differential algebraic equation (PDAE). The PDAE involves additional algebraic variables that determine a moving coordinate frame (within which

the aforementioned patterns become stationary), and it imposes extra constraints that try to minimize the temporal changes of the spatial profile. The method generalizes to evolution equations that are equivariant with respect to the action of a (generally noncompact) Lie group, cf. [3] for some general theory.

The numerical approximation of the PDAE involves several approximation processes, such as restriction to a bounded domain with asymptotic boundary conditions and discretization in space and time. We show several applications of our method to systems of Ginzburg-Landau and FitzHugh-Nagumo type and we demonstrate how the moving frame can facilitate mesh adaptation and prevent certain patterns from leaving the computational domain. We briefly discuss some recent work [2],[5] on analytical aspects related to the freezing approach, such as the preservation of asymptotic stability for specific patterns and the influence of numerical approximations on the dicrete and the continuous spectrum of linearizations.

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CT14
Finite-Difference Modeling of Sonic Log in 3D Viscoelastic Media.

1. Sonic logs are very important borehole measurements providing knowledge about physical properties of surrounding rocks. In order to be able to recover physical properties of surrounding rocks by sonic data one should fully appreciate key peculiarities of elastic waves propagating through and around borehole imbedded within 3D heterogeneous elastic formations.

Most of the previous 3D FD studies are done for Cartesian coordinates. But, the use of these coordinates leads to saw-like representation of the sharpest interface of the problem - interface between fluid-filled borehole and enclosing rocks. In its own turn this provokes generation of rather strong artifacts known as "numerical scattering". We believe one should take special care to avoid this artifact because for the first of all correct simulation of sonic log should provide one with correct simulation of head P- and S-waves. These waves are of first arrivals and possess very important information about desired elastic property of borehole vicinity.

2. The main trouble the person faces on when dealing with FD scheme in cylindrical coordinate system is linear inflation of azimuth face of grid cells with radius increase. In order to compensate this inflation we perform periodical refinement of azimuth sampling. In order to couple grids after these refinement there is necessary to interpolate components of velocity and stress vectors. Our choice was to use advantage providing by 2π-periodicity of velocity and stress vectors with respect to azimuth and to use interpolation on the base of Fourier Transform. This interpolation possesses exponential accuracy and its Fast Fourier Transform (FFT) version is extremely fast.

In order to incorporate in the model objects of rather small scale (for example, it could be necessity to take into account completion of the well) we do also local refinement of radial step as well.

3. For numerical simulation of elastic wave propagation one has to truncate infinite physical domain to finite computational one. The most widespread approach to do that is surrounding of a computational domain by a special layer with intrinsic attenuation introduced in a special way that provides extremely low reflections on both interior and exterior interfaces. We used here our own development described in (Kostin et al., 2002).

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CT14
A MULTIGRID ALGORITHM FOR THE ACOUSTIC SINGLE LAYER EQUATION

We present a multigrid algorithm for the two dimensional acoustic single layer equation along a polygonal boundary. The use of multigrid strategies for positive-definite, negative-order pseudodifferential operators was first described in [1]. For the indefinite Helmholtz case the algorithm is closely related. Its convergence for low to moderate wave numbers is analysed using a pertubation type argument from [2]. Our numerical results demonstrate that the multigrid scheme works well as a linear solver and as a preconditioner.

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CT14
Numerical simulation of seismic and acousto-gravity waves in a heterogeneous Earth-Atmosphere model

In many theoretical studies, the Earth-Atmosphere interface is considered to be absolutely reflecting, the effects, related to the excitation of seismic waves in the Earth's crust and their interaction with the acoustic-gravitational waves in the atmosphere being neglected. Theoretical and experimental studies in the course of the recent decades have shown a close relation between lithospheric and atmospheric wave motions. Alekseev et al. [1] discovered the effect of acoustic-seismic induction, in which an acoustic wave from a powerful vibrator induced intense surface seismic waves at a distance of tens of kilometers due to the atmospheric refraction.
A specific feature of the numerical modeling of wave fields for a heterogeneous Earth-Atmosphere model is a considerable difference in velocities of seismic and acoustic waves. In this case, the use of explicit finite difference schemes brings about serious restrictions on the time step of a finite difference scheme and results in large computer costs.
A numerical-analytical solution for seismic and acoustic-gravitational waves propagation problem is proposed to a heterogeneous Earth-Atmosphere model [2]. Seismic wave propagation in an elastic half-space is described by a system of first order dynamic equations of the elasticity theory. The propagation of acoustic-gravitational waves in the atmosphere is described by the linearized Navier-Stokes equations. The proposed algorithm is based on the integral Laguerre transform with respect to time, the finite integral Bessel transform along the radial coordinate with a finite difference solution of the reduced problem along the vertical coordinate. The algorithm is numerically tested for the heterogeneous Earth-Atmosphere model for different source locations. The study was supported by grants 06-05-64149, 07-05-00538 from the Russian Foundation for Basic Research.

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CT15
Numerical Integration in the Discontinuous Galerkin Method for Nonlinear Convection-Diffusion Problems in 3D

In common with the standard finite element method, the discontinuous Galerkin finite element method is based on a piecewise polynomial approximation of the sought solution. However, in the the discontinuous Galerkin method the requirement of the conforming properties is omited. This allows to deal with general triangulations of the domain, in which the intersection of two neighbouring elements may be formed only by parts of their sides. We use the discontinuous Galerkin finite element method to the space-semidiscretization of a nonlinear nonstationary convection-diffusion problem. We approximate the convective terms with the aid of the numerical flux, and we consider symmetric as well as nonsymmetric variants of the discretization of diffusion, and the interior and boundary penalty. In practical computations the integrals appearing in the forms defining the discrete solution are evaluated with the aid of numerical integration. Regardless, in theoretical works almost only exact integration is considered. In [1] we studied the effect of numerical integration in 2D. In the present work we are concerned with the 3D problem. We show what is the effect of the evaluation of the volume and surface integrals by numerical quadratures. We estimate the error caused by the numerical integration and show how to choose numerical quadratures in order to preserve the accuracy of the method with exact integration.

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CT15
Mathematical models and numerical simulation of drug release from stents

Drug eluting stents (DES) are apparently simple medical implanted devices used to restore blood flow perfusion into stenotic arteries. However, the design of such devices is a very complex task because their performance in widening the arterial lumen and preventing further restenosis is influenced by many factors such as the geometrical design of the stent, the mechanical properties of the material and the chemical properties of the drug that is released.
In this framework, numerical simulation techniques play a relevant role in understanding what are the most appropriate choices for the optimal design of DES. The main computational difficulties arise from the need to deal with phenomena that take place on multiple scales in space and time. Concerning the space scales, we remind that DES for cardiovascular applications are miniaturized metal structures that are coated with a micro-film containing the drug that will be locally released into the arterial walls for healing purposes. The thickness of this film generally lays within the range of microns. As regards the time scales, we observe that the release of drug is deliberately very slow. In general, it persists until a few weeks after the stent implantation.
To address these topics, we start from a general model for mass transfer through heterogeneous media, consisting on an advection-diffusion-reaction equation for each different layer of material or tissue into the stent and the arterial walls, see for instance [1]. Such model has already been applied in [2] for computational studies

about drug release from stents. However, we point out that simulation studies based on this model involve extremely high computational costs and by consequence, to our knowledge, only studies concerning simplified stent geometries have been pursued so far. Starting from this point, we propose a reduced model for mass transfer from a thin layer, which significantly cuts down the computational cost for the simulation of the drug release from stents. Another difficulty arise from the fact that the release of the drug represents a stiff problem, whose numerical approximation requires the application of an adaptive stepping strategy. Combining these techniques it is possible to obtain simulations involving realistic expanded stent geometries, obtained in [3], and long time scales. The efficacy of our approach is demonstrated by means of numerical results concerning realistic situations.

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CT15
A posteriori error analysis of an augmented discontinuous formulation for Darcy flow

In the recent paper [3] it has been developed and stabilized a Discontinuos Galerkin (DG) method applied to Darcy flow. The method is stable and convergent for any combination of velocity and pressure interpolation, first-order and higher. Morevover the method is locally conservative in the sense that each element satisfies an exact mass balance.

On the other hand, if the solution of boundary value problem is not smooth enough, then the numerical method would need certain knowledge about the singularities of the solution. In order to overcome this difficulty, and adaptive strategy that automatically generates efficiently refined meshes would be most attractive.

In the framework of stabilized DG methods, in [1] we develop an augmented DG formulation for elliptic problems using piecewise Raviart-Thomas elements to approximate the vector (gradient) solution, while in [2] we present an a posteriori error analysis for such problems. Our purpose now is to extend/apply the a posteriori error analysis for Darcy flow problems.

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CT16
Exploring mixing dynamics inside microdroplets with a Level Set method

Flows of two immiscible fluids in microdevices allow to create emulsions where droplets moves through microchannels networks. Thanks to predominance of surface tension, a good control of the flow is achieved and those droplets have the same size and are used as microreactors to study very fast chemicals kinetics. Nevertheless a better understanding of hydrodynamics inside microdroplets is still needed in order to achieve flow control needed in mixing applications.

In this talk, we present numerical results of various mixing regimes inside microdroplets which can help in the design of microflows configurations with microdroplets achieving the flow control needed in practical applications. These simulations are obtained thanks to a new Level Set method developped in [2] which is inspired by [3] and involved a new *numerical stability condition* induced by surface tension - compared to the one presented by Brackbill et al. in the reference work [1] - as well as a *splitting method* which allows to shorten simulation times and allows to accurately compute asymptotic dynamics of microdroplets. As a matter of fact, in microfluidics, numerical stability constraint on the time step can be very demanding due to smallness of the time step associated to surface tension, compared to the one associated to the convective terms (i.e. CFL condition). Presented results are in good agreement with physical experiments and available results of the literature. In addition, this is the first such demonstration we are aware of in the context of numerical simulation of moving microdroplets in microchannels, where mixing dynamics dependance on confinement, droplet volume, injection velocity and viscosity ratio is studied.

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CT16
Adaptive finite element simulation of relaxed models for liquid-solid phase transition

We consider phase field models for liquid-solid phase transition based on a coupled system of the Cahn-Hilliard, the Allen-Cahn and the heat equation. In these models the sharp interface between different phases has been relaxed to a small transition area with a characteristic length acting as a regularization parameter for the underlying Stefan problem. Such models are extensively studied by physicists to understand the mechanisms of nucleation and other phenomena related to phase transitions (see e.g. [1,2,6]). Although an adaptive numerical treatment of these models is obviously advisable due to the localized transition zone between different phases, only first attempts at this issue have been pursued so far: The adaptive schemes employed are usually based on estimators for the energy error or on physically motivated heuristics (e.g. [3,7]) rather than on a rigorous estimation of the error in more relevant quantities.
The purpose of this work is to develop adaptive techniques for such problems that are based on error estimators for various quantities of interest, as presented for general parabolic problems by Eriksson and Johnson [4,5]. These rely on a discontinuous Galerkin approach for time stepping and the exploitation of a parabolic duality argument. For the biharmonic operator occurring in the Cahn Hilliard equation, a non conforming Galerkin method is employed to guarantee the full order of convergence on unstructured quasi uniform meshes. The developed techniques are numerically compared to other adaptive strategies. Mesh adaption is studied for different functionals of interest computed from the solution of the system under consideration. It is particularly studied in how far the developed methods remain stable when the regularization parameter for the interface relaxation is varied.

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CT16
Adaptive Multigrid Methods for Anisotropic Allen-Cahn Equations

Allen-Cahn equations are resulting from a phase–field approach to isothermal phase transitions. Anisotropic material properties, e.g., crystal lattices are taken into acount by anisotropic surface energies γ. Strongly varying solution behavior suggests adaptivity in time and space. However, unconditionally stable, implicit time discretizations require the solution of large, nonlinear and nonsmooth spatial problems in each time step. In particular, γ cannot be expected to be twice differentiable which excludes classical Newton linearizations.
In this talk we present fast and robust multigrid methods exploiting convexity rather than smoothness. Numerical experiments also illustrate the properties of various time discretizations as well as the performance of adaptive time stepping schemes and mesh refinement techniques.

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CT16
A free-boundary problem modelling crystal dissolution and precipitation in porous media

We study a convection-diffusion problem for chemical species on a variable domain. The normal velocity of the free boundary depends on the concentration of the species at the boundary. Solutions are computed by casting the problem in an Arbitrary Lagrangian Eulerian [1] setting and using a finite element method.
This problem is motivated by the study of crystal dissolution and precipitation in a porous medium [2]. We consider a porous medium that is fully saturated by a fluid in which cations (e.g. sodium ions) and anions (e.g. chlorine ions) are dissolved. In a precipitation reaction, n cations and m anions can precipitate in the form of one particle of crystalline solid (e.g. sodium chloride) attached to the surface of the grains (the porous matrix). The reverse reaction of dissolution is also possible. As a result of the precipitation and dissolution of crystals the geometry of the flow domain may change.
Computations for one and two dimensional settings are presented. For the one dimensional simulations, a coordinate transform and a finite difference method is used. Two different two dimensional configurations are studied: a perforated domain and a narrow rectangular channel. The two dimensional simulations use the Arbitrary Lagrangian Eulerian method. We compare solutions of the microscale model with solutions of upscaled, effective equations, and show a good agreement.

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CT17
Functional a posteriori error estimates for viscous flow problems

We discuss a posteriori error estimates of a new type that contain no mesh–dependent constants and are valid for any conforming approximation. An important property of the estimates is that they indeed provide *computable* and *guaranteed* bounds of errors. First estimates of such a type were obtained by a variational technique (see [1,2] and the references therein). Another method was suggested in [3]. It is based on transformations of integral identities. In the talk, we give an overview of the a posteriori error estimates derived for such models as Stokes [5], generalized Stokes problem and modified Stokes model with a polymerization term [4], models with non–quadratic dissipative potentials [6], and also for Navier–Stokes equations with small Reynolds numbers.

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CT17
STABILIZATION OF FINITE-DIFFERENCE SCHEME FOR STOKES PROBLEM

We present a new stabilized method for the Stokes problem. Staggered grids (components of the velocity field are computed in grid's crosspoints and pressure - in the cells' centers) are considered. We deal with second order discrete gradient operator which leads to high precision results. It has bidimensional kernel in 2D case and mesh-dependent kernel in 3D case (number of spurious pressure modes linearly depends on the quantity of discretization points). Due this fact LBB stability condition violates. Our method is independent of the space dimension and does not require choosing any mesh-dependent parameters. It always leads to symmetric linear systems. The new method is unconditionally stable and has simple and straightforward implementations. The stabilization strategy relies on projection operator whose action can be evaluated locally at the mesh level using only standart nodal data structures. As a result, an existing code can be easily modified to handle the stabilization procedures. Numerical experiments were held not only for traditional viscous fluid, but also for more complicated non-newtonian models (Bingham fluids).

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CT17
Numerical simulations of incompressible laminar flow for Newtonian and non-Newtonian fluids

This paper deals with numerical solution of laminar incompressible flows for Newtonian and non-Newtonian fluids through a branching channel. The motivation for numerical solution of the fluid flow in the branching channels arises in many applications, e.g. in the biomedicine, the solution of blood flow in cardiovascular system. One could describe these problems using Navier-Stokes equations and continuity equation as a mathematical model using two different viscosities (right hand side of Navier-Stokes equations). The unsteady system of Navier-Stokes equations modified by unsteady term in continuity equation (artificial compressibility method) is solved by multistage Runge-Kutta finite volume method. For steady numerical solution time dependent method with steady boundary condition is used. Steady state is achieved for $t \to \infty$ and followed by steady residual behaviour. For unsteady solution high compressibility coefficient β^2 is considered or dual time (iterative time) is used. The numerical results for two and three dimensional cases of flows in the branching channel for Newtonian and non-Newtonian fluids are presented and compared. Numerical model for simulation of flow in geometrically complicated domain representing arteries was developed and used in order to simulate flow in different cases.

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CT18
Inversion–based trajectory planning for the tem-

perature distribution in a parallelepipedon

In this contribution, an inversion–based approach is presented to solve the trajectory planning problem, i.e. the design of an open–loop control in order to realize a finite time transition between an initial and final state, for the evolution of the temperature distribution $x(z,t)$ in a hypercube or respectively a parallelepipedon governed by the (normalized) linear heat equation, i.e.

$$\frac{\partial x}{\partial t} = \Delta x = \sum_{j=1}^{n} \frac{\partial^2 x}{\partial {z_j}^2}, \quad z \in \Omega,\ t > 0, \tag{9}$$

where $\Omega = \{z \in \mathbb{R}^n,\ n \in \mathbb{N} : 0 < z_i < L_i,\ i = 1, 2, \ldots, n\}$ with $z = (z_1, z_2, \ldots, z_n)$. In addition, $\overline{\Omega}$ denotes the closure of Ω with boundary $\partial\Omega = \partial\Omega_0 \cup \partial\Omega_1$ for $\partial\Omega_0 = \{z \in \partial\Omega : z_n = 0\}$ and $\partial\Omega_1 = \partial\Omega \setminus \partial\Omega_0$. The local set of coordinates in $\partial\Omega_0$ is denoted as $\bar{z} = (z_1, z_2, \ldots, z_{n-1})$. Robin boundary conditions are considered with the boundary input $u(\bar{z}, t)$ acting on the surface $\partial\Omega_0$, i.e.

$$-b\frac{\partial x}{\partial n} + ax = \begin{cases} u, & z \in \partial\Omega_0,\ t > 0 \\ 0, & z \in \partial\Omega_1,\ t > 0. \end{cases} \tag{10}$$

with constant parameters a and b. Here, $\frac{\partial x}{\partial n} = \vec{n}\nabla x$ denotes the outward normal derivative. The considered trajectory planning problem aims at the design of a feedforward control $u(\bar{z}, t) \in L^2(\partial\Omega_0 \times [0, T])$, $T \in (0, \infty)$ in order to realize the transition from an initial stationary profile to a final stationary profile $L^2(\overline{\Omega}) \ni x^0(z) = x(z, 0) \longrightarrow x(z, T) = x^T(z) \in L^2(\overline{\Omega})$ along a prescribed path within the finite time interval $t \in (0, T]$, $T > 0$.

Motivated by the extensions of flatness–based methods to distributed–parameter systems defined on 1–dimensional domains (cf., e.g., [2]), for the solution of the considered trajectory planning problem a so–called basic output $y(\bar{z}, t)$ is determined, which allows to parameterize the state $x(z, t)$ as well as the input $u(\bar{z}, t)$. For this, the Riesz spectral properties of the system operator $Ax(z, t) = \Delta x(z, t)$ and Green's theorem are exploited in order to transfer (9), (10) into the respective spectral description $\frac{\mathrm{d}x_k(t)}{\mathrm{d}t} = \lambda_k x_k(t) + \kappa_{k_n} u_{\bar{k}}(t),\ x_k(0) = x_k^0,\ k = (k_1, ..., k_n),\ k_j \in I_j \subseteq \mathbb{N}$ with the Fourier–coefficients $x_k(t) := \langle x(z, t), \psi_k(z)\rangle$, $u_{\bar{k}}(t) := \langle u(\bar{z}, t), \varphi_{\bar{k}}(\bar{z})\rangle$, $\varphi_{\bar{k}}(\bar{z}) = 1/\kappa_{k_n} \frac{\partial \psi_k(z)}{\partial z_n}|_{z_n=0}$, $\kappa_{k_n} \sim k_n$ for $\bar{k} = (k_1, \ldots, k_{n-1})$. Here $\lambda_k \in \mathbb{R}$ and $\psi_k(z)$ denote the discrete eigenvalue and eigenfunction corresponding to the multiindex $k = (k_1, ..., k_n)$, $k_j \in I_j \subseteq \mathbb{N}$, respectively. Based on this spectral formulation, at first a formal state and input parametrization is systematically derived in terms of a basic output $y_{\bar{k}}(t) := \langle y(\bar{z}, t), \varphi_{\bar{k}}(\bar{z})\rangle$ via differential operators of infinite order. At second, it is shown that uniform convergence in $L^2(\Omega)$ of the Fourier series $x(z, t) = \sum_k x_k(t)\psi_k(z)$ and $u(\bar{z}, t) = \sum_{\bar{k}} u_{\bar{k}}(t)\varphi_{\bar{k}}(\bar{z})$ with coefficients $x_k(t)$ and $u_{\bar{k}}(t)$ parametrized in terms of the basic output can be verified by restricting $y_{\bar{k}}(t)$ to functions of certain Gevrey classes. It should be pointed out that the introduced basic output $y(\bar{z}, t)$ in many situations allows a physical interpretation. As an example, for $a = 1$, $b = 0$ it follows that $y(\bar{z}, t) = \frac{\partial x(z,t)}{\partial z_n}|_{z_n = L_n}$

In addition to the solution of the trajectory planning problem, the determined parametrizations in terms of the basic output represent exact solutions to the so–called controllability moment problems initially posed by Fattorini [1] when studying the reachable final profiles in $L^1(\Omega)$ for (9), (10) with $a = 1$, $b = 0$. For distributed–parameter control problems this in particular confirms the strong relation between (approximate) controllability and parametrizability in terms of a basic output.

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CT18
A numerical treatment of an inverse problem to nonlinear strongly degenerate parabolic equations.

In this paper we present a numerical method for the identification of parameters in the flux and diffusion functions of nonlinear strongly degenerate parabolic equations when the solution at a fixed time is known. We formulate the identification problem as a minimization of a suitable cost function and we derive its formally gradient by means of a first-order perturbation of the direct problem solution which is a linear strongly degenerate parabolic equation with source term and discontinuous coefficients. For the numerical approach, we assume that the direct problem is discretized by the Engquist-Osher scheme and obtain a discrete first order perturbation associated to this scheme. The conjugate gradient method permits to find numerically the physical parameters.

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CT18

Determination of a piecewise constant conductivity using boundary integral equations with application to EEG

We consider the three-dimensional inverse electrical impedance problem in the case of piecewise constant conductivities. Let $D \subset \mathbb{R}^3$ be a bounded domain, with boundary ∂D, representing the conducting medium, assumed to be made up of several layers. The electric potential u satisfies the equations:

$$\begin{array}{lll} \nabla(\sigma.\nabla u) = 0 & \text{in} & D \\ u = f & \text{on} & \partial D \\ \sigma_2 \dfrac{\partial u}{\partial n} = g & \text{on} & \partial D \end{array} \tag{11}$$

with σ, f and g respectively representing the conductivity in D, the electrical poential and the current density on ∂D.
We will assume that the geometry of the layers is known (for example, by means of MRI). Our aim is to identify the electrical conductivities of the differents layers of the medium (a head, in the case of EEG).
First, we present a uniqueness result with one measurement in the case of two layers.
Then, we solve numerically the inverse conductivity problem in the case of two or three layers. To that end, we use an iterative method where at each step, we solve a direct (Dirichlet or Neumann) problem. For these direct problems we have built an equivalent system of boundary integral equations.
Finally, we present some numerical results.

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CT18
Inverse Problems of Econometrics

In present paper a deterministic approach to the problem of construction of parameters of linear vector regression is offered. The maximal size of an error of each sample q_{ik} of the economical characteristic q_i is supposed known a priori, proceeding from experience of similar measurements and errors of measuring devices. The number of samples is minimal and equal the number of variables in researched economical process n^2. This fact allows to attribute offered algorithm to the fast algorithms of the analysis of the economical information.
As the samples are obtained from experiment it is supposed that the each sample q_{ij}, $1 \le i, j \le n$ has the error the value of which is known a priori:

$$|\, q_{ij} - q_{ij}^{ex} \,| \le \delta_i, \quad 1 \le j \le n, \quad i = 1, \dots, n. \tag{12}$$

where q_{ij}^{ex} is the exact sample of variable q_i. Such approach can have application for short time forecast of economical characteristics under uncertainties. Let us present a problem of construction of model of stationary connection between variables $q_1, q_2, \dots, q_n$ as a problem of the solution of linear system.

$$A_p z = q_1, \tag{13}$$

where $A_p z = z_1 q_2 + z_2 q_3 + \cdots + z_{n-1} q_n + z_n e,\ z = (z_1, z_2, ..., z_n)^T$, $q_i = (q_{i1}, q_{i2}, ..., q_{in})^T$, $i = 1, \dots, n$; superscript T denotes transposition; e being unit vector of dimension n; q_{ik} is k-th sample of variable q_i; $p = (q_{21}, q_{22}, \dots, q_{2n}, q_{31}, q_{32}, \dots, q_{3n}, \dots, q_{n1}, q_{n2}, \dots, q_{nn})^T$. The matrices A_p depend on vector p (or in general on vectors $q_2, q_3, \dots q_n$). Vector p can have values inside some closed region D since the vectors $q_2, q_3, .., q_n$ have been obtained with errors. The set of matrices $K_A = \{A_p\}$ in (2) correspond to the set D. At least one matrix from K_A is singular . The set of possible solutions to (2) with fixed matrix $A_p \in K_A$ is as follows: $Q_{\delta_1,p} = \{z : \| A_p z - u_{\delta_1} \|_U \le \delta_1\}$. The following inverse problems (extreme problems) can be considered as examples to find the some linear vector regressions z:

$$\begin{array}{rcl} \| z^s \|^2 & = & \inf\limits_{q_2} \inf\limits_{q_3} \dots \inf\limits_{q_n} \inf\limits_{z \in Q_{\delta_1,p}} \| z \|^2, \\ \| z^{s,b_n} \|^2 & = & \inf\limits_{q_2} \inf\limits_{q_3} \dots \sup\limits_{q_n} \inf\limits_{z \in Q_{\delta_1,p}} \| z \|^2, \\ & \dots & \\ \| z^b \|^2 & = & \sup\limits_{q_2} \sup\limits_{q_3} \dots \sup\limits_{q_n} \inf\limits_{z \in Q_{\delta_1,p}} \| z \|^2. \end{array} \tag{14}$$

The problem of construction of econometric model was chosen for test calculation on the data which are given in well known work.

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CT18
Nonsmooth Newton Methods for Set-Valued Saddle Point Problems.

We present a new class of iterative schemes for large–scale set–valued saddle point problems as arising, e.g., from optimization problems in the presence of linear and inequality constraints. Our algorithms can be either regarded as nonsmooth Newton–type methods for the nonlinear Schur complement or as Uzawa–type iterations with active set preconditioners. Global convergence of various inexact variants can be shown. Numerical experiments with discretized optimal control problems and a discretized Cahn–Hilliard equation illustrate the reliability and efficiency of the approach.

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CT19
Regularized Hyperbolic Problems for Optimal

Nodal Control of Gas Networks

We investigate gas networks which are considered as directed graphs. At every junction of the network one should be able to control the flow by increasing and/or decreasing the pressure. With the help of an interpretation we adopt this model for gas networks, traffic flow networks and by changing some parameters for water networks.
In a first step we consider only one gas pipeline where the flow is controlled on one end. The flow is modelled by nonlinear hyperbolic differential equations which allow - in contrast to elliptic or parabolic ones - only few results about the regularity of the solution. The numerical treatment of optimal control problems with hyperbolic constraints is therefore very complicated. We approach a discretization by regulizing the nonlinear hyperbolic equation obtaining a singular parabolic equation which offers us limited acces to results from the semilinear parabolic case. This enables us to discretize the boundary control problem by a finite element approach in the spatial dimension and by a semi-implicite time scheme. Developing a discretization for the complete optimal control problem we show unique solutions for both the continuous and the discrete problem. Moreover, consistency of the parabolic regulized state equation implies convergence of the discrete solution to the exact one. This model of one pipeline is extended to a junction of more than two pipes. The boundary constraints are replaced by mass conservation and a continuity requirement at the node. In addition, we control the flow at this junction and show some recent results.

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CT19
Approximate reduced SQP methods for model-based optimization

One of the major challenges in applied model-based optimization is the fact that the underlying process model and a sophisticated solver code is given in many cases and changes involve high costs in terms of code flexibility or application range. Therefore, one searches for methods which allow a fast numerical solution of the overall optimization problem and change the process model only in a weak form. Reduced SQP methods are considered as candidates for a respective algorithmic paradigm. However, solutions to linearized models and adjoint equations usually can only be provided approximatively. Therefore approximate variants are used and investigated. Theoretical, as well as, numerical results for the challenging problem of aerodynamic shape optimization are presented, which have been achieved during the German collaborative effort MEGADESIGN.

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CT19
Numerical Optimization in a Real-World Application

We consider a modern ship propulsion and steering system, the Voith Schneider Propeller. On the Voith Schneider Propeller, a rotor casing which ends flush with the ship's bottom is fitted with a number of axially parallel blades and rotates about a vertical axis. To generate thrust, each of the propeller blades performs an oscillating motion about its own axis. This is superimposed on the uniform rotary motion. Such an industrial device offers a whole variety of optimization problems that we will introduce and partly solve.
In this talk, we first introduce the performance of the Voith Schneider Propeller and show that it can serve as a model for general propulsion systems. In particular, we indicate mathematical problems arising from the consideration of a real-world problem.
The flow is modeled by the 3D instationary, incompressible Navier-Stokes equations that serve as constraint for the different optimization problems. As a first example, we consider the optimal steering. We indicate the mathematical structure of the target functional leading to specific optimization methods. We also indicate how AD (automatic differentiation) can or cannot be used in this framework. The second example concerns the shape optimization of the blades itself. Finally, we present some approaches to treat the complete system, when one or several propellers are embedded into the ship's hull. This in particular amounts the coupling of different methods and a particularly good description of the ship's hull.
This work has been done in cooperation with the Voith Turbo Marine company (Dr.-Ing. D. Jürgens, M. Palm, S. Singer) and in collaboration with my students J.C. Matutat, R. Deininger and R. Leidenberger.

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CT20
Modelling the Electrostatic Workpiece Charging during Electron Beam Lithography

Electron beam lithography provides a method which allows to print submicron structures onto a target, e.g. a mask blank or a Si-wafer. However, placement accuracy is reduced due to the charging of the

target. Modelling these placement errors, might provide a method for improving pattern placement.
During electron beam lithography, the pattern generator scans the target with an electron beam with varying dose D, which can be expressed as a function:

$$D: \begin{array}{rcl} \mathbb{R}^3 & \to & \mathbb{R}_0^+ \\ (x_0(t),\, y_0(t),\, z_0) & \to & D(x_0(t),\, y_0(t),\, z_0) \end{array} \tag{15}$$

Each shot of the pattern generator deposits charges inside the target which influences the trajectory of the electron beams of subsequent shots. These charges build up an electric potential, which is given by

$$\phi(\mathbf{r},t) = \frac{1}{4\pi\varepsilon_0} \int_{\mathcal{M}} q_e \frac{c(\mathbf{R},t)}{\|\mathbf{r}-\mathbf{R}\|_2} d\mathbf{R}\,. \tag{16}$$

Here, $\mathbf{r} = (x\,y\,z)^T$ denotes the position of the probe charge and $c(\cdot,t)$ is the charge distribution of the target. One can derive the following integro-differential-equation of motion by applying Newton's law:

$$\ddot{\mathbf{r}} = -\frac{q_e}{m_e} \nabla_{\mathbf{r}} \phi(\mathbf{r},t)\,. \tag{17}$$

The trajectory of the beam's electrons is given by equation (17) and proper initial conditions.
The beam deflection $(\delta x(x,y),\, \delta y(x,y))$ due to the already deposited charges are implicitly given by

$$\delta x(x_0,y_0) = x(t^*) - x_0 \qquad \delta y(x_0,y_0) = y(t^*) - y_0\,. \tag{18}$$

Hence, at the pattern surface of the target, there is a flux $\mathbf{j}$ of electrons:

$$\begin{aligned} &\mathbf{j}(x_0(t) + \delta x(x_0(t),y_0(t)), y_0(t) + \delta y(x_0(t),y_0(t))) \cdot \vec{e}_z \\ &\qquad = D(x_0(t),y_0(t),z_0)\,. \end{aligned} \tag{19}$$

Furthermore, the distribution of electrons inside the target is changing with time due to diffusion subjected to a potential which can be expressed by the following partial differential equation:

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = -\nabla_{\mathbf{r}} \cdot (d\nabla_{\mathbf{r}} c(\mathbf{r},t) + z\mu f c(\mathbf{r},t) \nabla_{\mathbf{r}} \phi(\mathbf{r},t))\,, \tag{20}$$

with d, z, f, μ denoting the diffusion coefficient, charge number, Faraday's constant and the mobility, respectively.
The partial differential equation (20) is coupled with the integro-differential-equation (17) via the Neumann boundary condition given in equation (19).
In this paper, the coupling of these equations will be studied and a computational method for simulating the electron beam lithography will be proposed.

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CT20
Stabilized FEM for incompressible flows: Equal-order vs. inf-sup stable approximation

A recent approach to the variational multiscale approach to incompressible flows consists in stabilization of the standard Galerkin finite element method using the local projection approach [1]. In the present paper, we take advantage of a general framework for the a-priori analysis of such methods given in [2] for linearized Navier-Stokes problems of Oseen type.
The case of equal-order approximation for velocity and pressure can be found in [1], [2]. The case of inf-sup stable finite element pairs is considered in [3]. Here, we give a critical comparison for a h/p-version of both variants. Numerical examples for incompressible Navier-Stokes flows support the discussion.

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CT20
Local time stepping for implicit-explicit methods on time varying grids

Our scope of interest is the accurate numerical simulation of conservation laws. The solutions of such systems of PDEs exhibit localized and moving singularities which require costly numerical schemes. At the same time realistic applications often require simulation of the phenomenon on very long time range. In multiphase flows an additional feature is the big discrepancy between two types of waves: a slow kinematic one which is the phenomenon of interest, and fast acoustic waves arising from the highly nonlinear physics.
This setup is a very good candidate for the adaptive method developped in [1]. Its gist consists in analyzing the smoothness of the solution by performing a wavelet-like transformation. The adaptive grid is designed by locally selecting the level of discretization beyond which the wavelet coefficients are negligible. The evolution of the adaptive grid at each time step in order to follow the displacement of the singularities of the solution strongly relies on the hyperbolic nature of the equations which ensures a finite speed of propagation. At this stage, the time step is monitored by the smallest space grid step and the CFL-like stability condition.
A recent extension of this method by Müller et al [2] consists in using a local time step. A macro time step, fit for the coarsest level of discretization, is subdivided into intermediate time steps. At a given intermediate time step, the solution is updated only on cells belonging to the current synchronization level or finer. Straigthforward application of this method to our system of PDEs in the

explicit scheme case is now extensively tested. The computing time ratio between the uniform grid scheme and the local time stepping scheme can be as high as 16.
As developed in [3], the discrepancy between kinematic and acoustic speeds specific to our problem can be advantageously dealt with in a Lagrangian projection formulation. This allows to resolve the acoustic part of the solution with an implicit scheme - therefore relaxing the prohibitive time step bound. The kinematic components are solved explicitely, which ensures the required precision. We present here the original local time stepping version of this *semi-implicit* scheme. It provides a computing time gain of 11.

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CT20
The Composite Mini Element - Coarse grid computation of Stokes flows on complicated domains

We introduce a new mixed finite element for the discretization of the Stokes equations with Dirichlet as well as slip boundary conditions. The basis of every finite element method is the subdivision, for instance a triangulation, of the physical domain. The approximation quality is determined by the maximal meshwidth of the triangulation, while the computational effort is determined by its number of elements. If the physical domain is very complicated, i.e. its boundary contains a huge number of geometric details, then the minimal number of triangles, that are necessary to resolve the domain and to preserve optimal order convergence, can be affected critically, even for locally refined meshes. In this case, the computational effort can be too large to solve it even on state-of-the-art computers.
In contrast to that, our approach decouples the minimal dimension of the approximation space from the domain geometry by adapting the shape of the finite element functions to the needs of the complex geometry and the imposed boundary condition. This approach allows low-dimensional approximations even for problems with complicated geometric details.
This new nonconforming mixed method for the Stokes equation, the composite mini element, is proved to be stable and linear (optimal order) convergent. The method can be viewed as a coarse scale generalization of the classical mini element approach, i.e. it reduces the computational effort while the approximation quality depends on the maximal mesh width in the usual way.

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CT21
Calibration of Interest Rate Volatility as a High-Dimensional PDE Problem

The objective of this work is the calibration of a time-homogeneous, hump-shaped volatility function to a time series of LIBOR rates. The observed data are used to estimate simultaneously the distribution of instantaneous forward rates as unobservable driving processes, and the model parameters.
Acknowledging the presence of observation noise in a Bayesian setting, we obtain parameter distributions that yield stable and accurate estimates together with measures for their uncertainty. We extend the approach in [1] to a more realistic setting and propose an efficient numerical strategy for the solution.
This is achieved by deriving a seven-dimensional Fokker-Planck equation for the posterior distribution (of four parameters and three forward rates) between observation dates, which is then solved on a sparse grid with techniques similar to the ones developed in [2].
We analyse to what extent the curse of dimensionality can be broken and demonstrate numerical results for observed LIBOR market data.

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CT21
Multiscale analysis of jump processes in finance – sparse tensor product based wavelet compression

Pricing financial derivatives where the underlying is modeled by multivariate Lévy processes yields high-dimensional parabolic partial integrodifferential equations. As described in [2], these equations are of the form $\partial_t u + \mathcal{A}u = 0$ on $[0,1]^d$ with $d \geq 2$ and non-local operator $\mathcal{A}$. Their numerical solution by Finite Element Methods requires an efficient discretization of $\mathcal{A}$.
Motivated by such financial models, for a wide class of anisotropic operators we present a new sparse tensor product based wavelet compression scheme using anisotropic tensor product wavelets. The scheme (asymptotically) reduces the complexity of the Finite Element stiffness matrix from originally $\mathcal{O}(h^{-2d})$ to essentially optimal $\mathcal{O}(h^{-1}|\log h|^{2(d-1)})$, where h denotes the meshwidth of the Finite Element discretization. It is based on a combination of concepts from [1], [3] and the references therein. The compression technique is neither limited to Lévy models nor to non-local operators only arising in finance.
Numerical results are presented.

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CT21
Fast pricing techniques for Multi-Asset Options.

Options on more than one underlying asset are called multi-asset options and belong to the class of exotic options. We aim for pricing multi-asset options numerically for an increasing number of dimensions.
In this presentation we present a novel pricing technique based on the risk-neutral expectation of the discounted payoff:

$$V(\mathbf{S}(t),t) = e^{-r(T-t)}\mathbb{E}_{\mathbf{Q}}V(\mathbf{S}(T),T), \tag{21}$$

where r is the risk-free interest rate, T the time to maturity, $\mathbf{S}$ the vector of values of the underlying assets and $\mathbf{Q}$ the risk-neutral probability measure. In [1] it is shown that the price can be computed by use of two Fourier transforms:

$$V(\mathbf{y}(t),t) = e^{-r(T-t)}\int_{\mathbb{R}^d}\left(\int_{\mathbb{R}^d} V(\mathbf{x}(T),T)e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x}\right)\phi(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{y}}d\mathbf{k}, \tag{22}$$

where $\mathbf{x}$ and $\mathbf{y}$ are the logarithmic values and $\phi(\mathbf{k})$ represents the characteristic function which is known explicitly for a certain class of processes which contains the GBM (Geometric Brownian Motion) and Lévy processes.
The numerical computation of equation (22) is done by discretizing on a regular grid with N_i points and replacing both integrals by a multi-dimensional multi-step trapezoidal rule. The computation of these finite sums can be done by rewriting the sums into the d-dimensional Fast Fourier Transform (FFT_d):

$$V(\mathbf{y}_m(t),t) \approx e^{-r(T-t)}\mathbf{IFFT_d}\left\{\phi(\mathbf{v}_n)\mathbf{FFT_d}\left(f\left(\mathbf{x}_k\right)\right)\right\} \tag{23}$$

This method is significantly faster corresponding to the PDE method. One of the reasons is that the time derivative term is not present in the standard multi-dimensional Black-Scholes equation. Therefore no time integration is needed for European options. We compare the results of this method with the sparse grid solution of the multi-dimensional Black-Scholes PDE [2].
By means of parallel computation we can efficiently compute the **FFT** on the full tensor-product grid. A parallel partitioning technique divides the array in even and odd points. This partitioning is repeated towards a single point.
In this way we can handle problems of medium sized dimensions (up to 8D) efficiently. We can go up in the dimensions, depending on the parallel computer at hand.

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CT21
Optimal Portfolio Allocation with Quasi-Monte Carlo Methods

Portfolio optimization is a widely studied problem in finance dating back to the work of Merton from the 1960s. While many approaches rely on dynamic programming, some recent contributions use martingale techniques to determine the optimal portfolio allocation.
Using the latter approach, we follow the work [1] and show how optimal portfolio weights can be represented in terms of conditional expectations of the state variables and their Malliavin derivatives. In contrast to other approaches, where Monte Carlo methods are used to compute the weights, here the simulation is carried out using Quasi-Monte Carlo methods in order to improve the efficiency. Despite some previous work on Quasi-Monte Carlo simulation of stochastic differential equations, we find them to dominate plain Monte Carlo methods. However, the theoretical optimal order of convergence is not achieved. With the help of a theorem from [2] and backed by some computer experiments on a simple model with explicit solution, we provide a first guess, what could be a way around this difficulties.
This work has been done in collaboration with Rüdiger Kiesel and Karsten Urban (both Ulm University).

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CT22
Non-conforming finite elements of arbitrary order for the Stokes problem on anisotropic meshes

Anisotropic meshes are characterized by elements with large or even asymptotically unbounded aspect ratio. Such meshes are known to be particularly effective for the resolution of directional features of the solution, like edge singularities and boundary layers.
We consider here the numerical solution of the Stokes problem in two-dimensional domains by non-conforming finite elements of higher order. The pressure is approximated by discontinuous, piecewise polynomials of order $r-1$. For approximating the velocity we discuss four non-conforming spaces of approximation order r.
For the stability of finite element methods for solving the Stokes problem it is necessary that the discrete spaces fulfil an inf-sup condition. All of the considered families fulfill this condition but only two of them have an inf-sup constant which is independent of the aspect ratio of the meshes. For these two families we show optimal error estimates on anisotropic meshes. The proof is restricted to rectangular triangulations with special properties.
The elements can be used also for Navier–Stokes equations.

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CT22
CONVERGENT DISCRETIZATIONS OF A NAVIER-STOKES-NERNST-PLANCK-POISSON SYSTEM

We introduce an electrohydrodynamic model that combines the incompressible Navier-Stokes equation with a Nernst-Planck-Poisson system and show existence of weak and strong solutions. In a first step, we propose a fully discrete scheme whose solutions satisfy a discrete energy law, entropy inequality, maximum principle as well as non-negativity, and establish convergence towards weak solutions. Then an efficient scheme is proposed, and convergence with optimal rates towards strong solutions is verified. Computational results are provided for numerical comparison of both schemes.

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CT22
A unified convergence analysis of local projection stabilisations applied to the Oseen problem

The discretisation of the Oseen problem by finite element methods suffers in general from two problems. First, the discrete inf-sup (Babuška–Brezzi) condition can be violated. Second, spurious oscillations occur due to the dominating convection. One way to overcome both difficulties is the use of local projection techniques.
These local stabilisation techniques are based on a projection $\pi_h : Y_h \to D_h$ from the underlying approximation space Y_h onto a discontinuous projection space D_h. Stabilisation is derived from additional weighted L^2-terms of the fluctuation $\kappa_h := id - \pi_h$ of the gradient of pressure and velocity (or only parts of the latter like the divergence or the streamline derivative). The key point in the analysis is a proper interpolation operator $j_h : H^1(\Omega) \to Y_h$ such that the interpolation error fulfils not only optimal error estimates but has also additional orthogonality properties with respect to D_h.
Studying the local projection method in an abstract setting, we show that the fulfilment of a local inf-sup condition between approximation and projection spaces allows to construct an interpolation with additional orthogonality properties. Based on this special interpolation, optimal a-priori error estimates are shown with error constants independent of the Reynolds number.
Applying the general theory, we extend the results of Braack and Burman [1] for the standard two-level version of the local projection stabilisation with low order finite elements on quadrilaterals and hexahedra to discretisations of arbitrary order on simplices, quadrilaterals, and hexahedra.
Moreover, our general theory allows to derive a novel class of local projection stabilisation by enrichment of the approximation spaces. This class of stabilised schemes uses approximation and projection spaces defined on the same mesh and leads to much more compact stencils compared the two-level approach.

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CT22
Benchmark proposal for incompressible two-phase flows

Numerical simulation of incompressible interfacial flows, such as two phase flows with immiscible fluids, is maturing at a rapid rate. Each year sees the publication of numerous improved schemes and methods for numerically simulating mixtures of immiscible fluids undergoing complex topology change. These new schemes address issues such as interface tracking and resolution, mass conservation, implementation of surface tension effects etc. With the focus on these issues it is perhaps not surprising that no rigorous, that is quantitative, benchmark configuration has been proposed for validation and comparison of interfacial flow codes to this date. Although fully three dimensional benchmarks are available, such as the collapse of a liquid column, they mostly only include visual measures for comparisons which are not sufficient for precise validation of numerical codes. This is in stark contrast to the field of incompressible laminar single phase flow for which dedicated benchmarks regarding *accuracy versus CPU cost* have been presented and accepted by the general CFD community.
With this in mind we proceed to propose two benchmark configurations and define relevant benchmark quantities to directly measure both topological parameters such as interface deformation, and also indirect ones, such as velocity measures. The task of the proposed benchmarks is to track the evolution of two dimensional bubbles in liquid columns. The configurations are simple enough to compute accurately yet also allow for very complex topology change, giving the interface tracking techniques of today an adequate challenge.
Results from preliminary studies are presented and discussed. These studies [1] were undertaken by 3 different participating groups. Two represented Eulerian level set finite element codes, and one represented a moving grid approach where the interface always is aligned with the cell edges. Moreover, we discuss the features of our new FEM level-set approach with implicit treatment of the surface tension and adaptive grid alignment which leads to improved robustness and accuracy results.

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CT23
Fishways design: An application of optimal control theory.

From the end of last century to the present times, it has been growing the interest in solving the ecological problems appearing when the hand of man acts on nature. One of these problems is the necessity to preserve and enhance stocks of diadromous (fish that migrate between freshwater to saltwater) and resident fish in our rivers. When a dam is constructed in a river, it is necessary to build a hydraulic structure that enables fish to overcome the dam to their spawning and other migrations. This hydraulic structure is known as fishway. There are several types of fishways, but in stream obstructions, a vertical slot fishway [1] is generally used. It consists of a rectangular channel built on a side of the dam, with a sloping floor, that is divided into a small number of pools by baffles with slots. Water runs downstream in this channel, through a series of vertical slots from one pool to the next one below. The water flow forms a jet at the slot, and the energy is dissipated by mixing in the pool. The objective of this type of fishways is that fish can ascend, using its burst speed, to get past one slot, and then, that it can rest inside the pool till the next slot is tried.
The main objective of this work consists of finding the optimal design of a vertical slot fishway. We look for the location and length of the baffles separating the pools, in order to obtain a suitable water velocity. In the zone of the channel near the slots, we look for a velocity suitable for fish leaping and swimming capabilities. In the remaining of the fishway, we look for a velocity close to zero for making possible the rest of the fish. Moreover, in all the channel, we try to minimize the flow vorticity.
First we introduce a mathematical formulation of the optimal design problem for a standard ten pools channel, where the state system is given by the shallow water (Saint-Venant) equations, the design variables are the location and length of the baffles, and the objective function is related to obtaining the aforementioned objectives on the water velocity. Next, by using the "domain derivative" (cf. [2]) we give a detailed expression for the gradient of the objective function *via* the adjoint system. Next, we propose a characteristics-Galerkin method for solving the state system, and two algorithms to solve the optimization problem: (a) a derivative-free algorithm, and (b) a gradient-type method computing the cost gradient by solving the adjoint system with the characteristics-Galerkin method. Finally, we show numerical results obtained for a standard ten pools fishway.

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CT23
An Optimal Control Problem in Adoptive Cellular Immunotherapy

Immunotherapy refers to the treatment capable to stimulate or restore the ability of the immune (defense) system to fight infection and disease. Immunotherapy (also called biological therapy or biotherapy) often employs substances called biological response modifiers

(BRMs). The body normally produces low levels of BRMs in response to infection and disease. Forms of biological therapy include monoclonal antibodies, interferon, interleukin-2 (IL-2), and several types of colony-stimulating factors.
Of particular interest here is the use of cytokines, which are protein hormones that aid in regulating aspects of cell growth and function during specific immune response. They act by changing the cells that produce them and altering the cells near them. Interleukin-2 (IL-2) is an important cytokine for lymphocytes activation, in mediating cell proliferation, promoting of other cytokines, and enhancing natural killer cell function. This use of cytokines to treat cancer is usually done in conjunction with adoptive cellular immunotherapy (ACI). During ACI, lymphocytes are taken from cancer pacients, then grown and activated in a manner which stimulates them to react to certain antigens. These cells are then infused into the pacient. The adopted lymphocytes invade the tumor cite and immunologically reject it.
In this paper we investigate a mathematical model described by a system of differential equations which model tumor-immune dynamics. The model introduces three populations: the activated immune system cells (or, effector cells), the tumor cells, and the concentration of IL-2 in the tumor-site compartment. The effects of the cytokine interleukin-2 on tumor-immune dynamics are analysed by means of an optimal control problem. The control variable describes the percentage of adoptive cellular immunotherapy given. The objective functional of the optimal control problem is defined such that to maximize the amount of effector and interleukin-2 cells and minimizing the number of tumor cells and the cost of the control. The boundedness of solutions of the state system and the existence of an optimal control for this problem are proved. We characterize the optimal control in terms of the solutions to the optimality system. Computational issues together with numerical findings are also presented. The biological significance of the results is discussed.

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CT23
Augmented Lagrangians for Optimal Control and Topology Optimization

We present applications of a method of semi–monotonic augmented Lagrangians, which was developed and proved to be optimal in [1] in terms of matrix analysis. The analysis was extended to an operator notation in [2] and applied to the Stokes problem preconditioned with a geometric multigrid. In this paper we proceed on with our approach to efficient solution of Karush–Kuhn–Tucker systems arising in optimal control and topology optimization.
The optimality (linear complexity) of the semi–monotonic augmented Lagrangian method relies on a particular update of the augmented Lagrange parameter, that insures an increase (semi–monotonicity) of the Lagrange functional, and on preconditioning of the inner products in both the primal variables and Lagrange multipliers. Then, one can prove a well–controlled bound of the augmented Lagrange parameter, which implies a uniform equivalence of Hessians of augmented quadratics. At the end, we present numerical results for applications in optimal control for image processing and topology optimization in magnetostatics.

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CT23
Discrete Gradient Flows for a Shape Optimization Problem

Shape optimization problems are ubiquitous in science, engineering and industrial applications. They can be formulated as minimization problems with respect to the shape of a domain Ω in R^d. If $y(\Omega)$ is the solution of a boundary value problem in Ω

$$Ly(\Omega) = 0, \tag{24}$$

and $J(\Omega, y(\Omega))$ is a cost functional, then we consider the minimization problem

$$\Omega^* \in \mathcal{U}_{ad}: \qquad J(\Omega^*, y((\Omega^*)) = \inf_{\Omega \in \mathcal{U}_{ad}} J(\Omega, y(\Omega)), \tag{25}$$

where $\mathcal{U}_{ad}$ is a set of admissible domains in R^d. If the problem is purely geometric, namely there is no state constraint (24), then we simply denote the functional $J(\Omega)$.
We present (see [1]) a variational method which explicitly and clearly leads first to design a flow $\Omega(t)$, starting from an initial configuration $\Omega(0)$ to a relative minimum $\Omega(\infty)$, that decreases the function $t \mapsto J(\Omega(t), y(\Omega(t))$, and next to discretize in time and space, thereby obtaining a natural descent direction. Here we summarize our approach which hinges on three essential features:

1. *Shape sensitivity analysis*: this allows us to express variations of bulk and surface energies with respect to domain changes and formalize the notion of shape derivative and thus shape gradient.
2. *Semi-implicit time discretization*: this is crucial in order to maintain an implicit computation of geometric quantities such as mean curvature and normal velocity but not the entire geometry. This can be realized without explicit parametrization of the domain boundary, and is sufficiently flexible to accommodate several scalar products for the computation of normal velocity depending on the application.
3. *Adaptive finite element method for space discretization*: this is important for the intrinsic computation of mean curvature as well as the control of local meshsize to increase resolution.

We make also explicit the concept of shape derivative of $J(\Omega)$ in the direction of a normal velocity V and we then indicate how to exploit this information to design different discrete gradient flows. Several numerical experiments will be discussed.

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CT24
A Multiscale Method for Earth Structure Determination from Normal Mode Splitting

The splitting function $c = \sum_{n=0}^{\infty}\sum_{j=1}^{2n+1} c_{n,j}Y_{n,j}$ is a radial average of three-dimensional heterogeneity of the Earth. Its coefficients are related to internal properties δm and the topography δd by

$$c_{n,j} = \int_0^a K_n^m(r)\delta m_{n,j}(r)\,dr + \sum_d K_n^d \delta d_{n,j}\ ,$$

where K_n denotes the degree-dependent sensitivity kernel of a given mode. We present a new multiscale method for the determination of δm and δd. At first, the splitting function c is decomposed by a spherical wavelet. Now it is possible to determine wavelet coefficients of δm and δd by a linear equation system. Then δm and δd can be reconstructed by wavelets on the three-dimensional ball. The main advantage of a wavelet method is its localisation property. If the wavelets are chosen appropriately it is also possible to reconstruct the harmonic and anharmonic part of the Earth's density separately, whereas gravitation based models provide only the harmonic part. Hence, we will be able to use our results to construct a multiscale Earth model from a combination of gravitational and seismic data.

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CT24
Multilevel Solutions of Stochastic Wick-type Heat Equations.

Numerical solutions of heat equations can be easily obtained by already existing numerical tools developed for solving time-dependent differential equations. Indeed, this is possible provided that all involved data are given in a deterministic manner. However, modeling realistic applications in heat conduction may require treatment of randomness in the equation under study. As an example of this random input, the conductivity in the material which may be not known apriori and only some of its statistical properties are given. Other sources of randomness are the heat source, initial and boundary conditions. Taking into account all these random effects, the model leads to the well-established stochastic heat equations. In practice, these equations belongs to multiscale problems and still represent a challenge in designing numerical algorithm for their solutions.
In this contribution, we are concerned with stochastic heat equations of Wick type. As a special case, we consider the Wick-stochastic heat equation with the conduction coefficient is taken as exponential of white noise. To perform a rigorous study of stochastic effects in the heat equation we employ techniques from Wick calculus, see [1,2,3,4] among others. The differentiation respect to time and space along with the product operations are perform in a distribution sense. Using the Wiener-Itô chaos expansion for treating the randomness, the governing equation is tranformed into a system of uncoupled deterministic heat equations to be solved for each chaos coefficient by canonical numerical methods for partial differential equations. In our study, we formulate a finite element method for spatial discretization and a backward Euler scheme for time integration. To speed up the algorithm, we formulate a multilevel solver for the algebraic equations. Once the chaos coefficients are obtained, statistical moments for the stochastic solution are carried out. Numerical results are presented for stochastic heat equations in both one and two space dimensions.

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CT24
Fast Approximation on the 2–Sphere by Optimally Localizing Approximate Identities

A method to construct approximate identities on the 2–sphere which have an optimal localization is introduced. This approach can be used to accelerate the calculations of approximations on the 2–sphere essentially with a comparably small increase of the error. The localization measure in the optimization problem includes a weight function which can be chosen under some constraints. For each choice of weight function existence and uniqueness of the optimal kernel can be proved as well as the generation of an approximate identity in the bandlimited case. Moreover, the optimally localizing approximate identity for a certain weight function is calculated and numerically tested.

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CT24
A wavelet-based dynamically adaptive scheme for viscous Burgers equation

This paper is concerned with the design, theoretical and computational issues of dynamically adaptive wavelet method for viscous Burgers equation. The adaptivity in the context of wavelet discretization insists in how to choose which wavelet coefficients to keep and which to discard. A specific difficulty is that the singularities might move in time and so the set of indices of significant wavelet coefficients at each time step is updated.

Our aim is to design an asymptotically optimal algorithm in the sense that storage and number of floating point operations, needed to resolve the problem with desired accuracy, remain proportional to the problem size when the resolution of the discretization is refined, so the computational complexity for all steps of our algorithm is controlled.

We follow some ideas from [2,4], where a general wavelet adaptive method for a large class of nonlinear equations has been proposed. The basis functions used for spatial discretization are the spline wavelets on the interval introduced in [3] which we modify to satisfy boundary conditions according to [1].

Numerical examples are presented for solution with steep front on a stationary wave and for a situation of a fast moving wave which also develops a steep front.

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CT25
PSI Solution of Convection-Diffusion equations with data in L^1.

We consider in this work convection-diffusion problems with source term in L^1. These problems model the behaviour of physical variables such as the kinetic turbulent energy in turbulent flows, the electric potential in a conducting fluid, and some others.
Let Ω be a bounded domain of $\mathbb{R}^d$ ($d = 2$ or 3). We consider the following stationary convection-diffusion problem:

$$(P)\begin{cases} a\cdot\nabla u-\mu\Delta u=f, & in\ \Omega\\ u=0, & on\ \partial\Omega\end{cases}$$

where $a \in L^\infty(\Omega)$ with $\nabla\cdot a = 0$, $\mu > 0$ and $f \in L^1(\Omega)$.
This problem has a unique solution u by transposition. Moreover this unique solution belongs to $W_0^{1,q}(\Omega)$ for every q with $1 \le q < N'$.
In [1], we analyze the numerical solution of the Laplace equation with data in L^1 by $\mathbb{P}_1$ finite element schemes. The key ingredient is that the matrix of the system is an M-matrix. With this sole assumption we prove that u_h tends to u in $W_0^{1,q}(\Omega)$, for $q < N'$.
In this work, we study the numerical solution of problem (P) by $\mathbb{P}_1$ finite element schemes, where we have used non linear Fluctuation Splitting (FS) methods, in particular Positive Streamwise Implicit (PSI), to discretize the convection term and centered schemes for diffusion term. These FS schemes ensure a positive discretization of the convection operator. To increase the accuracy of the discretization, we use non-linear FS schemes. Our discretization again allows to obtain an M-matrix as matrix of the system. This property allows us to obtain a priori estimates sufficient to deduce that u_h is bounded in $W_0^{1,q}(\Omega)$. In this case, the convergence analysis is more envolved than in [1], due to the fact that the discrete problem is non linear.

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CT25
Anisotropic space–time adaption for advection-diffusion problems

We deal with the approximation of a time-dependent advection-diffusion problem. The cGdG method based on space-time finite elements, piecewise constant in time and continuous affine in space, is employed [3]. In particular, we are interested in the advection-dominated case: it is a challenging setting, due to the possible presence of steep internal and boundary layers, which can also move in time. With a view to an effective procedure providing us with an accurate and computationally fair solution, we resort to both space and time adaptivity. Two are the key points: the derivation of an a posteriori error estimator where the contributions of the spatial and temporal discretization are split, and a suitable balance of these two contributions via a proper adaptive procedure. This is accomplished by extending to the time dependent case the anisotropic interpolation error estimates in [4,5] and by generalizing the a posteriori error estimator of [6] to the advection-diffusion regime. Concerning the scientific panorama, the approximation of model parabolic equations in the case of optimization problems is studied in the recent preprint [8]. However, while in this last case the interest is for a goal-oriented analysis, we aim at controlling a suitable energy norm of the discretization error as in [1,2]. A model parabolic problem in the framework of anisotropic grids has been only considered in [7], as far as we know. However, a sound time adaption is not addressed, in favor of a heuristic approach, and the backward Euler scheme is adopted. In this communication we address the theoretical framework, and the resulting adaptive algorithm for the simultaneous management of the time step and of the anisotropic spatial grid is validated on some numerical test cases.

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CT25
Analysis of an Euler implicit-mixed finite element scheme for reactive transport in porous media

The need of accurate and efficient numerical schemes to solve reaction-convection-diffusion equations modelling transport in porous media is well recognized. Inappropriate numerical methods can lead to a totally false prediction of the evolution of a contaminated site, with unforeseeable consequences (see [1]). Here, I present and analyse an Euler implicit-mixed finite element scheme (EI-MFE), based on the lowest order Raviart-Thomas elements for the equation

$$\partial_t(\Theta c) - \nabla \cdot (D(\Theta, \mathbf{Q})\nabla c - \mathbf{Q}c) = \Theta R(c), \tag{26}$$

with c denoting the concentration, D the diffusion-dispersion coefficient and R a reaction term. The water content, Θ, and the water flux, $\mathbf{Q}$, are obtained by solving the Richards' equations, which modells water flow through soil including the unsaturated regions near the surface. The Richards' equation is a degenerate elliptic-parabolic equation, and it is a challenge by itself to numerically solve it. This is done here by an EI-MFE scheme, based again on the Raviart-Thomas lowest order elements. The error analysis for this scheme has been already presented in [2], for the case of a Lipschitz continuous saturation, and extended in [3] for the case of only Hölder continuity. The error arising in solving the water flow evidently influenced the quality of the finite element approximation of the solution of (26). Similar techniques with the ones used in [2, 3] will be now employed to analyse the EI-MFE scheme for the transport equation. The main result presented here will give an explicit order of convergence of this fully discrete numerical scheme for (26) in a very general framework. Especially the low regularity of the solution of the Richards' equation has been taken in account. At the end, illustrative numerical studies will be shown.

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CT25
A comparative study of mixed finite element and multipoint flux approximations of flows in porous media

Reliable and efficient simulations of subsurface flows and contaminant transport phenomena are desirable in hydrological and environmental investigations, in civil and environmental engineering and for industrial oil exploration studies. The ability to model and simulate complex flows and reactive transport processes in composite soil formations is important from the point of view of physical realism. *Mixed finite element methods* (cf. [2, 3]) and finite volume based *multipoint flux approximations* (cf. [1]) have become popular in recent years for discretizing flow problems in porous media due to their inherent mass conservation properties and the fact that they provide flux approximations as part of the formulation. These fluxes are usually of greater importance than the pressure head itself since they gover accompanying transport processes and are responsible for the availability of chemical species.

In this contribution the application of first-order accurate Raviart-Thomas and second-order accurate Brezzi-Douglas-Marini mixed finite element methods to a sequence of problems, from *single phase*

Darcy flow to *variably saturated flow* decribed by the *nonlinear parabolic-elliptic degenerate Richards equation* with solutions of weak regularity, is studied carefully. The numerical performance properties of the either discretizations are analysed and theoretical error estimates are presented. Moreover, the impact of the higher order Brezzi-Douglas-Marini flux approximation on accompanying multicomponent reactive transport phenomena is investigated. This is also done for real world field scale case studies.
Finally, the mixed finite element techniques are compared to multipoint flux approximations. Appreciable advantage of the multipoint flux approach is its lower algorithmic complexity. This might be the key reason for its widespread application in flow simulators in particular of oil industrial companies. Again, the comparison is done for a sequence of flow problems. Steady and unsteady flow problems in homogeneous and heterogeneous soils with solutions of different regularities are studied. Moreover, a new theoretically result regarding the equivalence of the Raviart-Thomas and the multipoint flux approach for single phase Darcy flows is presented.

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CT26
How to upgrade flow solvers to involutive and avoid LBB condition?

We propose to use the involutive form of the system of PDEs in numerical computations. We illustrate our approach by applying it to Stokes and Navier-Stokes systems. As for the solution of differential algebraic equations the approach requires solution of extra equations for derivative consequences. The extra calculation cost is negligible while the discrete form becomes much simpler to handle. For instance, one consequence is that discretization need not verify the classical LBB stability condition.
The approach is very general and can be useful for a wide variety of systems not as well known as fluid flow equations.
We also show that we can improve the performance of existing solvers providing 'involutive' upgrades.
The ingredients are illustrated on several academic flow calculations in two and three dimension. In particular, we show the impact of the involutive formulation to capture a special solution with singularity in cylinder geometry. We show that the approach improves the calculated solution with a Navier-Stokes solver using Chorin projection and level set to account for complex boundaries.

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CT26
Calibration of discretization and model parameters for turbulent channel flow

We consider the calculation of the turbulent incompressible flow in a plane channel at $Re_\tau = 395$. The problem is discretized using the BDF(2)-scheme in time and a collocated unstructured finite volume scheme in space using the interpolation by Rhie and Chow [1]. In a first basic step, we calibrate different discretization parameters and model parameters of the standard Smagorinsky LES model using the DNS data basis of [2]. The best results for first and second order statistics of the flow are obtained with a central discretization of the convective term together with appropriate values of the Smagorinsky constant C_S and with the definition of the filter width Δ following [3]. In a second step, we address a non-zonal hybrid method for combining the calibrated LES-model with an advanced RANS-model as a near-wall model [4]. First results of the approach are presented.

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CT26
The third order WLSQR scheme on unstructured

meshes with curvilinear boundaries

The work deals with the development of the high order finite volume method for Euler and Navier–Stokes equations. The accuracy of the scheme is improved by a piecewise quadratic interpolation of cell averaged data. The interpolation procedure [1] is based on the weighted least square approach and gives a scheme similar to the weighted ENO scheme [3]. Thanks to single stencil reconstruction with smooth non-linear weights, the resulting scheme posses extremely good convergence to steady state.
The article presents simplified analysis of the interpolation step as well as several numerical experiments concerning both the stability and the order of accuracy of the scheme.
The importance of good approximation of the boundary will be emphasized. The simple interpolation procedure based on the ideas of ENO reconstruction is described. This procedure allows us to easily handle piecewise smooth boundaries with corners.
The efficiency of the third order scheme will be presented using several numerical examples ranging from the simple scalar initial value problems to the compressible turbulent flows in complex geometries.

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CT26
Finite Volume Methods in Numerical Modelling of Electrochemical Flow cells

Electrochemical devices like fuel cells and thin layer flow cells are a rich source of mathematical problems to be solved analytically and numerically.
Besides giving an overview on these devices, we discuss in more detail ongoing work in modeling and simulation of differential electrochemical mass spectroscopy in thin layer flow cells. This is a method to gain more information about electrocatalytic reaction processes. In order to obtain detailed information about this process, one needs to go beyond the assumption of ideal mixing in the flowing electrolyte. In the talk, a rather general model of this process based on the Nernst-Planck-Poisson System coupled to Navier-Stokes and Darcy flow, and detailed reaction kinetics based on Langmuir and Frumkin models for adsorption is proposed.
Setting up a finite volume based numercial model for this process starts with assuming transport of a dissolved species in Hagen Poiseuille flow. It is verified that in the cases of an infinite strip electrode (2D calculation in a cell cross section) and of a circular electrode (3D calculation), the known Leveque type asymptotics for the limiting current are reproduced by the method. The ability to do so is strongly intertwined with meshing issues.
We discuss the extension of this model to more general cases and the way to handle it based on finite volume methods.

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CT27
A predictor-corrector approach to flux limiting for finite element discretizations of transient convection problems

A new approach to algebraic flux correction for finite element discretizations of convection-dominated transport problems is proposed. The positivity constraint is enforced in a nonlinear way by means of an artificial diffusion operator which is constructed edge-by-edge [1]. The resulting perturbation of the algebraic system to be solved is decomposed into skew-symmetric internodal fluxes which consist of a stationary part and 'mass antidiffusion'. The former is limited using a multidimensional flux limiter of TVD type [1,2] in the framework of an iterative defect correction scheme. Upon convergence, the rejected antidiffusion and the contribution of the consistent mass matrix are included using an explicit FCT algorithm [3] as applied to the converged end-of-step solution. This predictor-corrector strategy combines the advantages of FCT and TVD schemes in a very simple and efficient way. Moreover, it is readily applicable to nonlinear problems, unlike the general-purpose flux limiter introduced in [2].
A conservative flux decomposition of the convective term [1,4] is employed to construct an unconditionally positivity-preserving high-resolution scheme on the basis of the second-order accurate Crank-Nicolson time-stepping. In order to circumvent the CFL-like condition, the fully implicit backward Euler method is used to compute the provisional TVD solution at the predictor step. The difference between the explicit and implicit part of the convective flux is recovered in the course of FCT correction. As a result, the numerical solution remains nonoscillatory for arbitrary time steps and (almost) second-order accuracy can be achieved in a safe way. The performance of the new algorithm is illustrated by application to scalar transport problems as well as to the compressible Euler equations.

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CT27
Numerical solution of 2D and 3D unsteady viscous flows

The work deals with numerical solution of unsteady incompressible viscous flow described by the system of Navier-Stokes equations. The system is solved by implicit artificial compressibility methods using two modifications. The first one uses large artificial compressibility parameter and the iterative solution approximates unsteady evolution of flow. The second approach introduces dual time (artificial time) into the system of equations, where first time serves as iterative time only and the second one is physical time. Later approach is found more robust and reliable.
The discretization in space uses finite volume cell-centered method with third order AUSM type upwind approximation for convective terms. The viscous terms are computed by second order central approximation on dual finite volume grid. The structured grids consist of quadrilateral or hexahedral finite volumes in 2D and 3D respectively. Multi-block arrangement is used.
The computational results are presented for unsteady 2D laminar flow over circular cylinder in a channel for $Re = 100$ and in uniform upstream flow for $Re \in (0, 140 >$. Unsteady 3D case of turbulent synthetic jet flow is also presented. All numerical results are compared with corresponding experimental data or with numerical results of other authors.

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CT27
The coupling of two scalar conservation laws by a Dafermos regularization.

We are interested in the coupling of two different scalar conservation laws. Such a problem arises, for example when modeling a flow in a medium with discontinuous porosity, with possible applications in numerical modeling of singular pressure drop.
This problem is known to present difficulties because of the existence of non-conservative terms and also due to its resonant behavior. In this talk, we present our global approach that consists in considering the two half-space scalar problems as a single one supplemented with an equation, leading to a 2×2 system, and then to introduce the viscous regularization proposed by C.M. Dafermos in [1]. This regularization will select some 'entropy' solutions.
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CT27
Well-balanced high-order MUSTA Schemes for non-conservative hyperbolic systems.

We introduce a Multi-Stage (MUSTA) approach for constructing upwind numerical schemes for nonconservative hyperbolic systems:

$$\frac{\partial W}{\partial t} + \mathcal{A}(W)\frac{\partial W}{\partial x} = 0, \quad x \in \mathbb{R},\ t > 0. \tag{27}$$

MUSTA schemes for hyperbolic conservation laws were introduced in [1] as an approximate Riemann solver based on a GFORCE scheme and a predictor-corrector procedure. They have simplicity an generality as its main features. Here we use the concept of path-conservative numerical schemes introduced in [2], which extends the concept of conservative schemes for systems of conservation laws, to generalize GFORCE schemes to the nonconservative case and then MUSTA schemes, treating the predictor-corrector procedure as a reconstruction operator.
In particular, we obtain well balanced MUSTA schemes for solving coupled systems of conservation laws with source terms:

$$\frac{\partial W}{\partial t} + \frac{\partial F}{\partial x}(W, \sigma) = -B(W, \sigma)\frac{dW}{dx} + \tilde{S}(W, \sigma)\frac{d\sigma}{dx}. \tag{28}$$

How to get a high-order scheme based on a suitable first order numerical scheme and a reconstruction operator can be found in [2]. In particular, resulting schemes will be shown for GFORCE and MUSTA as base first order numerical schemes.
Numerical implementations for the Shallow-Water equations with depth variations are reported in the case of one and two layer flows. The results are compared with those obtained with a generalized Roe method in [3] and some other well balanced methods .

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CT28
New results on overlapping Schwarz methods.

New results have recently been obtained concerning the classical two-level additive Schwarz preconditioners. In the theory for domain decomposition methods, we have often assumed that each subdomain is the union of a small set of coarse triangles or tetrahedra. In this study, we present extensions of the existing theory to accommodates subdomains with much less regular shape.
One important goal is to extend our analytic tools to problems on subdomains that might not even be Lipschitz and to characterize the rates of convergence of our methods in terms of a few, easy to understand, geometrical parameters of the subregions. We believe that this goal now has been reached fully for scalar elliptic and linear elasticity problems in two dimensions.
We have also designed a new family of overlapping Schwarz methods, which in a certain sense is a hybrid algorithm since we borrow and extend coarse spaces from iterative substructuring methods. Methods based on such choices are known to be very robust even in the presence of large local changes of the materials being modeled by the finite element models. An extra attraction is that the overlapping Schwarz methods can be applied directly to problems where the stiffness matrix is available only in its fully assembled form. Important progress has also been made on almost incompressible elasticity and mixed finite element models. One of our results is the first of its kind for this family of saddle point problems and overlapping Schwarz methods.

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CT28
Overlapping Additive Schwarz preconditioners for degenerated elliptic problems

In this paper, we consider some degenerated boundary value problems on the unit square. These problems are discretized by piecewise linear finite elements on a triangular mesh of isosceles right-angled triangles. The system of linear algebraic equations is solved by a preconditioned gradient method using a domain decomposition preconditioner with overlap. We prove that the condition number of the preconditioned system is bounded by a constant which independent of the discretization parameter. Moreover, the preoconditioning operation requires $\mathcal{O}(N)$ operations, where N is the number of unknowns. Several numerical experiments show the preformance of the proposed method. This a joint work with S. Nepomnyschikh (Novosibirsk).

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CT28
Solution of 2D semicoercive contact problems by BETI method.

In this work we are concerned with a semicoercive 2D model problem which we solve by the Boundary Element Tearing and Interconnecting (BETI) method. After decomposing the domain into non–overlapping subdomains, we employ the symmetric representation of the local Steklov–Poincaré operator to obtain the related boundary variational inequality. This boundary weak formulation is further rewritten as a problem to find a minimizer of the corresponding energy functional. Moreover, since the Steklov–Poincaré operator is defined only implicitly, we have to use its suitable approximation. Using the Ritz method we get the quadratic programming problem with both equality and inequality constraints. Finally, we switch to the dual problem and employ the preconditioning by the projector to the “natural coarse grid”. To solve the resulting problem numerically, we use the recently proposed optimal algorithms for the solution of bound and equality constrained quadratic programming problems. These are based on the semimonotonic augmented Lagrangians and gradient projections. We also present the numerical experiments that indicates the numerical scalability of the algorithm.

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CT28
Optimal Total FETI algorithm for contact problems in elasticity

We shall first briefly review the FETI based domain decomposition methodology adapted to the solution of frictionless multibody contact problems in linear elasticity. We use modification that we call TFETI (Total FETI) [1] which enforces Dirichlet boundary conditions by Lagrange multipliers. The main advantage of the Total FETI algorithm is that each subdomain has the same, a priori known rigid body modes contrary to standard FETI method which requires effective identification of these free rigid body modes. As a result, we shall obtain a convex quadratic programming problem with a simple bounds and linear equality constraints. The classical results concerning the solution of linear elliptic boundary value problems give that the condition number of the Hessian of the quadratic form is bounded independently on the discretization parameter.
In the second part we shall present our algorithms for the solution of resulting quadratic programming problems. The unique feature of these algorithms is their capability to solve the class of quadratic programming problems with spectrum in a given positive interval in O(1) iterations. The algorithms enjoy the rate of convergence that is independent of conditioning of constraints and the results are valid even for linearly dependent equality constraints.
Finally we put together our results on approximation of variational inequalities and those on quadratic programming to develop algorithms for the solution of both coercive and semi-coercive variational inequalities and show that the algorithms are scalable [2]. We give results of numerical experiments to demonstrate numerical scalability of the algorithms presented that was predicted by the theory.

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CT29
The application of complex boundary elements method to free boundary seepage problems

We use the complex boundary elements method in order to study the infiltration of the water from a channel into the porous ground. The complex potential for the velocity of the infiltrating water is $f(z) = \varphi(x,y) + i\psi(x,y)$. One has to study the following free boundary value problem:

$$\Delta\varphi(x,y) = 0,\ \Delta\psi(x,y) = 0,$$

and the boundary conditions $\varphi = 0$ on the contour of the channel, $\psi = const.$, $\varphi + ky = 0$ on the free lines separating the wet portion of the soil from the dry one. Discretizing the Cauchy formula and taking into account the boundary conditions we describe an iterative procedure which allows to calculate the shape of the free lines, the rate of seepage and the functions $\varphi(x,y)$ and $\psi(x,y)$ on the boundary. In the case of the channel having the shape of an arc of cycloid the numerical results are compared with known analytical results [1].

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CT29
PDAS-method for a hemivariational inequality

The main topic is focused on non-smooth optimization methods. As the reference physical model we consider a membrane (thin film) being in contact with a rigid obstacle such that the cohesion force between the membrane and the obstacle is meaningful.
From an optimization point of view, the cohesion model is described by minimization of a cost functional (of the potential energy) subject to contact conditions, which is non-convex and non-differentiable. Thus, the principal difficulty of its investigation is connected with the absence of necessary and sufficient optimality conditions for finding a (non-unique) solution. The constrained minimization problem is represented by a hemivariational inequality being under the consideration, see [1] for the account of hemivariational inequalities. To manage the problem, we rely on a primal-dual formulation, which treats the displacement, contact and cohesion forces as independent variables.
We construct a *primal-dual active set* (PDAS) method to find a solution of the problem, and we analyze its global convergence properties in continuous and finite-dimensional spaces. The common advantage of PDAS-methods lies in the fact that they are associated to generalized Newton methods, see [2–5]. The non-smooth variational analysis of non-convex problems and their perturbation are presented in the related works [6,7].

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CT29
Advances in nonlocal electrostatics

Proteins are responsible for nearly all chemical reactions in the human body. They can also be important weapons to fight diseases. To find a fitting reactant to an ailment, hundreds of thousands of possible partners are tested in laboratory.
The number of tests could be significantly reduced, if it was possible to calculate the electric field of the virus and of all possible reactants efficiently, as they cannot react with one another if their fields do not fit. The environment where they come together is structured like water. To describe the electrostatic field of a molecule in water, we have to deal with nonlocal electrostatics because of the hydrogen bond network. In contrast to local electrostatics, the nonlocal approach proves quite challenging, since the relation between the electric field and the displacement field is much more complicated than in the local case. The genuine formulation (see for instance [1]) involves a differential equation for the potential inside the molecule and a integro-differential equation on the outside.
There has been an approach to slightly simplify the model and use some softer interface conditions, see [2]. It seems to work well, but the resulting system of equations is not equivalent to the original one anymore.
We will present a system of four partial differential equations in each domain, which is equivalent to the original model. For the spherical symmetric special case of an ion with charge located at the origin, an analytical solution will be given. The presented problem is an interface problem. The structure of the surface and the size of an biomolecule seem to exclude numerical calculations using finite element methods and therefore we want to use boundary element methods. Thus we will also present a fundamental solution for the operators involved in the PDE-formulation, show their ellipticity, and give a boundary integral formulation of the problem.

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CT29
Mixed fem-bem coupling for non-linear transmission problems with Signorini contact

Here we generalize the approach in [4] and discuss an interface problem consisting of a non-linear partial differential equation in $\Omega \subset \mathbb{R}^n$ (bounded, Lipschitz, $n \geq 2$) and the Laplace equation in the unbounded exterior domain $\Omega_c := \mathbb{R}^n \setminus \bar{\Omega}$ fulfilling some radiation condition, which are coupled by transmission conditions and Signorini conditions imposed on the interface. The interior pde is discretized by a mixed formulation, whereas the exterior part of the interface problem is rewritten using a Neumann to Dirichlet mapping (NtD) given in terms of boundary integral operators.
We treat the general numerical approximation of the resulting variational inequality and discuss the non-trivial discretization of the NtD mapping. Assuming some abstract approximation properties and a discrete inf-sup condition we prove existence and uniqueness and show an a-priori estimate, which generalizes the results in [4]. Choosing Raviart-Thomas elements and piecewise constants in Ω and hat functions on $\partial\Omega$ the discrete inf-sup condition is satisfied [1]. We present a solver based on a modified Uzawa algorithm, reducing the solution procedure of the non-linear saddle point problem with an inequality constraint to the repeated solution of a standard non-linear saddle point problem and the solution of a variational inequality based on an elliptic operator. Finally, we present a residual based a-posteriori error estimator compatible with the Signorini condition and a corresponding adaptive scheme, see [5].
Some numerical experiments are shown which illustrate the convergence behavior of the uniform h-version with triangles and rectangles and the adaptive scheme as well as the bounded iteration numbers of the modified Uzawa algorithm, underlining the theoretical results.

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CT30
A 'TVD-like' Scheme for Conservation Laws with source terms.

An important interest area of research in Computational Fluids Dynamics applications, is the numerical approximation of solutions of conservation laws with source terms. An interesting example are the shallow water equations, where the bottom topography of the waterbed leads to source terms of geometric nature that often need specialized numerical treatment.
The theoretical foundations of high-resolution TVD schemes for homogeneous scalar conservation laws and linear systems of conservation laws have been firmly established through the work of Harten [2], Sweby [4], and Roe [3]. These TVD schemes seek to prevent an increase in the total variation of the numerical solution, and are successfully implemented in the form of flux-limiters or slope limiters for scalar conservation laws and systems. However, their application to conservation laws with source terms is still not fully developed.
In this talk we analyze the properties of a second order, flux-limited version of the Lax-Wendroff scheme which preserves the TVD property, in the sense that it avoids oscillations around discontinuities, while preserving steady states [1]. Our technique is based on a flux limiting procedure applied only to those terms related to the physical flow derivative/Jacobian.

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CT30
On path-conservative numerical schemes for hyperbolic systems of conservation laws with source terms.

This work is concerned with the numerical approximation of Cauchy problems for one-dimensional hyperbolic systems of conservation laws with source terms or balance laws. These systems can be studied as a particular case of nonconservative hyperbolic systems (see [2,3,4]).
The theory developed by Dal Maso, LeFloch and Murat [1] is used in order to define the weak solutions of nonconservative systems: an interpretation of the nonconservative products as Borel measures is given, based on the choice of a family of paths drawn in the phase space. Even if the family of paths can be chosen arbitrarily, it is natural to require this family to satisfy some hypotheses concerning the relation of the paths with the integral curves of the characteristic fields [5]. The notion of path-conservative numerical scheme introduced in [6], which is a generalization of that of conservative scheme for systems of conservation laws, is also related to the choice of a family of paths.
In this work we present an appropriate choice of paths in order to define the concept of weak solution of the particular case of balance laws, together with the notion of path-conservative numerical scheme for this particular case and some properties. The well-balance property of these schemes is also considered. The final goal is to prove for the particular case of balance laws a Lax-Wendroff type convergence result: if the approximations provided by a path-conservative scheme converge to some function as the mesh is refined, then this function is a weak solution of the balance law if both the definitions of path-conservative scheme and weak solution make reference to the same family of paths.

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CT30
A WAF type method for non-homogeneous Shallow Water Equations with pollutant

In this work we study the extension of a WAF type method (*Weighted Average Flux*, see [1,4,5]) to Shallow Water Equations with topography and pollutant.
By considering a Riemann problem, the numerical flux of WAF method is defined by the space average over the control volume of the flux function at time $t = \Delta t/2$; where by Δt we denote the time step. The flux function at intermediate waves is approximated using HLLC flux.
Following the idea introduced in [2] and [3], firstly we focus on describing the numerical viscosity introduced by WAF method. Using this information we propose an extension of WAF method to the non-homogeneous case. We prove that the proposed scheme is asymptotically well-balanced in the sense defined in [2].
Finally, some numerical tests are presented, comparing with analytical solutions and HLLC solver.

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CT30
High order two dimensional schemes for coupled shallow water-transport systems.

This work is concerned with the development of *high order* two-dimensional numerical schemes (see [1]) using the *finite volume* method, for modeling the *transport* of a substance in a fluid, like for example, a pollutant disposal.
The mathematical model consists of the coupling of a one layer shallow water system and a transport equation:

$$\frac{\partial hC}{\partial t} + \frac{\partial q_x C}{\partial x} + \frac{\partial q_y C}{\partial y} = SC_s, \tag{29}$$

being h the thickness of the fluid layer, q_x, q_y the flux for each main direction, $S(\mathbf{x}, t)$ the pollutant sources (measured in m^2/sec), $C(\mathbf{x}, t)$ the averaged concentration of the pollutant, and C_s the concentration of the pollutant at the sources.
This coupling gives rise to a new linearly degenerate field in the system. If initially the substance occupies only a region of the fluid, the boundaries of this region move following a contact discontinuity (see [6]). Thus, to approximate sharply the evolution of a pollutant it is necessary to develop numerical methods that are able to capture precisely the contact discontinuities associated to these kind of systems (see [4]).
We compare the results obtained using different high order schemes: a bi-hyperbolic reconstruction scheme (see [5]), a reconstruction of states scheme based in [3], and an artificial compression technique (see [2]), all of them for structured and unstructured meshes. Finally, numerical experiments to validate the correct behavior of the different schemes are presented.

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CT31
A domain decomposition method for second order nonlinear equations.

In this communication we give a result of existence and present a numerical analysis of weak solutions for the following quasi-linear elliptic problem in one and two dimensions:

$$\begin{cases} -Au(x) + G(x, Du(x)) = F(x, u(x)) + f(x) \ \text{ in } \Omega \,, \\ u(x) = 0 \ \text{ on } \partial\Omega \end{cases} \tag{30}$$

where A is a second order derivatives operator in one dimension and the Laplace operator in two dimensions, G, F are Caratheodory non negative functions. The function f is given finite and non negative. The domain $\Omega \subset \mathbb{R}^N$, $N = 1, 2$ is open and bounded.
Such problems arise from biological, chemical and physical systems and various methods have been proposed to study the existence, uniqueness, qualitative properties and numerical simulation of solutions.
In the one dimensional case we consider a situation where f is irregular , more precisely a non negative measure in $(0, 1)$ and where the growth of G with respect to $Du = u'$ and F with respect to u are arbitrary.
In the two dimensional case we assume $f \in L^1(\Omega)$, the convexity of $s \to G(x, s)$ and that $G(x, s)$ is sub-quadratic w.r.t. s.
The general algorithm for the numerical solution of these equations is one application of the Newton method to the discretized version of problem (30), but at each iteration the resulting system can be indefinite. To overcame this difficulty we introduce a domain decomposition method. Then in the first step of the algorithm we compute a super solution using a domain decomposition method. In the second step we compute a sequence of solutions of an intermediate problem obtained by using the Yosida approximation of G. This sequence converges to the weak solution of the problem (30). We present numerical examples.

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CT31
Space-time higher order discretizations of non-stationary nonlinear convection-diffusion problems

We deal with a numerical solution of a scalar non-stationary nonlinear convection-diffusion equation, which exhibits a model problem for the solution of the system of the compressible Navier-Stokes equations. The space semi-discretization is carried out with the aid of the discontinuous Galerkin finite element method (DGFEM), which is based on a piecewise polynomial discontinuous approximation, for survey, see [1], [2].
It is possible to use a discontinuous approximation also for the time discretization [3] but the most usual approach is the application of the method of lines. In this case, the resulting system of the ordinary differential equations (ODEs) is often discretized by the explicit Runge-Kutta methods since these schemes have a high order of accuracy and they are simple for implementation. Their drawback is a strong restriction to the length of the time step. In order to avoid this disadvantage it is suitable to use an implicit time discretization but a full implicit scheme leads to a necessity to solve a nonlinear system of algebraic equations at each time step which is rather expensive.
Therefore, we develop a higher order unconditionally stable (or a scheme with a large domain of stability) time discretization technique which do not require a solution of nonlinear algebraic problem at each time step. We present two approaches.

i) a use of backward difference formulae (BDF) for linear terms and a higher order explicit extrapolation for nonlinear ones,

ii) a combination of implicit and explicit Runge-Kutta schemes for linear and nonlinear terms, respectively.

We analyse these approaches and derive a priori error estimates in the discrete analogous of the $L^\infty(0,T;L^2(\Omega))$-norm and the $L^2(0,T;H^1(\Omega))$-seminorm.

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CT31
Numerical Simulation of Barium Sulphate Precipitation

The precipitation of barium sulphate is modeled by a population balance system describing
- an incompressible flow field (Navier–Stokes equations),
- an isothermal chemical reaction (nonlinear convection–diffusion–reaction equation),
- a population balance equation for the particle size distribution (linear transport equation).

The solution of each individual equation possesses its difficulties:
- in applications, the flow is often turbulent,
- it is important that one obtains oscillation–free solutions for the concentrations in the chemical reaction,
- the particle size distribution depends not only on time and space but also on one or even more properties of the particles (interior coordinates); that means, one has to solve an equation in $\mathbb{R}^d$, $d \geq 4$ in applications.

It turns out that the simulation of population balance systems is rather challenging.
We will present first steps in the simulation of the precipitation of barium sulphate. The flow and the chemical reaction will be considered in a two–dimensional domain. The particle size distribution possesses one interior coordinate (the diameter of the particles). For the particles, nucleation and growth are modeled. Topics included into the talk are the discretization of the individual equations and numerical simulations for different physical and chemical parameters.

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CT31
Numerical Analysis of Generalized Newtonian Fluids

The numerical analysis of problems with p-structure is quite different from problems which are linear in the main elliptic term. E.g., in order to get optimal error estimates one needs to measure the error not in the usual $W^{1,p}$-norm, but in a so-called quasi-norm or some equivalent quantity. In the talk we present some recent progress which provides optimal results for different problems with p-structure, including results for generalized Newtonian Fluids.

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CT32
An analyis of a FETI-DP algorithm on irregular

subdomains in the plane.

In the theory for domain decomposition algorithms of the iterative substructuring family, each subdomain is typically assumed to be the union of a few coarse triangles or tetrahedra. This is an unrealistic assumption, in particular, if the subdomains result from the use of a mesh partitioner in which case they might not even have uniformly Lipschitz continuous boundaries. The purpose of this study is to derive bounds for the condition number of these preconditioned conjugate gradient methods which depend only on a parameter in an isoperimetric inequality and two geometric parameters characterizing John and uniform domains. A related purpose is to explore to what extent well known technical tools previously developed for quite regular subdomains can be extended to much more irregular subdomains. Some of these results are valid for any John domains, while an extension theorem, which is needed in this study, requires that the subdomains are uniform. The results, so far, are only complete for problems in two dimensions. Details are worked out for a FETI–DP algorithm and numerical results support the findings. Some of the numerical experiments illustrate that care must be taken when selecting the scaling of the preconditioners in the case of irregular subdomains.

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CT32
Pointwise constraints in space and time - on the stability and numerical robustness of pointwise constraints for stationary and dynamic problems in elasticity

The usage of pointwise constraints is very attractive due to their simplicity and locality. In the context of variational formulations, however, pointwise evaluation is often connected to dual quantities as a delta distribution, which might be uncomfortable as a test function. We show different possibilities how to interpret pointwise constraints in a weak sense and discuss the quantitative properties of the resulting discretization schemes. Furthermore, localization techniques for non–local constraints are presented. This is done in the framework of efficient multiscale solution methods for constrained minimization problems in elasticity, thereby connecting the discretization of the constraints with the development of efficient solution methods. As particular examples, we will consider dynamic contact problems, where the constraints have to be discretized in time as well as in space.
Since local constraints are much easier to handle form the algorithmic point of view, we finally discuss localization techniques for coupled constraints. This is done along the modeling and numerical treatment of certain biological materials as, e.g., articular cartilage.

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CT32
Multidimensional Coupling in a Human Knee Model

We present a new way to couple linear elastic three-dimensional bodies to slender objects modelled as one-dimensional nonlinear Cosserat rods. Starting from a full 3d nonlinear elastic formulation we derive suitable coupling conditions for a reduced model consisting of a 3d linear elastic body and a 1d nonlinear elastic rod. These involve the total force and torque transmitted through the interface as well as its averaged position and an average orientation. The resulting domain decomposition problem is solved using a Dirichlet-Neumann algorithm.
The configuration space of a discrete special Cosserat rod is $\mathbb{R}^{3n} \times \mathrm{SO}(3)^n$. We present an ∞-norm Riemannian trust-region algorithm for the minimization of the rod energy functional on this nonlinear space. In conjunction with a nonsmooth Newton multigrid method as the inner solver this yields an efficient method with provable global convergence.
We use this coupling approach to model a human knee joint, where the bones are modelled using 3d linear elasticity and the ligaments as 1d rods. The use of rods for the ligaments decreases the overall number of degrees of freedom and avoids meshing problems. The additional problem of modelling the contact between the bones is treated using a mortar element discretization and a nonsmooth Newton multigrid method for the solution of the resulting discrete system.

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CT32
A domain decomposition method derived from the use of Lagrange Multipliers for elliptic problems.

The primal hybrid formulation for second order elliptic problems uses Lagrange multipliers to inforce the continuity of the solutions across interfaces via the duality $H^{-1/2} - H^{1/2}$, see for instance the works of Raviart-Thomas [4], Roberts-Thomas [5]. The coupling of the different subdomains is performed through the Lagrange multipliers while the coercive form in the formulation does not relate these different subdomains. Therefore, we have observed that the application of some iteration techniques like Uzawa or Conjugate Gradient to the dual problem for the multipliers yield domain decomposition methods geometrically convergent with a mesh independent ratio. This property is shared with other well known methods like the Dirichlet-Neumann method proposed by Marini-Quarteroni [3] and the one by Lube-Müller-Otto [2].

Usually, for numerical discretizations, the duality $H^{-1/2} - H^{1/2}$ is worked out by means of some projection operator onto the L^2 space on the interfaces, see for instance work of Ben Belgacem [1]. In our approach we use Riesz representation and replace the duality with the $H^{1/2}$ scalar product that is explicitly computed. Therefore no consistency errors appear.

The computation of the $H^{1/2}$ scalar product for the discrete basis functions on the interface is performed once as long as the mesh does not change on it. Comparing this computational work with the accuracy benefit that we obtain we believe it is worthwhile for applications were the interfaces are not complicated.

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CT33
Thermo-magneto-hydrodynamic simulation of melting induction furnaces with cylindrical symmetry

This work deals with mathematical modelling and numerical simulation of induction heating furnaces for axisymmetric geometries. The induction furnace consists of a helical coil surrounding a cylindrical crucible charged with the material to be melted.

In order to perform a numerical simulation of the furnace the physical process is expressed as a coupled-nonlinear system of partial differential equations arising from thermo-magneto-hydrodynamic phenomena. The problem is formulated in a radial section of the domain by assuming cylindrical symmetry (see [3]).

The simulation of the process is quite complex, since it needs the solution of an eddy current problem, a thermal model with change of phase, and a hydrodynamic one for the molten region of the material. Moreover, all of the models are coupled because physical parameters depend on temperature, the heat source in the thermal problem is the Joule effect and the liquid domain of the hydrodynamic model depends on temperature. On the other hand, buoyancy and Lorentz forces appear in the hydrodynamic model, and the velocity of molten metal appears in the convective term of the heat equation.

The present work starts from the problem and the algorithms proposed in [1] and [2] and introduces the hydrodynamic model and the convective heat transfer in the heat equation. The electromagnetic problem is discretized using a finite element method, whereas the thermal and the hydrodynamic problems are approximated using Lagrange-Galerkin methods. To deal with the coupling between the models and the non-linearities we employ different iterative fixed point algorithms.

Finally, some numerical results obtained in the simulation of an industrial furnace used for silicon purification are shown.

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CT33
A new formulation of the eddy current problem with input current intensities as boundary data

This paper deals with a new formulation and finite element approximation of the time-harmonic eddy current model in a bounded domain with non-local boundary conditions. This problem arises when coupling the full field equations with circuits; on the common interface between the two models, the boundary data for the domain where the eddy current model is considered are either input current intensities or voltages. (See [3], [4], [5], [6].)

There are only few papers analyzing the low-frequency Maxwell system with this kind of boundary condtions. Its finite element approximation has been studied in [2] where the problem is formulated in terms of the magnetic field and the input current intensity is imposed by means of Lagrange multipliers.

We propose a new formulation and the associated finite element approximation of the eddy current problem with input current intensities as boundary data considering as main unknowns the electric field in the conductor Ω_C and the magnetic field in the insulator Ω_I. (See [1] for such an hybrid formulation.) The magnetic field in the dielectric is decomposed as the sum of the gradient of a function in $H^1(\Omega_I)$ plus an harmonic field. The harmonic field is univocally determined by the given input current intensities, hence the unknowns of the problem reduce to the electric field in the conductor and a scalar magnetic potential in the insulator. For the finite element approximation of the problem, the harmonic field is replaced by a linear combination of generalized gradients of n discrete functions, where n is the Betti number of Ω_I. Finally we briefly discuss the set of boundary conditions that are compatible with the prescription of the input current intensities.

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CT33
External finite element approximations of a 2D Maxwell eigenvalue problem with curvilineair boundary

The electromagnetic resonances occuring in cavities are modelled by a Maxwell eigenvalue problem (EVP). This EVP is given by the following set of equations for the triple $(\omega, \mathbf{E}, \mathbf{H})$:

$$\begin{array}{rcllcll}
\nabla\times\mathbf{E} &=& -i\omega\mu\mathbf{H} & & & & \text{in } \Omega\\
\nabla\cdot(\mu\mathbf{H}) &=& 0 & & & & \text{in } \Omega\\
\nabla\times\mathbf{H} &=& i\omega\epsilon\mathbf{E} & & & & \text{in } \Omega\\
\nabla\cdot(\epsilon\mathbf{E}) &=& 0 & & & & \text{in } \Omega\\
\mathbf{E}\times\mathbf{n} &=& 0 & \text{and} & (\mu\mathbf{H})\cdot\mathbf{n} &= 0 & \text{on } \Gamma_\tau\\
\mathbf{H}\times\mathbf{n} &=& 0 & \text{and} & (\epsilon\mathbf{E})\cdot\mathbf{n} &= 0 & \text{on } \Gamma_\nu
\end{array}$$

Here, ω is the unknown freqency (characterising the time harmonic behaviour) and $\mathbf{E}$ and $\mathbf{H}$ represent the electric and magnetic field vectors, respectively. ϵ and μ are material parameter functions. Moreover, Ω is the domain with boundary Γ, the latter being divided into two distinct parts Γ_ν and Γ_τ.
This EVP is recasted in a variational form to allow the use of finite element approximations. For simplicity we restrict ourselves to the 2D case, which corresponds with a thin cavity or can arise from translation symmetrical settings.
Many authors have pointed out one has to be very carefull while approximating electromagnetic eigenmodes, since spurious modes are known to slip into the approximated spectrum. To avoid those spurious modes the use of edge elements is now established. At present conditions to assure the correctness of the approximation are known, see [1].
To the author's knowlegde, however, this far all convergence results require the domains considered to be triangulated exactly, therefore in practice being restricted to polyhedrical domains. We extend the known convergence results to include curvilinear boundaries. To this end, we allow for triangulated domains Ω_h which are not completely included in the domain Ω. As in [2], we do require all vertices of $\partial\Omega_h$, to be situated on $\partial\Omega$.
In this work we present convergence results for external finite element approximations of Maxwell EVPs for h (the mesh parameter) tending to zero, thereby extending the results of [2].

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CT33
Modified boundary integral equations for electromagnetic scattering problems

For exterior electromagnetic scattering problems, the boundary integral equation method is a suitable choice for a numerical approach, because only the boundary has to be discretised, and the Silver-Müller radiation condition is incorporated. However, the unique solvability of the original problem can get lost in particular when eigenfrequencies of the scattering body appear. A first approach to overcome this problem is to use the approach of Brakhage and Werner, who introduced a combined field integral equation for the acoustic scattering problem. But this approach is considered usually in $L_2(\Gamma)$, where uniqueness results are based on Gardings inequality and Fredholms's alternative. However, the compactness of certain boundary integral operators is needed, i.e. the boundary must be assumed to be sufficiently smooth. That's why modified boundary integral equations were introduced which are formulated in the energy function spaces to ensure unique solvability also for Lipschitz polyeders.
In this talk a modified boundary integral equation will be presented that in comparison to already existing approaches neither uses a compact operator in the formulation nor uses the Hodge decomposition.

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CT34

On solving nonsymmetric saddle-point systems arising in FDM

The classical fictitious domain method (FDM) enforces boundary conditions in PDE's by Lagrange multipliers defined on the boundary γ of the original domain ω [1]. Therefore the computed solution has a singularity on γ that can result in an intrinsic error. The basic idea of our modification consists in introducing new control variables (instead of Lagrange multipliers) defined on an auxiliary boundary Γ located outside of $\overline{\omega}$ [3]. In this approach, the singularity is moved away from $\overline{\omega}$ so that the computed solution is smoother in ω and the discretization error has a significantly higher rate of convergence in ω.
The respective finite element discretization leads typically to a nonsymmetric saddle-point system

$$\begin{pmatrix} A & B_1^\top \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} \hat{u} \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \tag{31}$$

where an $(n \times n)$ diagonal block A is possibly singular and $(m \times n)$ off-diagonal blocks B_1, B_2 have full row-rank and they are highly sparse. Moreover, m is much smaller than n and the defect l of A, i.e., $l = n - rank\, A$, is much smaller than m. For solving such systems, it is convenient to use a method based on the Schur complement reduction. If A is singular, the reduced system has again a saddle-point structure. Fortunately after applying orthogonal projectors, we obtain an equation in terms of λ only that can be efficiently solved by the projected variant of the BiCGSTAB algorithm [3]. This procedure generalizes ideas used in FETI domain decomposition methods [1], in which A is symmetric, positive semidefinite and $B_1 = B_2$.

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CT34
A dual dropping approximate inverse preconditioner for solving general linear systems of equations.

In this presentation we discuss numerical techniques based on least-squares minimization for computing a sparse approximation of the inverse of a nonsingular matrix. The approximate inverse can be used as a preconditioner of explicit type for an iterative Krylov method [1] as well as a smoother for multigrid methods [2]. This class of algorithms may be especially attractive for parallel computations because the preconditioning operation reduces to form a sparse matrix-vector product. Additionally, approximate inverses are generally less prone to instabilities for solving highly nonsymmetric and/or indefinite systems compared to preconditioners of implicit type. The most critical computational issue is the selection of the nonzero pattern because in general the inverse of an irreducible matrix is structurally dense. The idea is to keep the pattern structure reasonably sparse while trying to capture the "large" entries of the inverse, which are expected to contribute the most to the quality of the preconditioner.
We present a novel adaptive strategy for selecting the nonzero pattern and for refining the approximate inverse [3]. The resulting preconditioner is constructed using a dual dropping strategy and is refined after its computation by using spectral low-rank matrix updates that may enhance its robustness on tough problems. Preliminary experiments on a set of sparse matrices arising from different application fields are shown to illustrate the effectiveness and analyse the numerical stability of the proposed algorithm.

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CT35
Dynamic Iteration for Transient Simulation of Shape Memory Alloys

Shape Memory Alloy (SMA) materials have an enormous potential in technological applications like aviation, medicine and robotics among others. This calls for simulation tools and techniques that are able to describe the relevant effects of SMA behavior. Both mathematical models and appropriate numerical simulation schemes have to be developed. In our case the model described by Helm [1] presents major challenges since it consists of a heterogeneous coupled system of partial differential and differential-algebraic equations (PDAEs) where continuum models describe the evolution of deformation and temperature. State of the art solution methods in most cases use return mapping algorithms comparable to low order implicit integration schemes with fixed stepsize. So far, the use of finite element methods to simulate shape memory behavior has mainly focused on the isothermal case. Only few papers about the thermomechanic coupling exist. By the interpretation of the multiphysical problem as PDAE the range of applicable solution methods widens. Semidiscretization in space leads to coupled subsystems, consisting of structural mechanics, heat equation and evolution equations. Their different properties each call for the use of adapted time integration schemes with step size control. Therefor these subsystems have to be decoupled, which can be realized by a dynamic iteration scheme

[2,3]. Up to now this iterative approach is mainly utilized for simulation of large scale integrated circuits under the name of 'waveform relaxation' [4]. Numerical computations show that it can be adopted successfully also for the simulation of transient material behavior for instance of shape memory alloys. Not only the assignment of adapted integration schemes but also the possible parallelization of the computation are benefits of this method. Furthermore its ability to decompose the domain into several subdomains is of interest in connection with parallel computing.

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CT35
A hybrid numerical scheme for aerosol dynamics.

Aerosol coagulation, i.e. the merging of aerosol particles to larger clusters, is commonly described by the Smoluchowski equation. Of special interest is the phenomenon of "gelation", i.e. the formation of "macroparticles". A useful tool for the numerical simulation is the application of Monte Carlo simulations [1]. However, stochastic effects may change qualitative properties, e.g. they may cause the transition from stable states to metastable ones [2,3], for example in the presence of sinks or in combination with spatial diffusion.

In [4], a deterministic scheme for the space homogeneous system has been formulated and analyzed. It has been shown, that the scheme exhibits monotone convergence with respect to some moment of the solution. This gives rise to an efficient error control, at least for certain model problems. Moreover, the scheme is capable of resolving the gelation process with high precision. It turns out that the most efficient system is a hybrid code with a stochastic component for the simulation of higher regions of the state space.

The talk introduces the numerical scheme, discusses its properties in comparison to stochastic schemes and presents numerical examples of the gelation process in diffusive environments.

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CT36
Application of FETI method for 2D quasistatic contact problems with Coulomb friction

The mathematical model of this problem leads to a system of implicit variational inequalities for the deformation and its velocity. After the full discretization (in time and space) we obtain a system of static contact problems with local Coulomb friction for increments at each time level. These problems are solved by the method of successive approximations combined with the dual formulation of each iterative step. To solve large scale problems a FETI type domain decomposition technique is used. Numerical results will be presented.

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CT36
A posteriori error analysis of penalty domain decomposition methods for linear elliptic problems

In this work we place ourselves in the framework of penalty domain decomposition techniques, as introduced by Lions (Cf. [2]). We use a posteriori error analysis, with the purpose of designing strategies for optimizing the combined choice of the penalty parameter and the adaptation of the grid. Otto and Lube develop in [3] a similar approach to estimate free parameters in a domain decomposition techniques.

We choose as a test problem the Dirichlet problem for the Poisson equation:

$$-\Delta u = f \quad \text{in} \quad \Omega, u = 0 \quad \text{on} \quad \partial\Omega. \qquad (32)$$

Here, Ω is a bounded open set of $\mathbb{R}^d$, $d \geq 1$. Given a simple decomposition of Ω into two non-overlapping subdomains Ω_1 and Ω_2, set $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$. We consider the penalised approximation

$$\begin{cases} -\Delta u_1 & = & f & \text{in} & \Omega_1, \\ u_1 & = & 0 & \text{on} & \Gamma_1, \\ \partial_{\mathbf{n}_{12}} u_1 & = & \frac{1}{\varepsilon} b(u_1 - u_2) & \text{on} & \Gamma, \end{cases}$$

$$\begin{cases} -\Delta u_2 & = & f & \text{in} & \Omega_2, \\ u_2 & = & 0 & \text{on} & \Gamma_2, \\ \partial_{\mathbf{n}_{21}} u_2 & = & \frac{1}{\varepsilon} b(u_2 - u_1) & \text{on} & \Gamma, \end{cases}$$

where b is an injective linear bounded boundary operator on Γ. b reduces to the identity for $L^2(\Gamma)$ penalty (Cf. [1]). Also, we introduce in this work $H^{1/2}_{00}(\Gamma)$ penalty. In this case, b is a distributed operator on Γ.

Our a posteriori error analysis yields independent error indicators for both penalty and discretization errors that allows to develop strategies to provide relevant error reductions: We determine an optimal value for the penalty parameter for a fixed grid that yields a penalty error of the same size as the discretization error, with an minimal computational effort. Also, we determine both optimal values for the penalty parameter and optimal grids that allow to reduce the error below a targeted value, also with a minimal computational effort. We finally discuss the computational benefits of using $H_{00}^{1/2}(\Gamma)$ penalty versus $L^2(\Gamma)$ penalty, and present some numerical results that exhibit the good performances of our adaptive strategies.

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CT36
BETI-DP methods for potential equations in unbounded domains

Boundary element tearing and interconnecting (BETI) and dual-primal BETI (BETI-DP) methods, introduced by Langer and Steinbach [3] as the boundary element counterpart to the well-known finite element tearing and interconnecting (FETI) and FETI-DP methods, see, e. g., [1, 2], are robust domain decomposition (DD) solvers for partial differential equations. These methods have proved to be parallely scalable and the condition number of the corresponding preconditioned system is rigorously bounded by $C(1+\log(H/h))^2$ where the constant C is independent of the subdomain diameter H, the mesh size h, and moreover of the coefficient which is here assumed to be piecewise constant on the subdomains, see, e. g., [5].
In this talk, we give the analysis for BETI and BETI-DP methods where one of the subdomains is unbounded, i. e. one of the subproblems is an exterior problem with a radiation condition. Under appropriate assumptions the condition number can be bounded by $C(1 + \log(H_F/h))^2$ where H_F denotes the maximal diameter of the interfaces between adjacent subdomains. In particular C can be shown to be robust with respect to the diameter of the complement of the unbounded domain. We sketch the idea of the proof and give some numerical results.

This work was supported by the Austrian Science Foundation (FWF) under grant SFB F013.

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CT37
Newton-like solver for elastoplastic problems with hardening and its local super-linear convergence.

We discuss a solution algorithm for quasi-static elastoplastic problems with linear hardening. After discretization in time, such problems can be described by the minimization of a functional, which depends on the plastic strain non smoothly, and on the displacement and a hardening parameter smoothly. For the most relevant models of hardening, the minimizers for the plastic strain and the hardening parameter can be calculated explicitely. By substitution, one obtains a minimization functional which depends on the displacement only.
A theorem of J. J. Moreau from convex analysis states, that this functional is differentiable and the derivative can be computed explicitely. This is a non trivial result, since the original functional depends non smoothly on the plastic strain, and the plastic strain minimizer depends non smoothly on the displacement.
However, the second derivative of the energy functional does not exist. As a remedy, we utilize a concept of slanting functions, which was recently developed by X. Chen, Z. Nashed and L. Qi. A Newton-like method, exploiting slanting functions of the energy functional's first derivative, is proposed. The local super-linear convergence of this method is shown in the FE-discrete case, and sufficient regularity assumptions are formulated, which imply the local super-linear convergence also in the spatially continuous case.

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CT38
DAE-Index of Real Gas Flow Equations

The modeling of flow problems is based on conservation principles. In fluid dynamics the three fundamental principles are the conservation of mass, momentum and energy. For a one-dimensional inviscid flow we obtain the 1D-Euler gas equations

$$\begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (\rho E + p) u \end{pmatrix}_x = 0 \qquad (33)$$

which form a system of partial differential equations of first order for the four unknown states ρ,u,p and E. The closure conditions - relations between pressure, density and internal energy- complete the system. The conservation principles are also valid in the case of chemically reacting gas flow. It is the closure equations, i.e. pressure and internal energy laws, and the initial resp. boundary conditions that are different from one application to the other. Although in many cases (like high pressure or low temperature) not appropriate, the ideal gas law $pV = n\mathcal{R}T$ is very often preferred to the real gas law due to its simplicity.
In our investigation, we restrict to the one-dimensional case with real gas closure equations and different sets of boundary conditions and study the influence, the analytical properties and the numerical consequences due to the DAE-index of such choices.

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CT38
A road traffic model with overtaking: Oscillatory patterns.

We investigate microscopic models of the road traffic, see [1]. In particular, we consider *car-following* models for a single-line traffic flow on a circular road. The model is characterized by a choice of a particular *optimal velocity function* (OV) which is related to each individual driver. In [2], it was shown that periodic solutions (cycles) of the model are due to the Hopf bifurcation. Nevertheless, one can check that many cycles become *non physical* for large parameter regions.
The analysis shows that a trajectory becomes non physical since an event which can be interpreted as a collision with the preceding car. The natural action of a driver at that moment would be to overtake the slower car. In [3], we proposed a model of an overtaking. It *implicitly* defines a maneuver consisting of deceleration/acceleration just shortly before/after the event. The maneuver is fully defined by the OV of the driver. The resulting model is no longer smooth. In [3], we also hinted at a large variety of oscillatory solutions (*oscillatory patterns*) of this new model.
In our presentation, we formulate our model as a particular *Filippov system*, see [4]. We define selected oscillatory patterns as invariant objects of this Filippov system. We use the standard software (AUTO97) to continue these patterns with respect to a parameter.

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CT39
Optimal shape design of quasi-1D Euler flows with discontinuities

Optimal shape design aims at finding the minimum of a functional (objective function) by controlling the PDE that models the flow using surface (domain boundaries) deformation techniques. As a solution to the enormous computational resources required for classical shape optimization of functionals of aerodynamic interest, one of the best strategies is to use in a systematic way methods inspired in control theory. To do this one assumes that the flow is controlled by the aerodynamic surface. The problem is then to find the surface that minimizes the given functional (typically lift or drag), which depends on the flow solution.
Minimization is often achieved by means of iterative gradient-descent methods, which require the computation of the gradients of the objective function with respect to the variables it depends on (design variables).
One of the key ingredients in the application of control theory methods relies on the usage of adjoint techniques to simplify the computation of gradients. Some of the groundbreaking works in this field are due to J.-L. Lions [3], followed by the developments of O. Pironneau [4], who was a pioneer in the application to CFD. A. Jameson [2] was the first to apply these techniques to aeronautical design problems.
In the present work we will restrict our attention to optimal shape design in systems governed by the Euler equations with discontinuities in the flow variables (shock waves). We first review some facts on the state-of-the-art of control theory applied to optimal shape design in systems governed by the Euler system [1]. We then study the adjoint formulation, providing a detailed exposition of how the derivatives of functionals may be obtained when a discontinuity appears. Conflictive terms that directly depend on the discontinuity position will be analyzed. Several technical and numerical difficulties, as imposition of internal boundary conditions or the choice of design variables, will be discussed. Different solutions and alternatives adopted in practical implementations will also be commented. Finally, recent results on this field will be shown, together with some numerical experiments.

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CT39
Sensitivity Analysis of Optimal Load Changes for a Fuel Cell PDAE Model

Molten carbonate fuel cells are well suited for stationary power production and heat supply. In order to enhance service life time, hot spots, resp. high temperature gradients inside the fuel cell have to be avoided. In conflict with that, there is the desire to achieve faster load changes while temperature gradients stay small. For the first time, optimal fast load changes have been computed numerically, including a parametric sensitivity analysis [1], based on a mathematical model of Heidebrecht [2].
Mathematically speaking, we have to compute optimal boundary control functions for an optimal control problem with a (nonlinear) integro partial differential-algebraic equation system as a constraint. Due to the continual model updates during the project time, we chose the approach "first discretize, then optimize".
The numerical procedure is based on a method of lines approach via spatial discretization and the solution of the resulting very large scale DAE optimal control problem by a nonlinear programming approach.

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CT40
Local projection stabilization for the Oseen system on anisotropic meshes

The classical local projection method as well as residual-based stabilization techniques, as for instance streamline upwind Petrov-Galerkin (SUPG), are only optimal for isotropic meshes. Here we extend the local projection stabilization (LPS) for the Navier-Stokes [2,3] system to anisotropic quadrilateral meshes. In this work [1] we describe the new method and prove an a priori error estimate. This method leads on anisotropic meshes to qualitatively better convergence behavior than other isotropic stabilization methods. By means of two numerical test problems the capability of the method is illustrated.

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CT40
A comparative study of efficient iterative solvers for generalized Stokes equations

We consider a generalized Stokes problem with parameters $\xi \geq 0$ (size of the reaction term) and $\nu > 0$ (size of the diffusion term). This problem is discretized on a tetrahedral grid with a pair of conforming finite element spaces that is *inf-sup* stable. The main topic of the work is a study of efficient iterative solvers for the resulting discrete saddle point problem. In particular the efficiency (robustness) of the solvers with respect to variation in the mesh size parameter and in the problem parameters ξ and ν is studied. We investigate a coupled multigrid method with Braess-Sarazin [1] and Vanka type [2] smoothers, a preconditioned MINRES method and an inexact Uzawa method [3]. In the latter two methods multigrid preconditioners are used for the scalar problems for each velocity component. We present a comparative study of these methods. We give an overview of the main theoretical convergence results known for these methods. We also investigate the efficiency of the different methods by means of numerical experiments. For a three dimensional problem, discretized by the Hood-Taylor $\mathcal{P}_2 - \mathcal{P}_1$ pair, we give results of numerical experiments. It turns out that all methods show good robustness properties with respect to variation in the mesh size and in the parameters ξ and ν.

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CT41
Computing nonclassical solutions of scalar conservation laws with a sharp interface and fully conservative scheme

We are interested in computing nonclassical weak solutions of an initial-value problem for a scalar conservation law of the form

$$\begin{cases} \partial_t u + \partial_x f(u) = 0, \;\; u(x,t) \in \mathbb{R}, \;\; (x,t) \in \mathbb{R} \times \mathbb{R}^{+*}, \\ u(x,0) = u_0(x), \end{cases} \tag{34}$$

supplemented with the validity of a *single* entropy inequality

$$\partial_t U(u) + \partial_x F(u) \leq 0. \tag{35}$$

In these equations, t is the time, x is the one dimensional space variable, $f : \mathbb{R} \to \mathbb{R}$ is a (smooth) flux function, while $U : \mathbb{R} \to \mathbb{R}$ and $F : \mathbb{R} \to \mathbb{R}$ are (smooth) functions such that U is convex and $F' = U'f'$. Importantly, f is taken to be *nonconvex* in this study.
When f is convex, it is well-known that entropy condition (36) is sufficient to select a unique *classical* solution of (34). When f fails to be convex, it is necessary to supplement (34)-(36) with an additional selection criterion called *kinetic relation* from [1]. More precisely, in this case the Riemann problem associated with (34)-(36) still admits a one-parameter family of solutions, which may contain shock waves violating Lax shock inequalities : the so-called *nonclassical shocks*. In order for the uniqueness to be ensured, a *kinetic relation* needs to be added along each nonclassical discontinuity connecting a left state u_- to a right state u_+. It takes the form $u_+ = \varphi^\flat(u_-)$ where $\varphi^\flat$ is the *kinetic function*.
The numerical approximation of nonclassical solutions is known to be very challenging. The main difficulty is the respect of the kinetic relation at the discrete level. In this talk, we present a *sharp interface and fully conservative* scheme (the first one of this type up to our knowledge) for capturing those discontinuities whose dynamics is driven by a kinetic function. The resulting algorithm provides numerical results in full agreement with exact ones, whatever the strength of the shocks are. Some stability properties of the proposed strategy will be given.
This work fits into a joint research program on multiphase flows between CEA-Saclay and Laboratoire J.L. Lions.

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CT41
Convergence of Adaptive Finite Element Methods for the p-Laplace Equation.

We study adaptive finite element methods for the p-Laplacian Equation using piecewise linear, continuous functions. The error is measured by means of the quasi-norm of Barrett and Liu. We provide residual based error estimators without a gap between the upper and lower bound. We show linear convergence of the algorithm which is similar to the one of Morin, Nochetto, and Siebert. Moreover, we show that the algorithm produces (almost) optimal meshes with respect to the degress of freedom. This extends the results of Stevenson to the non-linear case. All results are obtained without extra marking for the oscillation. Abstracts should briefly outline the main features, results and conclusions as well as their general significance and contain relevant references.

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CT41
Finite elements for spatially correlated stochastically perturbed parabolic equations

We present a finite element method for the pathwise approximation of processes which are solutions of stochastic PDE's of the form

$$\partial_t u - \Delta u(t) + f(u(t)) = \dot{W}_t, \text{ on } D$$

where $\dot{W}$ is a time-space noise.
The main focus is on how to handle the discretization the time-space noise in the case of higher-dimensional non-rectangular domains where Fourier/wavelets bases are not easily obtained. In this case, to ensure well-posedness, the noise has to be correlated in space. We study the case in which the correlation is given via

$$\mathbb{E}[\langle \dot{W}_t, \phi\rangle\langle \dot{W}_s, \psi\rangle] = (t \wedge s) \int_D q(x,y)\psi(y)\phi(x)dy =: \langle Q\psi, \phi\rangle$$

where q is a fixed correlation function and Q is the correlation operator.
Our approach to the problem consists in a direct approximation of the correlation operator Q, avoiding its Fourier/wavelets expansion as found in the literature, by basing the computations on q. This

approach allows us to treat general domains D in $\mathbb{R}^d$, with $d = 1, 2$ and 3, as shown by the numerical examples.

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CT41
Exact Stekhlov-Poincaré maps for planar stress in general domains.

We present two explicit series-based representations of Stekhlov-Poincaré maps on general regions, for a time-harmonic elastic scattering problem.
Consider the model problem of computing the scattered elastic wave from a bounded, coated obstacle, D. We surround the obstacle by an artificial boundary denoted by Σ. We describe this in the context of a planar stress problem, though the analysis can be carried out for the planar strain problem analogously.
We assume the incident wave is time-harmonic, allowing us to rewrite the problem as a boundary value problem on the infinite region exterior of D. If we knew the Stekhlov-Poincaré (Dirichlet-to-Neumann) map, $\mathcal{G}$, on Σ, we could model the problem as

$$\begin{cases} -div(\mathcal{A}\mathcal{D}(u)) = 0, & x \in \mathbb{R}^2 \setminus \overline{D} \\ u|_{\Gamma_d} = g, \text{ or } \mathcal{B}u = h, & x \in \partial D, \\ \mathcal{B}u = \mathcal{A}\mathcal{D}(u) \cdot \hat{n}_\Sigma = \mathcal{G}u & x \in \Sigma. \end{cases}$$

The goal is to prescribe an explicit Stekhlov-Poincaré map on Σ, which can be used as a nonreflecting artificial boundary condition. That is, given the displacement u on Σ, we wish to accurately and efficiently compute the traction $T = \mathcal{G}u$, so that there are no reflections from the artificial boundary.
Clearly, if Σ is such that the exterior of this curve yields a seperable geometry, then following the ideas of Givoli and Keller, and subsequently Grote and Keller, we can write a series representation for the operator $\mathcal{G}$. In this talk, we shall describe two different approaches to determine a series representation on more general artificial boundaries, which are perturbations of a circle. We prove analyticity of these maps as a function of this perturbation, but also present results demonstrating the validity of the representations to large deformations. We also establish some results describing the error incurred by truncating these series representations.
The significance of these maps is that they allow one to more closely approximate the actual scattering obstacle. This permits devoting computational resources to the near-field.

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CT42
Stabilization and Acceleration of Iterative Solvers for Linear Systems of Equations: Exploiting Recursive Properties of Fixed Point Algorithms

Here we describe three algorithms for stabilization and acceleration of iterative solvers for large systems of linear equations. More specifically, we describe Reduced Rank Extrapolation (RRE), Minimal Polynomial extrapolation (MPE), and Recursive Projection Method (RPM) applied to iterative solvers in linear algebra.
The fixed-point function of many iterative methods for the solution of large systems of linear equations generates Krylov subspaces during iterative process. The Jacobian of the fixed-point function for a specific iterative method has a recursive property that links spectral content of errors in the initial solution to the spectral content of the errors at any iteration. The recursive property of the Jacobian of the fixed-point function can be used to construct improvements to existing iterative methods by using it to either minimize errors in the Krylov subspace or to construct orthogonal projectors that separate stable and unstable components of the solution.
The use of the recurrence relation to express errors in the current iterate relative to the true solution by using the the minimal polynomial of the iteration matrix for a given iterative method leads to extrapolation methods in Krylov subspaces [1]. Here coefficients of minimal polynomial are computed so that the error is minimized in some sense. Depending on conditions that are imposed on coefficients, RRE and MPE methods result. RRE and MPE algorithms are used for acceleration and stabilization of iterative solvers for linear systems of equations.
By recognizing that the recurrence relation of the Jacobian of the fixed-point function generates Krylov space, stable and unstable bases of this space can be identified. This is achieved through a process of basis orthogonalization by using a modified Gramm-Schmidt procedure and by identifying unstable basis as eigenvectors associated with eigenvalues outside of the unit circle in complex plane. The idea of Recursive Projection Method (RPM) [2] is to use this basis to construct stable and unstable orthogonal projectors. These two projectors are used to separate stable and unstable parts of the solution, thus resulting in a stabilized algorithm.
Numerical experiments show that the use of RRE, MPE and RPM algorithms significantly improve performance of stationary iterative methods. Moreover, they significantly improve performance of Algebraic Multigrid Methods when applied to large systems of linear equations. Use of stabilization algorithms extend the applicability range of stationary iterative and Algebraic Multigrid methods into linear systems whose matrix violates M-matrix properties. This is achieved without modifications to the basic iterative algorithms by embedding them into RRE, MPE and RPM algorithms. Performance gains are illustrated on very large problems obtained by Finite Volume and Finite Element discretizations.

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CT42
Special iterative method for solution of transport-dominated convection-diffusion problems

Convection-diffusion equation with Dirichlet boundary conditions and small parameter at the higher derivatives in the incompressible medium has been considered. The standard 5-point central difference scheme on the regular mesh has been used for approximation of the problem and it's transformation by regular ordering to the system

$$Au = f, \tag{36}$$

where A is matrix u is the vector of unknown, f is the vector of the right part. In the case of central difference approximation of the convective terms operator A can naturally be expressed as a sum of symmetric positive definite operator A_0 and skew-symmetric operator A_1. A_0 is a difference analogue of the Laplace operator, A_1 is a difference analogue of the convective terms. Thus, system with non-symmetric positive real matrix A is constructed.
It is well known, that difficult to solve the linear equation systems (36) because matrix can lose property of diagonal dominant and become strongly nonsymmetric, i.e.

$$\|A_0\|_* << \|A_1\|_*$$

where$\|\&\|_*$ is some matrix norm.
Let us approach (36) by considering the iterative method of the following form:

$$y^{n+1} = Gy^n + \tau f, \quad G = B^{-1}(\omega)(B(\omega) - \tau A), \tag{37}$$

where f, $y_0 \in H$,H is an n-dimensional real Hilbert space, f is the right part of (36), A, $B(\omega)$ are linear operators (matrices) in H, A is given by equation (2), $B(\omega)$ is invertible, y_0 is an initial guess, y_k is the k-th approach, $\tau, \omega > 0$ are iterative parameters, u is the solution that we obtain, $e^k = y^k - u$ and $r^k = Ae^k$ denote the error and the residual in the k-th iteration, respectively.
Consider the next choice of operator B

$$B = (B_C + \omega K_U)B_C^{-1}(B_C + \omega K_L), B_c = B_c^*, \tag{38}$$

where $K_L + K_U = A_1, K_L = -K_U^*$, $B_C = B_C^*$. Operator B_C can be chosen arbitrarily, but has to be symmetric. This method is called two-parameters product triangular (TPTM) method. Convergence of TPTM has been considered and proved. We compare TPTM to the conventional SSOR procedure.
Numerical experiments show that in considered particular cases the behavior of methods is closely related to the technique of choosing the matrix B_C.

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CT42
Fractional Step Runge-Kutta-Nyström methods and order reduction

In this communication we deal with the efficient numerical integration of problems like

$$\left\{ \begin{array}{rcll} u_{tt}(x,t) & = & Au(x,t) + f(x,t), & x \in \Omega, \quad 0 \le t \le T < \infty, \\ u(x,0) & = & u_0(x), & x \in \Omega, \\ u_t(x,0) & = & u_{t,0}(x), & x \in \Omega, \\ \partial u(x,t) & = & g(t), & x \in \partial\Omega, \quad 0 \le t \le T < \infty, \end{array} \right. \tag{39}$$

where Ω is a bounded spatial domain and A is a self-adjoint and negative definite differential operator.
One of the most common techniques to solve this problem consists of using the method of lines, discretizing firstly in space and then in time; or the other way round, doing the time discretization before the spatial one. As for the time integration, one possible way is to write problem (39) as a first order in time differential equation in order to use known methods for their numerical integration (like Runge-Kutta methods). Other possible choice is to use methods that have been specifically designed for the numerical integration of second-order in time problems, like Runge-Kutta-Nyström methods (RKN).
Fractional Step Runge-Kutta-Nyström methods (FSRKN), introduced in [4], are an efficient alternative to the use of RKN methods when multidimensional problems like (39) are integrated. The use of FSRKN methods allows us to avoid the stability problems of explicit RKN methods and besides, they have the advantage of having a low computational cost per stage when they are compared with other classical time integrator methods, like implicit RKN methods. To reduce the computation cost, the differential operator is split as a sum of simpler operators in a certain sense. After that, a time integration is made, by using a FSRKN method subordinated to such partition; in this way, only one part of the split acts in an implicit way in every intermediate stage.
When the boundary conditions depend on time, the order reduction problem appears; such drawback has already been studied for RKN and Fractional Step Runge-Kutta methods [1, 2, 3]. From the ideas used in [1,3], it is shown that by changing in an adequate way the values that the stages take at the boundary, this order reduction can be reduced and, in certain cases, the classical order is obtained.

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CT42
A High Performance Parallel Linear Algebra Toolbox: Building Blocks for a Parallel Algebraic Multigrid Solver

The *Parallel Toolbox*, a high performance parallel linear algebra toolbox written in the C++ programming language is introduced. The toolbox provides building blocks for the construction of advanced parallel multilevel solvers. A parallel algebraic multigrid solver is used as a testbed for problems in fluid mechanics and biomedical engineering.

The toolbox automatically generates the necessary parallel communication for unstructured distributed finite element meshes. The communication complexity is handled by the toolbox with only a few simple user accessible routines.

A key design goal for the toolbox is to use only *almost linear* algorithms in the components of the toolbox to achieve optimal computational scaling with respect to problem size and number of processors. Benchmarks on high performance computing clusters are presented to validate the viability of the approach.

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CT43
Local Projection Stabilizations for Inf-sup Stable Finite Elements applied to the Oseen Problem

In many solvers for the non-stationary, incompressible Navier-Stokes equations the problem is split into linearized auxiliary problems of Oseen type.

In this talk we give a full a priori analysis for finite element discretizations using local projection methods. Especially, the choice of the stabilization parameters is discussed. In contrast to existing papers [1], [3] we assume inf-sup stable velocity-pressure pairs. The theoretical results are validated by numerical experiments.

Finally the results are compared briefly with residual-based stabilization methods, cf. [2], [4].

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CT43
Higher order finite elements on pyramids

We present a construction of high order finite elements for H^1, $H(\mathrm{curl})$, $H(\mathrm{div})$ (and L^2) on a pyramid which are compatible with existing tetrahedral and hexahedral high order finite elements and satisfy the commuting diagram property.

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CT43
Bilinear shell elements and boundary layers.

The performance of low-order finite elements when modelling shell structures is one of the scientifically open questions in computational mechanics. The focus of this study is on the response of best bilinear finite elements to boundary layer-type deformations of shells.

Our mathematical approach to this problem is based on simplified reformulations of the original (3D) elements in the context of shallow shells, see reference [1]. In addition, the error analysis becomes more transparent if the ‘layer problem’ is isolated as an energy minimization problem of its own kind. The locking effects that may arise in the finite element model can then be analyzed within a such subproblem of the original ‘shell problem’, see reference [2].

Here we consider shell layers generated by straight lines (boundary lines, line loads,. . .) and concentrate on the following main layer modes:

1. The line layer that decays in the length scale $L \sim \sqrt{Rt}$ from the layer generator, where t is the thickness of the shell and R measures the total curvature of the shell. This case is characterized as a “*simple edge effect*” and is possible in all shell geometries.

2. The line layers that decay in the length scales $L \sim \sqrt[n]{R^{n-1}t}$ ($n = 3, 4$) from the layer generator. These two cases are referred as “*generalized edge effects*” and they arise in hyperbolic ($n = 3$) and parabolic ($n = 4$) shell geometries when the layer generator is a characteristic line of the mid-surface of the shell.

Our theoretical predictions supported by computational experiments indicate that parametric error amplification effects occur in all cases, and that the case of hyperbolic degeneration ($n = 3$) appears to be the worst case in this sense.

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CT43
On efficient solution of linear systems arising in *hp*-FEM

We discuss the *hp* version of the finite element method (*hp*-FEM) for 2D linear elliptic problems, see e.g. [2–4]. There are three types of basis functions in this case: vertex, edge, and bubble functions. The classical technique of the static condensation, see e.g. [1,2], decouples the linear algebraic equations for bubble functions from the equations for the other two types of the basis functions. This condensation of the degrees of freedom (DOFs) corresponding to the bubble functions (the internal DOFs) can be done in parallel element by element and, moreover, no fill-in appears in the resulting Schur complement system for vertex and edge DOFs.
In the presentation, we show how to continue and condense out the edge DOFs to decouple them from the vertex DOFs. The price for this decoupling is however the presence of more non-zero elements in the system for vertex DOFs. We will present various numerical experiments to discuss and compare the efficiency of the described approaches.
Further, we will mention possible extensions to 3D, we will comment on the connection of the static condensation of internal DOFs with the ILU preconditioning and on the connection with the orthogonalization of basis functions [5].

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CT44
Schwarz domain-decomposition for an external magnetostatic problem

We model non-linear ferromagnetic effects using different formulations of the magnetostatic problem – the reduced scalar potential, the mixed form of reduced scalar potential formulation and the reduced vector potential with and without the Coulomb's gauge.
An overlapping domain-decomposition Dirichlet-Dirichlet technique is proposed [1,3] to solve the underlying problems on unbounded domains. In the near-field, adjacent to the ferromagnetic object, we employ finite element discretizations, while the far-field, going to infinity, is modelled through the Poisson representation formula.
In this way, we circumvent the need to store and invert full matrices, which usually occur when using techniques based on boundary element method on fictitious boundary. In case of complicated industrial geometries, the order of these full matrices is about 10^5, reaching thus up-to-date limits in computer hardware and CPU time. The domain-decomposition technique, however, permits to solve industrial problems on standard computer equipment in a reasonable time. Besides comparing our approach to other known techniques on a simple testcase, we estimate its CPU and memory costs and its convergence speed.
To illustrate the performance of the proposed method, we present a simulation of ferromagnetic effects on a typical testcase for the electrolysis of aluminium. During the process of aluminium production, high densities of electric current are used to produce pure liquid aluminium out of aluminium oxide. These currents induce huge magnetic fields, which interact with the liquid aluminium, causing important flows inside the electrolytic cell. The forced flow may ultimately develop instabilities, causing damages to the electrolytic cell. To predict the aluminium flow, magnetic forces acting on the fluid must be calculated. Taking into account the effect of induction (Biot-Savart's law) is not sufficient, we must include also the non-linear ferromagnetic response of the metallic container of the electrolytic cell.
Due to complicated shell-geometry of the metallic container [2], techniques based on boundary elements on the boundary of the container are too expensive to use. Even if the container is inscribed into a ball, these methods are still quite costly. On the other hand, with the domain-decomposition technique we solve this testcase more efficiently and we can even perform several levels of mesh refinement.
The study has been sponsored by the Swiss CTI grant no. 6437.1 IWS-IW and Alcan-Péchiney.

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CT44
Mixed Conforming Elements for the Large-Body Limit in Micromagnetics

We consider the large-body limit of the Landau-Lifshitz minimization problem introduced by DeSimone in 1993: Find a minimizer $\mathbf{m} : \Omega \to \mathbb{R}^d$ with $|\mathbf{m}| \leq 1$ a.e. of the bulk energy

$$E(\mathbf{m}) = \frac{1}{2}\int_{\mathbb{R}^d} |\nabla u|^2\,dx + \int_\Omega \phi^{**}(\mathbf{m})\,dx + \int_\Omega \mathbf{f}\cdot\mathbf{m}\,dx.$$

Here, $\Omega \subset \mathbb{R}^d$, for $d = 2, 3$, is the spatial domain of the ferromagnetic material, ϕ^{**} is the (convexified) anisotropy density, and $\mathbf{f} : \Omega \to \mathbb{R}^d$ is an applied exterior field. The magnetic potential $u : \mathbb{R}^d \to \mathbb{R}$ is related to the magnetization $\mathbf{m}$ by the magnetostatic Maxwell equation

$$\operatorname{div}(-\nabla u + \mathbf{m}) = 0 \quad \text{in } \mathcal{D}'(\mathbb{R}^d). \tag{40}$$

In our discretization we replace the entire space $\mathbb{R}^d$ in the energy functional E and in the potential equation (40) by a bounded Lipschitz domain $\widehat{\Omega}$ containing Ω and stipulate $u \in H^1_0(\widehat{\Omega})$ as the boundary condition on $\partial\widehat{\Omega}$. We consider a mixed $P^0(\mathcal{T})$-$S^1_0(\widehat{\mathcal{T}})$ finite element discretization of $(\mathbf{m}, u)$ for the corresponding (and equivalent) Euler-Lagrange equations. Since conforming elements appear to be unstable for the pure Galerkin discretization, we append to the Galerkin discretization a consistent stabilization term. Moreover, the side constraint $|\mathbf{m}_h| \leq 1$ is replaced by a penalization strategy.
In this the talk, we discuss the well-posedness of the discrete problem and the corresponding error analysis. We comment on the extension of the analysis to higher-order elements and the efficient treatment of the full space equation (40). Numerical experiments illustrate the theoretical results.

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CT44
Analysis of a Centered Flux Discontinuous Galerkin Method for Maxwell's Equations on Cartesian Grids

The Discontinuous Galerkin (DG) method on Cartesian grids using a centered numerical flux [1,2] is investigated. It is shown that the DG discretization can be expressed in terms of properly defined, discrete vector analytic operators. Under certain conditions, this discrete operators inherit important algebraic properties, e.g. $\operatorname{div}\operatorname{rot} = 0$, from their analytic counterparts. In particular, in this case a discrete Gauss law is exactly fulfilled if discrete currents and charges are defined in a proper manner. This result is of particular interest for the usage of the method as a building block within a Particle-In-Cell algorithm for the numerical solution of the Maxwell-Vlasov equations [1]. Performing a dispersion analysis, the wave propagation properties of the semi-discrete DG method is investigated [3]. Writing the semi-discrete DG equation as a Hamiltonian system, the time integration is performed by explicit symplectic methods of various orders. For some of these methods, the stability and dispersion properties are analyzed. The theoretical findings are complemented by numerical simulations.

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CT44
Functional type a posteriori error estimates for Maxwell's equations

A posteriori error estimation in the context of Maxwell's equations is still under active development. First a posteriori error estimates derived for finite element solutions of the eddy-current and time-harmonic problems are quite recent. These estimates are residual based and contain several unknown, mesh dependent constants, thus in practice they serve only as error indicators. This situation creates a need for practically computable, guaranteed a posteriori error estimates.
In this talk, we present functional type a posteriori error estimates for the eddy-current and time-harmonic simplifications of the Maxwell's equations with zero tangential boundary conditions (corresponding to a PEC-surface). Functional type a posteriori error estimation is well established for several other types of problems (see Neittaanmäki, Repin [1]), but it has not been previously applied in this context.
Estimate for the eddy-current case is based on a direct application of a technique from Hannukainen, Korotov [2]. The resulting a posteriori error estimate does not contain any unknown constants, is applicable to any admissible approximation of the solution, and is practically computable.
Functional type a posteriori error estimate for the time-harmonic problem is based on applying an adjoint problem to establish a connection between the L^2-norm of the error and the residual. The same technique is applied in the derivation of a residual based error estimate in Monk [3]. In this case, the functional type upper bound contains one unknown constant, which is dependent only on the parameters of the original problem.

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CT45
An augmented Lagrangian approach to linearized problems in hydrodynamic stability

The solution of linear systems arising from the linear stability analysis of solutions of the Navier–Stokes equations is considered. Such stability analysis leads to the solution of an eigenvalue problem, in particular, to the determination of eigenvalues close to the imaginary axis. Shift-and-invert type methods are often used for the solution of the eigenvalue problem, leading (on the continuous level) to systems of the form: Given a mean velocity field U, a forcing term $\mathbf{f}$, a scalar $\alpha \geq 0$ and a viscosity coefficient ν, find a velocity-pressure pair $\{\mathbf{u}, p\}$ which solves

$$\begin{aligned} -\nu\Delta\mathbf{u} - \alpha\mathbf{u} + (U\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)U + \nabla p = \mathbf{f} &\quad \text{in} \quad \Omega\,, \\ -\operatorname{div}\mathbf{u} = 0 &\quad \text{in} \quad \Omega\,, \\ \mathbf{u} = \mathbf{0} &\quad \text{on} \quad \partial\Omega \end{aligned}$$

Due to indefiniteness of the submatrix corresponding to the velocities, this system poses a serious challenge for iterative solution methods. In this talk we discuss the extension of the augmented Lagrangian-based block triangular preconditioner introduced by the authors in [1] to this class of problems. We prove eigenvalue estimates for the velocity submatrix and deduce several representations of the Schur complement operator which are relevant to numerical properties of the augmented system. Numerical experiments on several model problems demonstrate the effectiveness and robustness of the preconditioner over a wide range of problem parameters. Some further details can be found in [2].

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CT45
On Some Uniqueness results of Incompressible Flow through Cascade of Profiles

The paper is concerned with the theoretical analysis of the model of incompressible, viscous, stationary flow through a plane cascade of profiles. The boundary value problem for the Navier-Stokes system is formulated in a domain representing the exterior to an infinite row of profiles, periodically spaced in one direction. Then the problem is reformulated in a bounded domain of the form of one space period and completed by the Dirichlet boundary condition on the inlet and the profile, a suitable natural boundary condition on the outlet and periodic boundary conditions on artificial cuts. Specially, we study the question of uniqueness of the weak solution of this problem for linear boundary condition, and for nonlinear modification of the ”do nothing” type of boundary condition (proposed by C. H. Bruneau, F. Fabrie in [1]). Let us recall that the uniqueness of a weak solution of the stationary Navier–Stokes equation with nonhomogeneous Dirichlet–type boundary data is known to hold only if certain norm of the boundary data and the external body force is “sufficiently small” in comparison with the viscosity. Then the weak solution can be constructed so that it lies in a “sufficiently small” ball and the theorem on uniqueness says that the solution is unique, not only among solutions in the same ball, but in the class of all weak solutions. (See e.g. the books by R. Temam [2] and G. P. Galdi [3]) This paper contains a result of a similar type. However, in case of nonlinear boundary condition, we can show only uniqueness in the class of “sufficiently small” solutions.

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CT45
Justification of the splitting scheme for the large-scale ocean circulation problem

In a cylinder Ω in the Cartesian coordinates we consider the system of primitive equations describing large-scale ocean dynamics [1], [2]

$$\begin{aligned} &\hat{\mathbf{u}}_t - \nu\triangle\hat{\mathbf{u}} + \nabla' p + \mathbf{u}\cdot\nabla\hat{\mathbf{u}} = \mathbf{0}, \quad p_z = -g\rho, \\ &\operatorname{div}\mathbf{u} = 0, \quad \rho_t - \nu_1\triangle\rho + \mathbf{u}\cdot\nabla\rho = 0; \end{aligned} \tag{1}$$

here $\mathbf{u} = (u_1, u_2, u_3)$, $\hat{\mathbf{u}} = (u_1, u_2)$, $\nabla' = (\partial_x, \partial_y)$. We complete (1) with appropriate initial and boundary conditions.
For numerical solution to (1) we consider the splitting scheme of the Chorin type. Convergence of the splitting scheme is proved with the help of technique from [3] and [4].

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CT45
Numerical and analytical research of multimode solutions of the Jeffery – Hamel problem

The unknown till now multimode both symmetric and asymmetric solutions of the Jeffery – Hamel problem [1] for viscous flow in plane confusor by small, moderately big, and asymptotically big values of Reynolds' number Re in all permissible range of confusor angle are constructed and studied. These solutions depend singularly on Re by its asymptotically low values. Some new hydrodynamic effects have been established and commented. The present work is a development of previous investigation of authors [2, 3] where the modified method on advanced convergence is proposed and developed. An essence of this method is also stated in present report.

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CT46
Edge stabilization of higher order elements for convection diffusion equations

We investigate the edge stabilization method of Burman and Hansbo [1,2] for higher order finite elements applied to a convection diffusion equation with a small diffusion parameter ε. Performing numerical experiments, it turns out that strongly imposed Dirichlet boundary conditions lead to relatively bad numerical solutions. However, if the Dirichlet boundary conditions are imposed on the inflow part of the boundary in a weak sense and additionally on the whole boundary in an ε-weighted weak sense due to Nitsche [3] then one obtains reasonable numerical results. In many cases, this holds even in the limit case where the parameter of the edge stabilization is zero, i.e., where the standard Galerkin discretization is applied.
We present an analysis which explains this effect. Furthermore, we investigate an adaptive procedure based on the weak discretization of the Dirichlet boundary conditions.
For finite elements of degree larger than two, we propose the use of non-standard basis functions which essentially reduce the number of additional couplings caused by the edge stabilization. Thus, the edge stabilization method will become more attractive from the implementational point of view.

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CT46
On the choice of parameters in stabilization methods for convection–diffusion equations.

This contribution is devoted to the numerical solution of scalar convection–diffusion equations by means of the finite element method. If convection dominates diffusion, the solution of the continuous problem typically possesses interior and boundary layers which cannot be resolved properly unless the mesh is extremely fine. This often leads to spurious oscillations in the numerical solution. In particular, the solutions of the classical Galerkin finite element discretization are typically globally polluted by spurious oscillations. Therefore, various stabilization techniques have been developed during the last three decades to remove or, at least, to diminish these oscillations. Let us mention the streamline upwind/Petrov–Galerkin (SUPG) method proposed by Brooks and Hughes [1], the Galerkin/least–squares method introduced by Hughes, Franca, and Hulbert [2] or the various (often nonlinear) SOLD methods recently reviewed in [3].
An important drawback of many stabilized methods is that they contain stabilization parameters for which a general 'optimal' choice is not known and whose definitions usually rely on heuristic arguments. On the other hand, it is well known that the choice of these parameters may often dramatically influence the accuracy of the discrete solutions. The aim of the presentation is to discuss the choice of the stabilization parameters for various stabilization techniques (SUPG method, some of the SOLD methods) and to present theoretical and numerical results comparing various approaches published in the literature.

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CT46
Mixed hybrid DG methods for convection-diffusion problems

A new method for convection-diffusion problems, composed of a mixed method for the elliptic part and a discontinuous Galerkin method for the convective part, is proposed and analyzed.
The two methods for the elliptic/hyperbolic subproblems are made compatible via hybridization, i.e., enforcing continuity of the solution via Lagrange-multipliers. This approach has several advantages, e.g.., it allows to eliminate the primal and flux variables on the element level and yielding a global system for the Lagrange-multipliers only. Moreover, the upwind character of the numerical scheme can be clarified easily.
The resulting method is analyzed with respect to a problem- and mesh-dependent norm that explicitly includes the Lagrange-multipliers. By utilizing the structure of the method as composition of two well-established methods, important properties like consistency and conservation can be deduced. Additionally, stability and boundedness of the resulting bilinearform are inhereted from the mixed / DG method for the elliptic/hyperbolic subproblems.
The performance of the proposed method is illustrated with numerical examples, and implementational details are discusse.

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CT46
A finite element model for bone ingrowth into a prosthesis

We consider a finite element method for a model of bone ingrowth into a prosthesis. Such a model can be used as a tool for a surgeon to investigate the bone ingrowth kinetics when positioning a prosthesis. The overall model consists of two coupled models, which are shortly explained.
The first model concerns the biological part. Mesemchymal stemcells migrate from the bone marrow into the cavity filled with granular tissue. Under the stresses and fluid flows present in the granular tissue, the stem cells differentiate into fibrous tissue, cartilage or bone producing cells. This model deals with the gradual bone ingrowth into the cavity or prosthesis. The model was constructed by Prendergast [1] and used by Andreykiv [2] for the modeling of bone ingrowth into a shoulder prosthesis. The model consists of a nonlinearly coupled set of diffusion-reaction equations.
The second model deals with the mechanical part and computes the fluid flow and stresses in the bone and prosthesis. These quantities are needed for the biological model to determine which types of cells the stem cells differentiate to, and hence the output of this mechanical model is needed as input for the biological model. As an input the mechanical quantities change as the bone moves into the granular tissue. Hence, the resulting bone portion from the first model is needed for this model. This second model consists of poro-elasticity equations due to Biot, see the work due to Bear [3] for instance.
The two models are coupled and so far no sensitivity analysis of the parameters involved has been carried out. This will be a topic in the presentation. Further, various strategies of coupling between the two models will be addressed in terms of accuracy and efficiency sustained by numerical experiments. In this work the experiments will be rather academic, but we expect our insights to be incorporated into models with more realistic geometries.

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CT47
Integrodifferential approach in the linear theory of elasticity

Some possible modifications of the governing equations of the linear theory of elasticity are considered. The stress-strain relation is specified by an integral equality instead of the local Hooke’s law. The modified integro-differential boundary value problem is reduced to the minimization of a nonnegative functional over all possible displacements and equilibrium stresses under differential constraints. The semi-inverse method is applied to derive this new minimum variational principle. The relations between the proposed approach and the minimum potential and complementary energy principles are considered. The method under consideration enables one to construct effective local and integral bilateral estimates of a numerical solution.
A numerical algorithm based on polynomial approximations of unknown functions (stresses and displacements) is developed and applied to linear elasticity problems. The algorithm consists of specified steps. In the fist step the independent variables are approximated by finite polynomial series. After that, equilibrium equations and boundary conditions are satisfied. As the result the unconstrained minimization problem for quadratic functional arises. The bilateral estimation criteria of solution errors are proposed in order to analyze the algorithm convergence rate.
The numerical results obtained by applying the integrodifferential approach and the conventional variational methods are compared. The possibilities of FEM realization of the variational principle proposed are discussed.

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CT47
FEM realization based on integral strain-stress relations

The method of integrodifferential relations is applied to solve linear elasticity problems and can be considered as an alternative to conventional variational approaches. The local stress-strain relation (Hooke's law) is replaced by a generalized integral equality and the original boundary value problem is reduced to minimization of a quadratic nonnegative functional under differential constraints. This variational statement of an elasticity problem allows to construct an adaptive FEM algorithm for effective analysis of the stress-deformed state of an elastic body. In the algorithm piecewise polynomial functions in the Bezier-Bernstein form over an arbitrary domain triangulation are used to approximate displacement and stress fields. These spline approximations must satisfy given boundary conditions, interelement compatibility and stress equilibrium equations.
Three nonnegative objective functionals are proposed and can be regarded as criteria of numerical solution quality. The numerical algorithm developed enables us to construct bilateral estimates for various integral characteristics (e. g., elastic energy and displacements). This FEM realization gives us the possibility to work out various strategies of p-h adaptive mesh refinement by using a local error estimate based on the difference of the potential energy density with complementary energy density.
The advantages of the developed finite element approach are illustrated on 2D static problems. This algorithm can be directly generalized to 3D linear elastic problems and applied to anisotropic structures. The case of more complex boundary conditions such as elastic (Winkler) base, "living" forces, etc. does not encounter any difficulties. The method can appear to be useful also in advanced beam, plate, and shell theories.

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CT47
Constraints Coefficients in *hp*-FEM.

Continuity requirements on irregular meshes enforce a proper constraint of the degrees of freedom that correspond to an irregular node, edge or face of the neighboring elements. This is achieved by using so-called constraints coefficients which are obtained from the appropriate coupling of shape functions on the master element (cf., e.g., [1], [2], [3], [4], [7]).
In this talk, a recursive procedure is presented for determining the constraints coefficients of hierarchical Gauss-Lobatto shape functions in 2D and 3D. The coefficients are available for arbitrary patterns of subdivisions even on multi-irregular grids. Numerical examples concerning adaptive *hp*-FEM are presented.
Furthermore, the application of constraints coefficients in cascadic multigrid schemes and time-dependent problems is discussed.

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CT47
p-Sparse BEM for weakly singular integral equation on a random surface

We consider the weakly singular boundary integral equation $\mathcal{V}u(\omega) = g$ on a randomly perturbed smooth closed surface $\Gamma(\omega)$ (cf. [2] for stochastic g). The aim is the computation of the moments $\mathcal{M}^k u := \mathbb{E}[\otimes_{i=1}^k u]$, $k \geq 1$, if the corresponding moments of the perturbation are known. The problem on the stochastic surface is reduced to a problem on the nominal deterministic surface Γ with the random perturbation parameter $\delta\beta(\omega)$. Note, that $u(\omega)$ depends nonlinearly on $\delta\beta(\omega)$.
Resulting formulation for the kth moment is posed in the tensor product Sobolev spaces and involve the k-fold tensor product operators $\mathcal{V}^{(k)} := \otimes_{i=1}^k \mathcal{V}$. The complexity of the standard full tensor product Galerkin BEM is $\mathcal{O}(N^k)$, where N is the number of degrees of freedom needed to discretize the nominal surface Γ. Based on [3], we develop a p-sparse grid Galerkin BEM to reduce the problem complexity to $\mathcal{O}(N(\log N)^{k-1})$ (cf. [1] for h-sparse grid Galerkin BEM with wavelets).

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CT48
Rosenbrock methods for Large-Scale Differential Riccati Equations

We consider the numerical solution of stiff differential Riccati equations (DREs). Rosenbrock methods have already given good results for a variety of stiff problems, e.g. chemical kinetics [2,3]. Moreover, they are very attractive for several reasons: they posses excellent stability properties (as they can be made A-stable or L-stable), they are easy to implement and they are suitable for parallelization [6]. We derive a matrix valued version of the Rosenbrock methods for DREs. It turns out that one Lyapunov equation has to be solved in each stage of the method. For the case in which the coefficient matrices of the Lyapunov equation are dense, the Bartels-Stewart method can be applied for solving the equations. Here, we focus on solving DREs arising in optimal control for parabolic partial differential equations. Typically the coefficient matrices of the DRE arising from these control problems have a certain structure (e.g. sparse, symmetric or low-rank). Thus, the solution of the resulting Lyapunov equation with Bartels-Stewart method is not feasible. We show that it is possible to efficiently implement Rosenbrock methods for large-scale DREs based on a low-rank version of the alternating direction implicit (ADI) iteration for Lyapunov equations [1,4,5].

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CT48
A second order scheme for solving optimization-constrained differential equations with discontinuities.

Dynamic optimization problems arise when coupling a minimization problem with ordinary differential equations. These problems appear for instance in computational chemistry when a system at equilibrium exchanges mass with a surrounding media.
We present here a numerical method for the simulation of dynamic phase transitions for a single atmospheric aerosol particle that exchanges mass with the surrounding gas. This system is described by a system of ordinary differential equations coupled with an inequality constrained optimization problem, which determines the thermodynamic equilibrium of the particle. This coupling induces discontinuities of the time-dependent variables. The key issues are the coupling of the differential equations with the constrained minimization problem and the accurate tracking of the discontinuities generated by the phase transitions inside the particle. These discontinuities appear when an inequality constraint of the minimization problem is activated or deactivated.
The ordinary differential equations are discretized in time and coupled with the first order optimality conditions of the minimization problem to form a differential-algebraic system of index one. We use a second order multistep method based on a predictor-corrector Adams scheme to detect the discontinuities by extrapolation of the trajectories. The features of the optimization problem are exploited in the exact computation of the derivatives of the optimization variables by using a sensitivity analysis. The main difficulty is the impossibility to define any explicit event function that characterizes the phase transition.
The order of convergence of our method is proved when inequality constraints are activated. Numerical results for atmospheric organic particles are presented and show the accuracy and efficiency of our approach.

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CT49
Space-and-Time Adaptive Calculation of Transient 3D Magnetic Fields

Transient magnetic fields are described by a parabolic initial-boundary value problem. Their discretization with geometric discretization schemes like the Finite-Element Method based on Whitney form functions results in nonlinear differential-algebraic systems of equations of index 1. As a result of external transient electric current excitations the magnetic field yields commonly thin layers of eddy currents in electric conductors and/or local nonlinear saturation effects have to be taken into account in ferromagnetic materials. A common approach in established simulation tools for solving this problem is the method of lines where the space is discretized adaptively at the beginning of the simulation and is then kept fixed within the adaptive time integration of the resulting time dependent equation. This approach, however, fails to take into account changes of the solutions in the regions of material related strong local field variation depending on the excitation wave form. This problem is solved using a coupled adaptive strategy for the spatial mesh discretization and for the time discretization similar to the approach used for advection-diffusion flow problems presented in [1]. Extending first results presented for two-dimensional magnetic field problems presented in [2], here a combination of error controlled spatial adaptivity for a three-dimensional FEM formulation based on Whitney form functions (using the AGM library [3]) and error controlled implicit Runge-Kutta schemes [4] and linear-implicit Rosenbrock-Wanner schemes [1] is used to reduce the number of unknowns for the nonlinear algebraic systems effectively and to avoid unnecessary fine grid resolutions both in space and time. The solution of the linearized curl-curl-type systems of equations is performed using algebraic multigrid schemes with hybrid smoothers provided by the Trilinos ML library [5]. Numerical results for 3d magnetic field simulations are presented using this approach.

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CT49
hp-FEM and High-Order BIE Method for Efficient Modelling of Photonic Crystal Materials with Negative Refraction

Photonic crystals (PC) have become a major subject of today's photonic engineering research. Such periodic dielectric structures may exhibit complete band gaps and possess a number of unusual electromagnetic effects, including negative refraction. These anomalous features allow considerable control over the light propagation and could lead to the development of materials that focus light to provide a superlens [1].
We predict a range of frequencies with negative refraction by calculating the band structure of a perfect photonic crystal and find dielectric pattern that optimizes the superlensing properties. The found pattern and range of frequencies are used to compute the transmitted fields of an excitation source through a finite crystal. Our method enables us to study photonic crystals with arbitrary lines of discontinuities of the dielectric material, including both smooth and polygonal interfaces.
The eigenvalue problem for the crystal with ideal periodicity is reformulated by the Floquet-Bloch transform [2] into a family of eigenvalue problems in the elementary cell, ordered by the quasi-momentum $\mathbf{k}$. The relation between quasi-momentum and frequency is the well-known band structure. We compute the eigenvalues with p - Finite Element (FE) for smooth interfaces and hp - adaptive FE [3] for polygonal interfaces of the dielectric pattern with our C++ library Concepts [4]. We refine the mesh geometrically towards corners of material interfaces and increase the polynomial degrees away from them. Therefore the eigenvalues converge exponentially both for smooth and polygonal interfaces.
To solve the electromagnetic transmission problem for the finite crystal we use a spectral Boundary Integral Equation (BIE) method where a reduction of the complexity of the computational scheme is achieved by using the Fast Fourier Transform (FFT). This approach leads to excellent error properties due to the use of a global periodic parametrisation of the interfaces. In addition, the singularity substraction technique is used for an accurate evaluation of the integral equation singularities.
Despite the obvious advantages exhibited by high-order methods, only limited attempts have been made so far to apply such methods to the characterisation of photonic nanomaterials. In this talk we demonstrate the use of the described high-order methods for the fast and accurate modelling of a superlens formed by PC material.

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CT49
An efficient iterative method for finite element discretizations, with application to 3D electromagnetic problems.

Construction of effective iterative methods for solving algebraic problems resulting from finite element discretizations is a topical challenge of numerical mathematics. The presented approach is a specific variant of the algebraic multigrid method [1-2] adapted for 3D electromagnetic problems. Construction of the proposed multigrid preconditioner consists of the following stages:

1. An original finite element grid is subdivided into non-overlapping superelements, each consisting of several neighboring cells.
2. "Inner" unknowns of each superelement are Gauss-eliminated, i.e. the Schur complement matrix for edge and face unknowns is constructed.
3. Prolongation operators on superelement edges and faces are derived basing on some natural 1D and 2D approximate representation of the 3D problem operator.
4. The prolongation operators are used for construction of the basic functions on the coarse grid.
5. The obtained coarse grid algebraic problem is solved (during the mutigrid iterative process) by a quasi-optimal Gauss direct method.

This two-level version of the method can be generalized to the multilevel one.
The method is applied to solving complex 3D time-harmonic electromagnetic problems discretized by the edge basic functions [3] on a cylindrical grid. Results of practical applications are presented.

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CT50
Numerical modelling of epidermal wound healing.

Wound healing, when it occurs, takes place due to the combination of several processes, such as reconstruction of the capillary network (neovascularization) [1], cell division and cell migration (wound contraction) [2] and scar modelling. Until now, these processes have been mathematically modelled independently and only for axisymmetric wound geometries. However, these processes do not take place in a complete sequential manner but partly overlap. In this work, we present a mathematical model for coupled neovascularization and wound contraction for general wound geometries. The model is based on the existence on an active layer surrounding the wound, where there is an increased activity of cellular growth, cellular division and production of growth factors that enhance wound healing. The model consists of a system of coupled diffusion-reaction equations that relate the oxygen concentration, the capillary density and the production of a generic growth factor that induces wound contraction in the regions where a certain threshold value is exceeded. The Level Set Method [3] is used to track the wound edge, and provides us with a straightforward identification of the active layer. Due to the thickness of the epidermis ($\approx$ 1mm), only two-dimensional problems are considered in this work. The numerical results show a non-continuous healing behavior due to the threshold condition imposed on the contraction rate, and the model is used to investigate the influence of the active layer thickness and the wound geometry on the healing process.

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CT50
Numerical Simulation and Optimization of Fracture Healing

The modeling of fracture healing processes is of great interest in biomechanics and medical research. A finite element model of a callus healing, which simulates the tissue differentiation process under biological and mechanical factors, was introduced in [1]. For this model an algorithm to estimate a healing time was applied.
Using this healing time, we applied an optimization algorithm to estimate an optimal healing time with respect to the stiffness of the fixation. However, using the simulation as black box function for the optimization process with optimization algorithms of low order does not lead to a satisfying result in the sense of efficiency and accuracy. To improve the results of the optimization process, we created an analytical model for the mechanical and biological processes of the healing simulation. Using these analytical models we applied more efficient optimization algorithms.

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CT50
Special efficient solutions for multicriterial transport problems

Some special type of min-efficient solutions for transport problems of cost-cost type, cost-time type, time-time type and time-cost type (see [1] and [2]) are considered and some theorems for their characterization are given.
Using these theorems, numerical algorithms for finding these special min-efficient solutions are constructed.
The structure of the set of these efficient solutions is studied. An application of these properties, in the problem of the organizing the mobile unit in order to take, collect and transport the smears for a cervical cancer screening, is given.

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CT50
Multiple Dynamic Programming Applied in Cervical Cancer Screening

An important aspect in planning a cervical cancer screening program is to organize the mobile unit in order to take, collect and transport the smears. Thus a medical unit goes in remote area in different villages and performs Pap tests. For each villages we know the number of the women which will be tested. We also know the time to perform a test and the time of reading the slide. The problem is to plane, for a given time period, the ways for the mobile unit such that the costs are minimum and the number of tests should be maximum. We keep into acount that the mobile unit goes every day from base and return home and the result of the test should be done in a maximum given time (laboratory response time).
In this paper we give an answer to this medical problem using a multiple dynamic programming model. Also we give an algorithm for determining the set of efficient points.
All this investigation is supported by the Research Grant, CEEX No. 125/31.07.2006, CanScreen, with the Romanian Ministry of Education and Research.

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CT53
An optimal control problem for stochastic elliptic pde's

In this talk we consider an optimal control problem for linear stochastic partial differential equations (SPDEs) with quadratic cost functionals and distributed stochastic control. Let $\mathcal{D}$ denotes an open, bounded spatial domain in $\mathbb{R}^d$ with a boundary $\partial\mathcal{D}$. Let ω be a random variable ranging in $\Omega = \mathcal{S}'(\mathbb{R}^d)$. As a prototype example of distributed control problems for SPDEs we will consider the minimization of the quadratic cost functional

$$\mathcal{J}(u,g) = \sum_{\alpha\in\mathcal{I}} \|u_\alpha - \overline{u}_\alpha\|^2_{H^1_0(\mathcal{D})} e^{k(2\mathbb{N})^\alpha} + \lambda \sum_{\beta\in\mathcal{I},\,|\beta|\le 1} \|g_\beta\|^2_{L^2(\mathcal{D})} e^{l(2\mathbb{N})^\beta} \tag{41}$$

subject to the elliptic SPDE for the state u and the stochastic control g:

$$-\Delta u(\mathbf{x},\omega) = f(\mathbf{x},\omega) + g(x,\omega)\,, \qquad \text{in } \mathcal{D}\times\Omega \tag{42}$$

$$u(\mathbf{x},\omega) = 0\,, \qquad \text{on } \partial\mathcal{D}\times\Omega \tag{43}$$

where $\overline{u}(x,\omega) = \sum_{\alpha\in\mathcal{I}} \overline{u}_\alpha(x)H_\alpha(\omega)$ is a desired state, $f = \sum_{\alpha\in\mathcal{I}} f_\alpha(x)H_\alpha(\omega)$ is a specified stochastic forcing term and $g = \sum_{\alpha\in\mathcal{I},|\alpha|\le 1} g_\alpha(x)H_\alpha(\omega)$ is the control term. Here $\mathcal{I}$ denotes the set of multi-indices $\alpha = (\alpha_i)$ where all $\alpha_i \in \mathbb{N}$ and only finitely many $\alpha_i \neq 0$ and $\mathcal{H}_\alpha$'s are the stochastic variables $\mathcal{H}_\alpha(\omega) = \Pi_{i=1}^\infty h_{\alpha_i}(\langle\omega, \eta_i(x)\rangle)$, $\omega \in \mathcal{S}'(\mathbb{R}^d)$ where h_n denotes the Hermite polynomial and the family $\{\eta_j\}_{j=1}^\infty \subset \mathcal{S}(\mathbb{R}^d)$ is an orthonormal basis for $L^2(\mathbb{R}^d)$. For this control problem we will set up a variational framework and prove the existence and uniqueness of an optimal solution. We will derive an optimality system of equations that the optimal solutions must satisfy. The orthogonality of $\mathcal{H}_\alpha$ enable us to reduce SPDEs like (1–3) to a system of uncoupled deterministic equations for the coefficients $u_\alpha(x)$. Standard deterministic numerical methods can be applied to solve it sufficiently accurately. The main statistics, such as mean, covariance and higher order statistical moments can be calculated by simple formulas involving only these deterministic coefficients. Moreover, in the procedure described above, there is no randomness directly involved in the simulations. One does not have to deal with the selection of random number generators, and there is no need to solve the SPDE equations realization by realization. Instead, uncoupled coefficient equations are solved once and for all. Moreover, one can reconstruct particular realizations of the solution directly from Wiener chaos expansions once the coefficients are available, see [1,2,3].

[1] H. Manouzi, T. Theting "Mixed Finite Element Approximation for the Stochastic Pressure Equation of Wick Type ", *IMA Journal of Numerical Analysis*, Vol. 24, pp. 587–604, (2004).

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CT53
Optimal shape design subject to variational inequalities

The shape and topological sensitivity analysis is performed for the obstacle problem using a penalization of the primal dual formulation. The shape derivative for the penalized problem can be defined and converges to an element of the subdifferential of the shape derivative for obstacle problem. The topological derivative for the obstacle problem can also be defined. These results are applied to the electomechanical machining problem, where we want to control the shape of the free boundary of the obstacle problem by the shape of the domain.

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CT53
Optimal Control of Complementarity Problems

In this talk we consider mathematical programs with complementarity constraints (MPCCs) in function space. Typical model problems are related to optimal control of variational inequalities (VIs) or parameter identification in VIs. Here we propose a relaxed Moreau-Yosida based path-following concept for both, the development of a first order optimality characterization as well as the design of a solution algorithm. Our first order conditions are close to strong stationarity in finite dimensions. The proposed algorithm uses a semismooth Newton method (with a locally superlinear convergence in function space) for solving the relaxed path-problems. The talk ends by a report on numerical tests.

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CT53
Multigrid Methods for Distributed Elliptic Optimal Control Problems

Multigrid schemes that solve distributed elliptic optimal control problems discretized by finite differences are presented. For the solution of these systems, a comparison is made between the MG/OPT method and the collective smoothing multigrid (CSMG) method. The resulting multigrid algorithms show that the convergence factors are mesh independent. Moreover, the convergence of the CSMG method does not deteriorate as the weight of the cost of the control tends to be sufficiently small. Examples are given to illustrate and validate both techniques.

[1] A. Borzì and K. Kunisch, "A Multigrid Scheme for Elliptic Constrained Optimal Control Problems", *Comp. Optim. Appl.*, Vol. 31, pp. 309–333, (2005).

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CT54
A third order method for Convection Diffusion Equations with Delay

The initial value problem

$$\begin{aligned} \frac{d}{dt}u - \varepsilon\nabla^2 u + k\cdot\nabla u &= f + \int_0^t K(s-t_1)u\,ds \quad \text{in } \Omega, \\ u &= \hat{u} \quad \text{on } \partial\Omega, \\ u &= u_0 \quad \text{in } \Omega, \text{for } t=0 \end{aligned}$$

and the prehistory problem

$$\begin{aligned} \frac{d}{dt}u - \varepsilon\nabla^2 u + k\cdot\nabla u &= f + \int_{t-d}^t K(s-t_1)u\,ds \quad \text{in } \Omega, \\ u &= \hat{u} \quad \text{on } \partial\Omega, \\ u &= u_{history} \quad \text{in } \Omega, \text{for } t\in[-d,0] \end{aligned}$$

will be discussed. K is a $C^1(\mathbb{R}\to\mathbb{R})$ function called kernel, $\varepsilon > 0$ is the diffusion coefficient and k the convection coefficient. Such equations appear for example in different contexts of heat conduction in materials with memory, viscoelasticity and population models (see e.g. [4] or [1] chapter 1). One problem concerning delay or memory problems is the data storage. While generally a lot of slow harddisk memory is available, the faster RAM of a workstation is still quite limited. So the goal is to keep all data which is necessary for the computation of the delay term in the fast RAM of a workstation. Thus data reduction in space e.g. using a grid hierarchy will be discussed and furthermore a method of third order in time for both problems is presented and combined with adaptivity. For higher Péclet numbers the stabilisation of the galerkin method is performed using streamline diffusion. Numerical results for different Péclet numbers are presented as well.

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[3] H.-G.Roos, M. Stynes and L.Tobiska, "Numerical Methods for Singulary Perturbed Differential Equations", Springer (Berlin, 1996)

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CT54
Asymptotic behavior of solution of elliptic pseudodifferential equation near cone.

For solving model pseudodifferential equation

$$(Au)(x) = f(x), \qquad x \in C_+^a, \tag{1}$$

where A is elliptic pseudodifferential operator with symbol $A(\xi)$, $c_1 \leq |A(\xi)(1+|\xi|)^{-\alpha}| \leq c_2,\ \xi = (\xi_1, ..., \xi_m),\ C_+^a = \{x \in \mathbf{R}^m :\ |x'| > ax_m,\ x' = (x_1, ..., x_{m-1}),\ a > 0\}$, the author has introduced the concept of wave factorization for symbol of elliptic operator [2], and for vanishing index of wave factorization the solution of equation (1) was written with help of integral operator

$$(G_m u)(\xi) = \lim_{\tau \to 0+} \int\limits_{\mathbf{R}^m} \frac{u(\eta', \eta_m) d\eta}{(|\eta' - \xi'|^2 - a^2(\eta_m - \xi_m + i\tau)^2)^{m/2}}$$

by the formula

$$\tilde{u}(\xi) = (A_{\neq}^{-1} G_m A_{=}^{-1} \tilde{lf})(\xi),$$

which is belonging to Sobolev-Slobodetskii space $H^s(C_+^a)$ under assumptions $f \in H^{s-\alpha}(C_+^a)$ and f admits continuation $lf \in H^{s-\alpha}$ $(\mathbf{R}^m)$. This implies such solution is belonging to class C^∞ inside a cone. An asymptotical representation for solution near cone is obtained, and it corresponds to well-known solution's asymptotics obtained earlier [1].

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Conference Venue

The conference is held at two locations at the campus of the Karl-Franzens University Graz.

Conference office, lecture rooms HS 15.01, HS 15.02, HS 15.03, HS 15.12, LS 15.01:
RESOWI-Center, Parts B and C,
Universitätsstraße 15
(Access via Geidorfgürtel)
8010 Graz.

Institute of Mathematics, lecture rooms HS 11.01, HS 11.02:
Heinrichstraße 36
8010 Graz.

How to get there:
See the map of the university quarter or the arial view of the campus for the location of the converence venue on the campus of the university on the next page.
See `www.uni-graz.at/imawww/pages/visitorinfo.html` for a description of the route from the airport and from the train station to the university.
To contact the conference office use:
`enumath07@uni-graz.at`

Restaurants, Cafés, Diners, and Snack-Bars

There is a great variety of breakfast, lunch, and dinner places in the immediate vicinity of the University, especially in Heinrichstraße and Zinzendorfgasse. The largest Restaurants are (see map of the university quarter on the next page, numbers 1-4)

1. *Mensa* (University restaurant and cafeteria). Three course meal for 6 €, salat bar, self-service. Open only for lunch (11:00–14:30). Room for up to 200 persons.
2. *Resowi Cafeteria.* Similar to Mensa. Room for up to 180 persons.
3. *Cafeteria in Heinrichstrae 36.* Three course meals for 6–7 €. Room for about 40 persons.
4. *Bierbaron.* Two course meal for 7–8 €. Traditional Austrian cuisine. Room for up to 100 persons.

Hospital, Pharmacy, Emergency numbers

Pharmacies can be found in Glacisstraße and in Heinrichstraße. The University Hospital is located at the End of Elisabethstraße. (15 Minutes walk from the University, see map).

Emergency telefone numbers in Austria are
Police: 133
Ambulance / Paramedics: 144
Emergency doctor: 141.

IT Support

Each lecture room is equipped with

- Notebook (MS Windows XP, Adobe Acrobat Reader, MS Powerpoint),
- Beamer,
- Overhead slide projector,
- Chalkboard.

1/4 hour before and during the lecture sessions stewards will be present in the lecture rooms who can help with the technical equipment. Participants are encouraged to transfer electronic slides by memory stick to the conference notebooks preferably half an hour before the session starts. Private notebooks can also be used but it must be checked if the display works properly prior to the begin of the session.
Please do not use your notebook computer in the lecture rooms during the sessions for private work or to browse the internet!

Wireless Network Access: To gain access select the wireless network named `KFU-Tagung` from the list of available networks and connect to it. You can then browse secured and unsecured web sites on the internet. Every other type of connection is prohibited by the firewall. The network is open and does not require a password. Wireless access is only possible in the immediate vicinity of the conference venue.

Use of public terminals: At the conference venue and at several other places on the campus you can find computer terminals which are available for public use. Use
Benutzername (username): `07t000ri`
Kennwort (password): `enumath07`
for login. Internet and several standard applications are available on the terminals. Every terminal is equipped with a USB connection which can be used to store data on your own USB drive. Please do not try to store data at any other place and do not try to change the settings of the terminals. Please do not forget to logout after using the terminals.
For questions concerning technical support please contact
`fabian.tschiatschek@uni-graz.at`
`wolfgang.ring@uni-graz.at`.

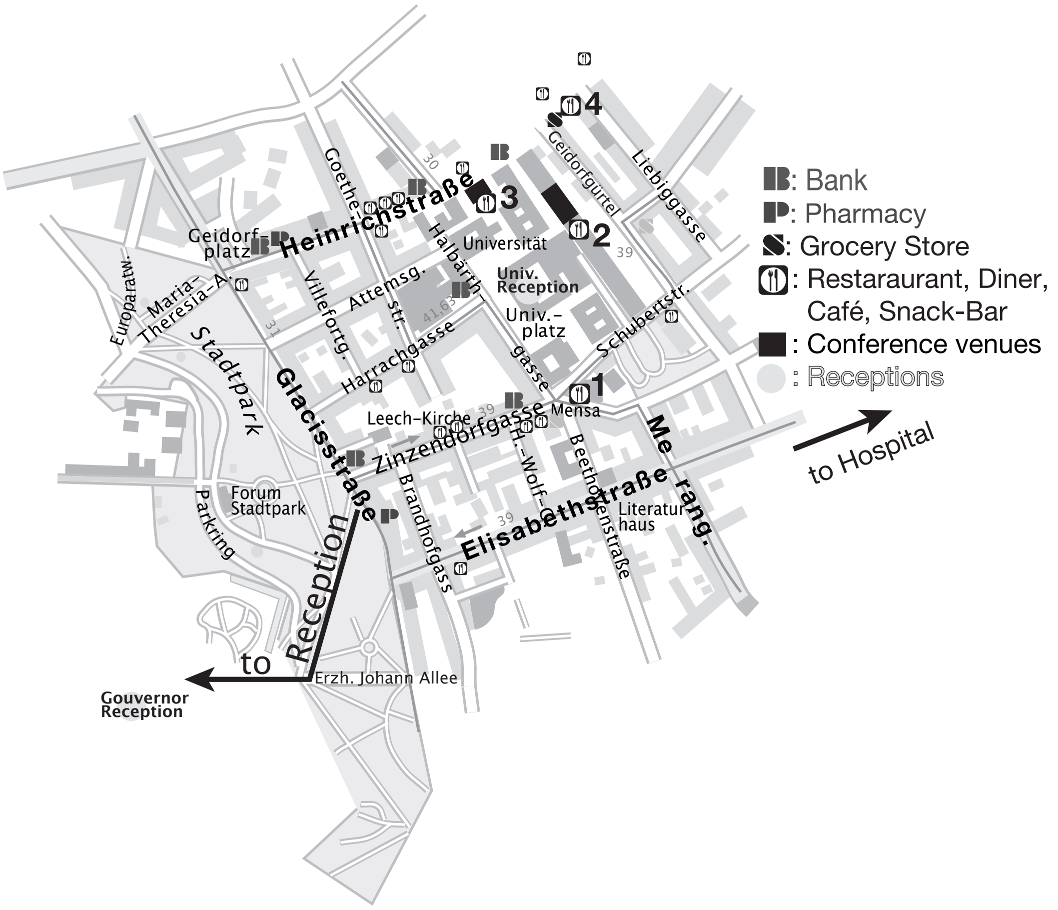


Figure 1: Map of the university quarter with conference venues and infrastructure.

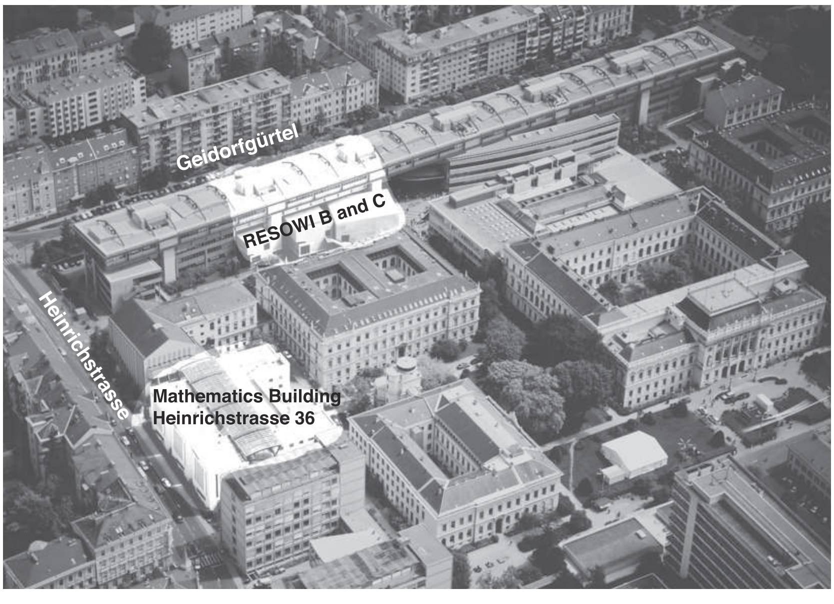
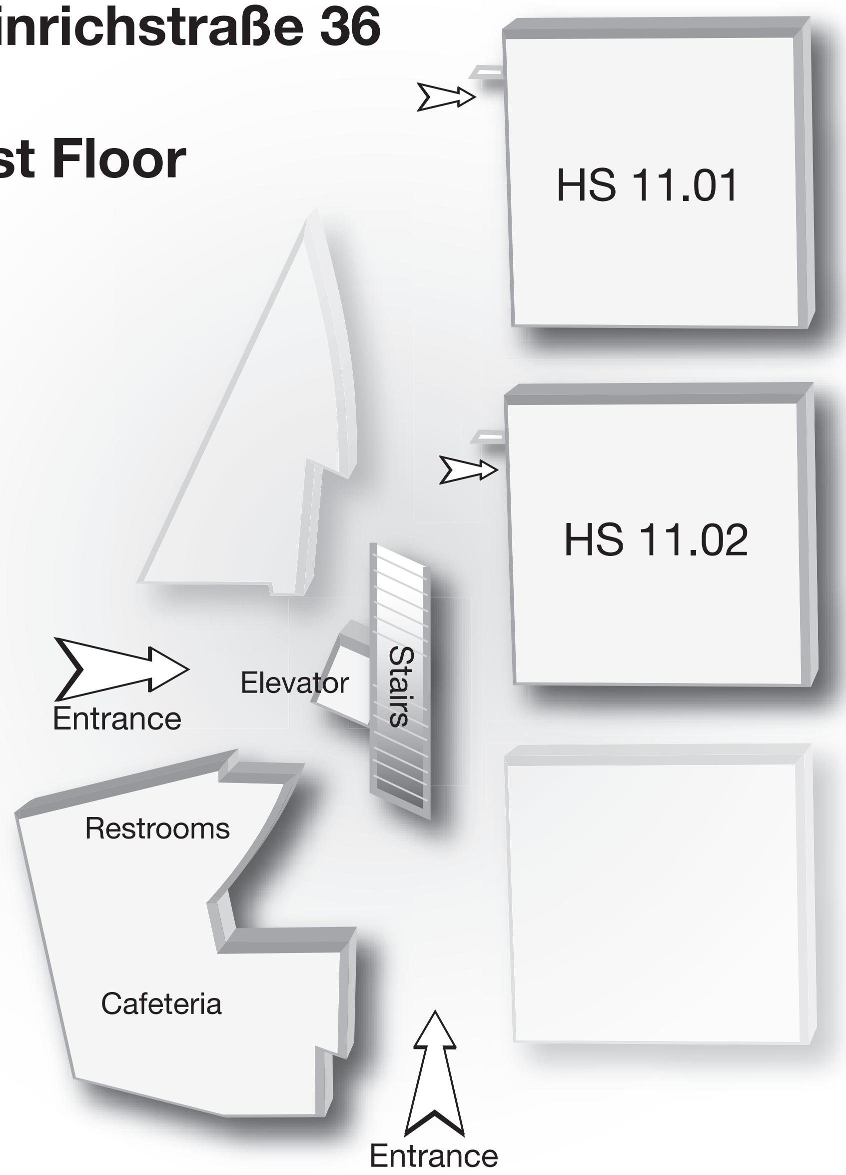


Figure 2: Arial view of the university campus.

Mathematics Building
Heinrichstraße 36

First Floor



RESOWI BUILDING

PARTS C and B
First and Second Levels