Universität Trier

First Indo-German Conference on

PDE, Scientific Computing and Optimization in Applications

September 8-10, 2004

Conference Program

First Indo-German Conference on PDE, Scientific Computing and Optimization in Applications

University of Trier, D–54286 Trier, Germany
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E–Mail: trapp@uni–trier.de
WWW: http://mathematik.uni–trier.de/indogerman04

Supported by

- ◇ The Deutsche Forschungsgemeinschaft (DFG)
- ◇ The Indian National Science Academy (INSA)
- ◇ Freundeskreis der Universität Trier

Proceedings:

There will be a special issue of the Journal of Computational and Applied Mathematics, for details see

http://www.mathematik.uni-trier.de/indogerman04/Proc.html

Invited Speakers

H. G. Bock, Heidelberg, Germany
M. Brokate, Munich, Germany
P. Dutt, Kanpur, India
O. Ghattas, Pittsburgh, USA
G. D. V. Gowda, Bangalore, India
R. Hoppe, Augsburg, Germany
M. Kirkilionis, Warwick, UK
N. Kroll, Braunschweig, Germany
V. Kumaran, Bangalore, India
M. Steinbach, Berlin, Germany

Organizing Committee

A. Adimurthi (Coordinator), Bangalore, India
H. G. Bock, Heidelberg, Germany
S. K. Dube, Kharagpur, India
S. M. Deshpandey, Bangalore, India
S. B. Hazra, Trier, Germany
R. Helmig, Stuttgart, Germany
G. Jayaraman, Delhi, India
H. Neunzert, Kaiserslautern, Germany
R. Ravindran, Bangalore, India
A. R. Roy, Kharagpur, India
E. W. Sachs, Trier, Germany
V. Schulz (Coordinator), Trier, Germany
V. D. Sharma, Mumbai, India
J. Sprekels, Berlin, Germany
R. Tichatschke, Trier, Germany

Local Organizers

S. B. Hazra, E. Hübner, F. Leibfritz, J. Maruhn, M. Ries, E. Sachs, M. Thieme-Trapp, R. Tichatschke, T. Voetmann

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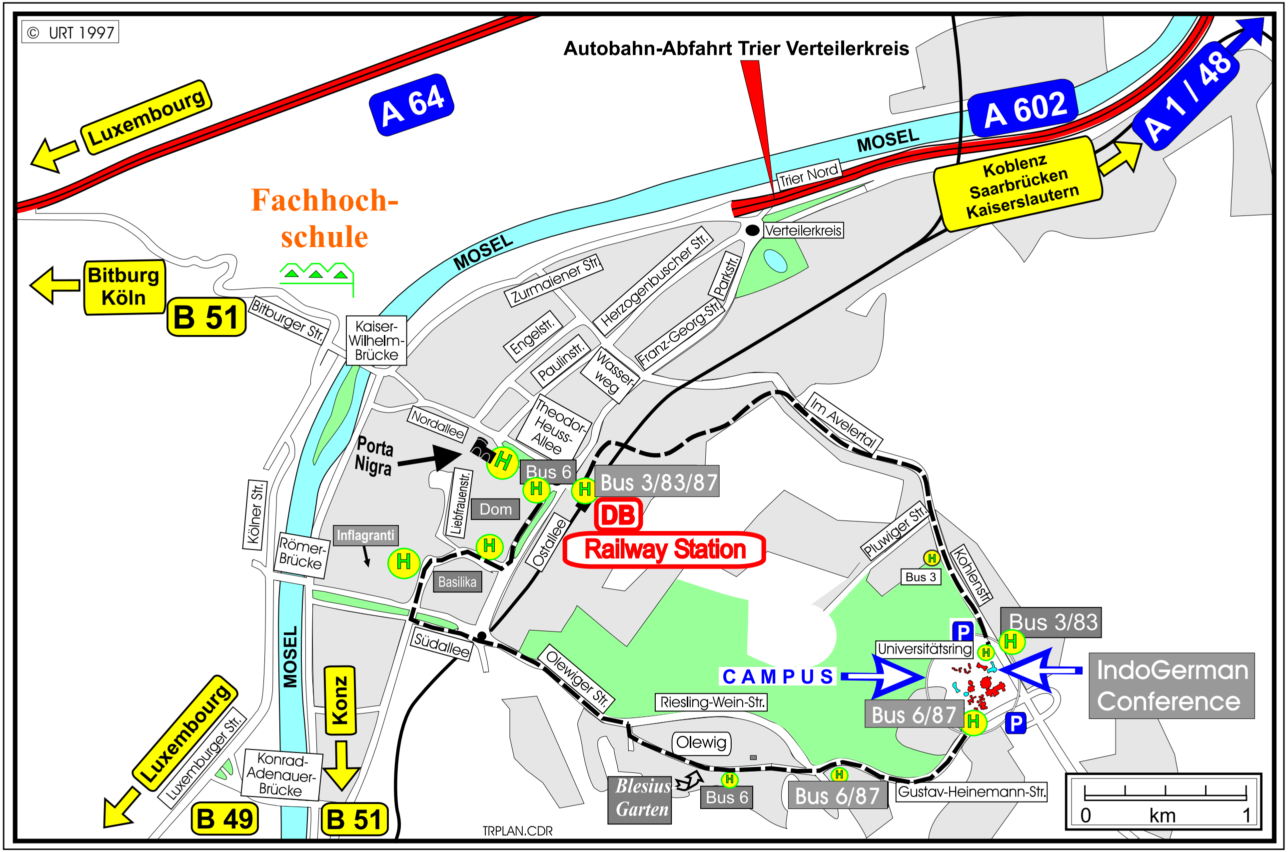
General Information

• Location:	University of Trier Department of Mathematics Building E Kohlenstraße 54286 Trier (follow the signs)
• Congress Office:	E 44
• Registration: (Congress Office)	Tuesday, September 7, 17:00 – 19:00 Wednesday, September 8, 08:00 – 16:00
• Lecture Room:	HS 10
• e-Mail Rooms:	E 02 / E 09 (Windows/Linux/Macintosh) Username and password are included in your welcome package
• Refreshments:	E 51

Travel information:

- **http://www.mathematik.uni-trier.de/abteilung/anreise.html.en**
- http://www.uni-trier.de/trier/trier-e.html
- http://www.mathematik.uni-trier.de/indogerman04
- http://www.trier.de/cityguide/

Please also refer to the maps on the following pages.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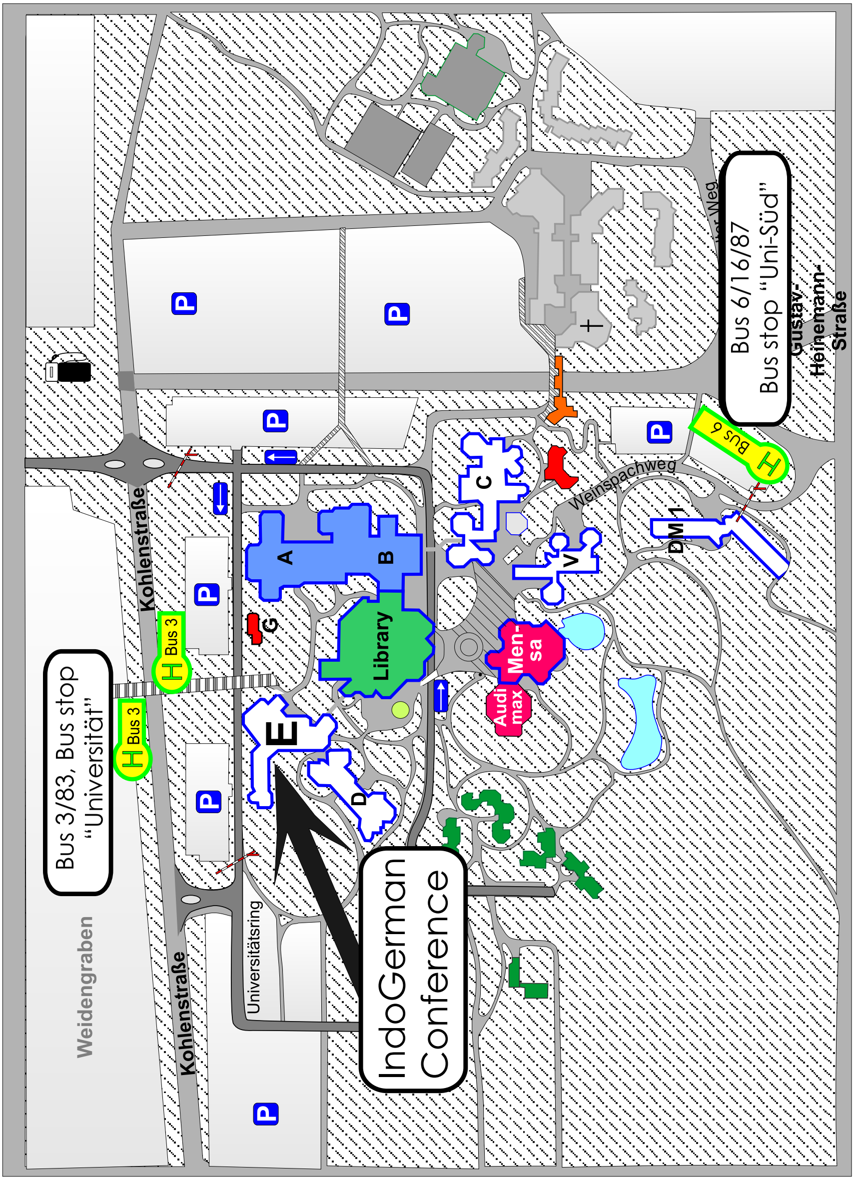
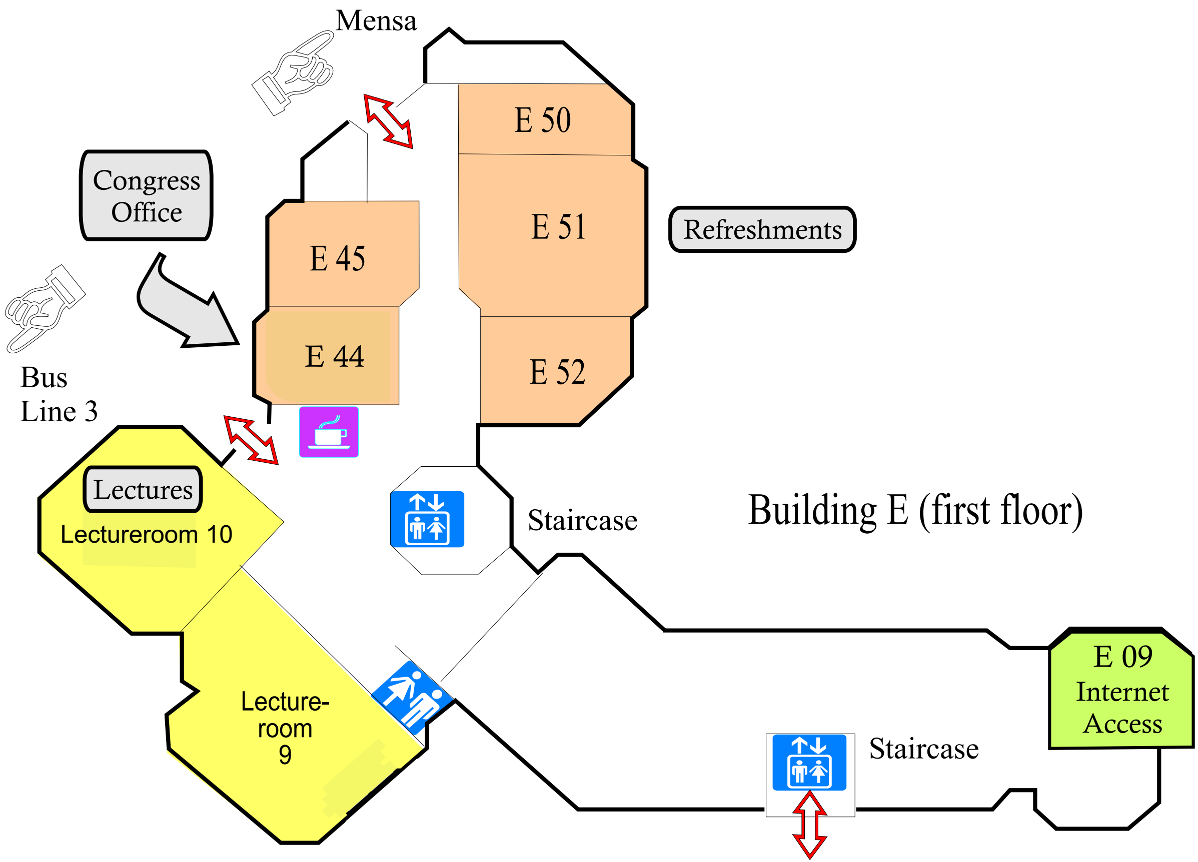


University Campus

First Floor of Conference Building E



Scientific Program

Wednesday, September 8, 2004

08:45 – 09:00 :	*Jäckel, M.* (Vice President, University of Trier): Opening

Morning Session 1. Chair: V. Schulz

09:00 – 09:45 : (IP)	*Dutt, P.:* Spectral Element Methods for Parabolic Problems on Parallel Computers
09:45 – 10:30 : (IP)	*Bock, G.:* Constrained Open-loop, Closed-loop Control and Real-time Optimization of Systems Governed by Large DE Models
10:30 – 11:00 :	**– Coffee Break –**

Morning Session 2. Chair: N. Kroll

11:00 – 11:25 :	*Voigt, A.:* BaF_2 for Microlithography Applications: Modeling, Simulation and Optimization of the Growth Process
11:25 – 11:50 :	*Dandapat, B. S.:* Free Surface Flow of a Liquid Film Over a Curved Rotating Disk
11:50 – 12:15 :	*Kashid, M.:* Computational Modelling of Slug Flow in a Capillary Millireactor
12:15 – 13:45 :	**– Lunch (Mensa) –**

Afternoon Session 1. Chair: P. Dutt

13:45 – 14:30 : (IP)	*Kirkilionis, M.:* The Mathematics of Cellular Behavior
14:30 – 14:55 :	*Dalal, D. C.:* Numerical Study of Unsteady Flow Through Arterial Stenosis
14:55 – 15:20 :	*Murthy A. S. V.:* Asymptotic and Numerical Analysis of a Simple Model for the Ramdas Layer

15:20 – 15:45 :	**– Coffee Break –**

Afternoon Session 2. Chair: M. Kirkilionis

15:45 – 16:10 : *Tsybulin, V.:* Conservation of Cosymmetry in PDE Discretization

16:10 – 16:35 : *Ainouz, A.:* Derivation of A Double-diffusion Model in Poro-elastic Media

16:35 – 17:00 : *Zahri, M.:* Wick-Stochastic Finite Element Solution of Reaction-Diffusion Problems

17:00 – 17:25 : *Maruhn, J.:* Cost-Optimal Static Super-Replication: Concept and Applications

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Optional Social Program:

18:30 – 21:30 : *Landesgartenschau 2004* (State Garden Show)
http://www.landesgartenschau–trier.de
Walk through the recreational area and/or listen to a Jazz concert of the Blue Drive band (18.30–20.00)
Entry fee: 5 € after 17:00

Thursday, September 9, 2004

Morning Session 1. Chair: A. Adimurthi

09:00 – 09:45 : (IP) *Kroll, N.:* Flow Simulation and Shape Optimization for Aircraft Design

09:45 – 10:30 : (IP) *Kumaran, V.:* Stability of Fluid Flow in Tubes and Channels with Flexible Walls

10:30 – 11:00 : **– Coffee Break –**

Morning Session 2. Chair: G. D. V. Gowda

11:00 – 11:25 : *Sawyer, W.:* A Scalable Implementation of the Finite-Volume Dynamical Core in the Community Atmospheric Model

11:25 – 11:50 : *Singh, A. K.:* An ODE Traffic Network Model

11:50 – 12:15 : *Adimurthi, A.:* Hamilton Jacobi Equations with Discontinuous Hamiltonian

12:15 – 13:30 : **– Lunch (Mensa) –**

13:30 – 13:45 : *Sarkar, D.* (Counselor for Science and Technology, Embassy of India, Berlin): Information about Indo-German cooperations, joint projects, possibilities

Afternoon Session 1. Chair: R. Tichatschke

13:45 – 14:30 : (IP) *Gowda, V.:* Conservation Laws with a Flux Function Discontinuous in Space

14:30 – 15:15 : (IP) *Steinbach, M.:* On PDE Solution in Gas Networks

15:15 – 15:45 : **– Coffee Break –**

Afternoon Session 2. Chair: M. Steinbach

15:45 – 16:10 : *Gauger, N.:* Efficient Aerodynamic Shape Optimization in MDO Context

16:10 – 16:35 : *Seaid, M.:* Multigrid Newton-Krylov Method for Radiation-Conduction in Semitransparent Media

16:35 – 17:00 : *Deka, B.:* Convergence of Finite Element Method for Second Order Elliptic Interface Problems

17:00 – 17:25 : *Voetmann, T.:* Weak Regularization for Signorini Problems with Friction

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18:30 – 20:00 : City Tour: Meeting point at the tourist information in front of Porta Nigra

20:00 – 22:00 : Conference Dinner: *Inflagranti*, Viehmarktplatz 13
Located at the Viehmarktplatz, meeting point in front of restaurant Inflagranti

Friday, September 10, 2004

Morning Session 1. Chair: H. G. Bock

09:00 – 09:45 : (IP)	*Ghattas, O.:* Eulerian Methods for Shape Optimization
09:45 – 10:30 : (IP)	*Hoppe, R.:* Interior-Point Methods in Shape Optimization
10:30 – 11:00 :	**– Coffee Break –**

Morning Session 2. Chair: E. W. Sachs

11:00 – 11:25 :	*Stadler, G.:* Semi-smooth Newton Methods for Contact Problems with Friction in Linear Elasticity
11:25 – 11:50 :	*Roy, A. R.:* A Fuzzy Soft Set Theoretic Approach to Decision Making Problems
11:50 – 12:15 :	*Kuhnert, J.:* Finite Pointset Method (FPM) for Two-phase and Low Mach Number Flows
12:15 – 13:45 :	**– Lunch (Mensa) –**

Afternoon Session 1. Chair: O. Ghattas

13:45 – 14:30 : (IP)	*Brokate, M.:* To Be Announced
14:30 – 14:55 :	*Wan, D.:* Efficient Multigrid-FEM Method for Simulation of Liquid-Solid Flows with Large Number of Moving Particles
14:55 – 15:20 :	*Sarma, M.:* Solving Non-linear ODE and PDE via Feed-forward Neural Networks
15:20 – 15:45 :	**– Coffee Break –**

Afternoon Session 2. Chair: R. Hoppe

15:45 – 16:10 : *Parsaei, M.:* Interaction of the Numerical Solution of Hyperbolic Equations with an Obstacle in the Flow Direction

16:10 – 16:35 : *Arora, R.:* Similarity Analysis and Evolution of Weak Discontinuities in a Van der Waals Gas

16:35 – 17:00 : *Danumjaya, P.:* Mixed Discontinuous Galerkin Finite Element Methods for the Extended Fisher-Kolmogorov (EFK) Equation

17:00 – 17:25 : *Hazra, S. B.:* Computation of Dilute Two-phase Flow in a Pump

Abstracts

Hamilton Jacobi Equations with Discontinuous Hamiltonian

Aditi Adimurthi **Thu 11:50**

TIFR Center, Bangalore, India, eMail: aditi@math.tifrbng.res.in

We prove the existence and uniqueness of a viscosity solution of Hamilton Jacobi equations in one space variable with Hamiltonian having discontinuity at x=0. Uniqueness is proved in a class of functions satisfying an interphase entropy conditon.

Derivation of a Double-diffusion Model in Poro-elastic Media

Abdelhamid Ainouz **Wed 16:10**

University Of Sciences and Technology, Algiers, Algeria, eMail: a.ainouz@wissal.dz

In this paper a Barenblatt-Biot consolidation model for flow in porous media is derived by means of the two-scale homogenization techniques. Starting with the time-dependent fluid flow in a two-component poroelastic medium separated by a thin periodic barrier and described by combining mass conservation equation with the Darcyś law, while for the displacement of the structure we use the general framework linear elasticity with the momentum balance equations and therefore this quasi-static assumption is the essence of the model for a consolidation problem. We assume that the period is too small compared with the size of the medium, with this in mind one is led to study the limiting behavior of the flow and the displacement in this porous elastic medium as the period tends to zero.

Similarity Analysis and Evolution of Weak Discontinuities in a Van der Waals Gas

Rajan Arora **Fri 16:10**

IIT Bombay, India, eMail: rajan@math.iitb.ac.in

The basic equations, governing the unsteady one-dimensional axisymmetric motion in a Van der Waals gas, are considered. Using the invariance group properties of the original system, the new autonomous system is found. The propagation of weak discontinuities is considered in the known particular solution of the autonomous system. The critical time, when these weak discontinuities culminate into a shock, is also determined for an ideal gas.

Constrained Open-loop, Closed-loop Control and Real-time Optimization of Systems Governed by Large DE models

GEORG BOCK **Wed 09:45**

IWR, Universität Heidelberg, Germany, eMail: bock@iwr.uni-heidelberg.de

The paper reports on recent progress in the real-time computation of constrained closed-loop optimal control, in particular the special case of nonlinear model predictive control, of large DAE systems arising e.g. from semi-discretization of instationary PDE. Through a combination of, a. o., a direct multiple shooting approach, a constrained Gauss-Newton method and an operation point embedding, a so-called "real-time iteration" approach has been developed in the last few years. One of the basic features is that in each iteration of the optimization process, new process data are being used. Through precomputation - as far as possible - of Hessian gradients and QP factorizations the response time to perturbations of states and systems parameters is minimized. In real experiments for a distillation column the new approach has been shown to be orders of magnitude faster than previous approaches based on application of off-line optimization methods. For the special class of NMPC problems to guarantee globally stable closed-loop controls, also the new approximate scheme is shown to be nominally stable. It is also shown how the approach can be further drastically accelerated by special algorithmic schemes for on-line feasibility and optimality improvement. In addition we report on strategies to reduce the computational effort for MoL approaches, and simultaneous state/parameter estimation and closed-loop NMPC control.
The paper is based on joint work of the Heidelberg optimization group (M. Diehl, E. Kostina, A. Schaefer, and J. P. Schloeder) and the Stuttgart process control group (F. Allgoewer, R. Findeisen).

To Be Announced

MARTIN BROKATE **Fri 13:45**

Universität München, Germany, eMail: brokate@ma.tum.de

Numerical Study of Unsteady Flow Through Arterial Stenosis

SWAPAN K. PANDIT, <u>DURGA C. DALAL</u> **Wed 14:30**

Indian Insitute of Technology Guwahati, India, eMail: durga@iitg.ernet.in

Velocity profile patterns corresponding to oscillatory, pulsatile and physiological pulsatile flow have been discussed using the incompressible Navier-Stokes equations in an abdominal aorta with a smooth isolated axisymmetric stenosis due to atheromatous plaque. Calculations are based on the HOC (Higher Order Compact) method. Results are obtained for unsteady flow in a 75% severity stenosis. Our results show that the velocity profiles not only depend on the flow parameters such as Reynolds no. and frequency no. (or Stokes no.) but also highly depend on the flow wave form. The results are well agreed with the previous experimental results qualitatively.

Free Surface Flow of a Liquid Film over a Curved Rotating Disk

B. S. Dandapat **Wed 11:25**

Indian Statistical Institute, Calcutta, India, eMail: `dandapat@isical.ac.in`

Transient profile of a non-planar thin liquid film on a non-planar rotating disk is studied. To study the effects of disk profile and the inertia of the liquid, nonlinear N-S equations describing the flow of a thin liquid film over non-planar disk along with the corresponding non-linear boundary conditions are solved by matched asymptotic expansion method to obtain the evolution equation for film height. This nonlinear evolution equation is solved by using the method of characteristics, and finally obtain the variation of film thickness at different time level with radial coordinate r numerically. It is shown that the profile of the liquid film eventually becomes similar to the shape of the rotating disk. Further it is shown that the non-uniformity of the disk gives the same rate of film thinning as the planar one. The present study has applications in microelectronics industry for coating the substrates with ultra thin film.

Mixed Discontinuous Galerkin Finite Element Methods for the Extended Fisher-Kolmogorov (EFK) equation

Palla Danumjaya **Fri 16:35**

IIT Bombay, Mumbai, India, eMail: `danu@math.iitb.ac.in`

We consider the following initial and boundary value problem. For $\gamma > 0$

$$u_t + \gamma\Delta^2 u - \Delta u + f(u) = 0,\ (x,t) \in \Omega \times (0,T] \tag{1}$$

with initial condition

$$u(0) = u_0,\ x \in \Omega, \tag{2}$$

and either of the boundary conditions

$$u = \Delta u = 0 \text{ on } \partial\Omega \times (0,T] \tag{3}$$

or

$$u = \frac{\partial u}{\partial \nu} = 0 \text{ on } \partial\Omega \times (0,T], \tag{4}$$

where ν is an outward normal, $f(u) = u^3 - u$ and $0 < T < \infty$. The different conforming finite element techniques which are used to approximate the solution of (1)–(3) or (4)

needs C^1-interelement continuity condition. In this paper, we relax continuity condition and discuss the discontinuous Galerkin mixed finite element method for the problems (P_1) and (P_2). We now split the equation (1) by setting $-\Delta u = v$, and using the boundary conditions (3) as

$$\left.\begin{array}{rcl} u_t - \gamma\Delta v + v + f(u) &=& 0,\ (x,t) \in \Omega \times (0,T], \\ -\Delta u &=& v, \\ u(0) &=& u_0,\ x \in \Omega, \\ u &=& 0, v = 0,\ (x,t) \in \partial\Omega \times (0,T]. \end{array}\right\} \qquad (P_1)$$

Using the other boundary conditions (4), we rewrite (1)–(2) and (4) as

$$\left.\begin{array}{rcl} u_t - \gamma\Delta v + v + f(u) &=& 0,\ (x,t) \in \Omega \times (0,T], \\ -\Delta u &=& v, \\ u(0) &=& u_0,\ x \in \Omega, \\ u &=& 0, \frac{\partial u}{\partial \nu} = 0,\ (x,t) \in \partial\Omega \times (0,T]. \end{array}\right\} \qquad (P_2)$$

In this paper, we have discussed the discontinuous Galerkin finite element method and derived *a priori* bounds using Lyapunov functional. Moreover, we have established *a priori* error estimates for the semidiscrete case.

Convergence of Finite Element Method for Second Order Elliptic Interface Problems

Bhupen Deka **Thu 16:35**

Indian Institute of Technology, Guwahati, India, eMail: bdeka@iitg.ernet.in

The purpose of this paper is to study the convergence of finite element approximation to the exact solution of a general elliptic interface problem. A general self-adjoint second order elliptic partial differential operator with discontinuous coefficients is considered. Optimal order error estimates in L^2 and H^1 norms are shown to hold when the global regularity of the solution is low and the interface is of arbitrary shape but is smooth. Further, the effect of numerical quadrature on finite element solution is also analyzed and the related optimal order estimates are derived.

Spectral Element Methods for Parabolic Problems on Parallel Computers

Pravir Dutt, P. Biswas, S. Ghorai **Wed 09:00**

Indian Institute of Technology, Kanpur, India, eMail: pravir@iitk.ac.in

We describe a spectral element method for solving parabolic initial boundary value problems on smooth domains using parallel computers. We divide the space domain into a number of shape regular triangles and quadilaterals of size h. We choose the time

step k proportional to h^2. At each time step we minimize a functional which is the sum of the squares of the residuals in the partial differential equation, initial conditions and boundary conditions in different Sobolev norms and a term which measures the jump in the function and its derivatives across inter-element boundaries in certain Sobolev norms. We can define a preconditioner for the minimization problem which allows the problem to decouple. We obtain error estimates for both the h and p version of this method.

Efficient Aerodynamic Shape Optimization in MDO Context

Nicolas R. Gauger **Thu 15:45**

German Aerospace Center (DLR), Germany, eMail: `nicolas.gauger@dlr.de`

The aerospace industry is increasingly relying on advanced numerical flow simulation tools in the early aircraft design phase. Today's flow solvers, which are based on the solution of the Euler and Navier-Stokes equations, are able to predict aerodynamic behaviour of aircraft components under different flow conditions quite well. Within the next few years numerical shape optimization will play a strategic role for future aircraft design. It offers the possibility of designing or improving aircraft components with respect to a pre-specified figure of merit, subject to geometrical and physical constraints. Consequently, extensive research effort has recently been devoted to the development of efficient optimization strategies for industrial aerodynamic aircraft design. Adjoint flow solvers are one of the components required in order to establish an efficient numerical optimization capability. The development of adjoint flow solvers and their application in multi-disciplinary optimization (MDO) context are presented.

Eulerian Methods for Shape Optimization

Volkan Akcelik, Alexandre Cunha, Omar Ghattas, George Biros **Fri 09:00**

Carnegie Mellon University, Pittsburgh, USA, eMail: `oghattas@cs.cmu.edu`

Our goal is to develop and apply scalable parallel algorithms for shape optimization of systems governed by partial differential equations. Target applications include design of artificial heart devices (for which the PDEs represent incompressible non-Newtonian flow) and design of linear accelerator cavities (electromagnetic eigenvalue problem).
Shape optimization problems present major challenges beyond those already encountered in fixed-geometry optimization problems. These include difficulties in maintaining a differentiable shape representation, in determining derivatives of response quantities with respect to the shape representation, and in maintaining a mesh that smoothly resolves the changing geometry. All of these are particularly challenging in 3D and on parallel computers. The geometry modeling and meshing complexities of the Lagrangian approach have lead us to pursue an Eulerian formulation, which solves the

shape optimization problem with respect to a fixed spatial description. This greatly facilitates parallel implementation.
Our approach integrates several contemporary ideas from scientific computing. From level set methods we borrow the idea of implicit shape representation by the zero isocontour of a level set function. But unlike level set methods, we avoid solving the Hamilton-Jacobi equation that evolves the level set function in "time" (which amounts to a steepest descent optimization method), in favor of direct Newton-Krylov solution of the nonlinear PDEs representing first-order optimality with respect to state, adjoint, and level set variables. Because there exist an infinite number of level set functions for a given shape, the optimization problem is ill-posed, and we must therefore employ a regularization functional to render the solution unique. As in phasefield methods, we use a characteristic function to denote interior and exterior regions. But because the exterior region is represented by boundary conditions, we appeal to distributed Lagrange multiplier variants of fictitious domain methods to incorporate the effect of these conditions.
Several shape optimization model problems, including ones in which the topology of the optimal shape differs from that of the initial, are solved on regular grids to demonstrate the method. Examples include segmentation of medical images and shape optimization of viscous incompressible flows. Numerical solution is effected through Galerkin finite element approximation of weak statements of the infinite dimensional Newton step. The implementation is done via Sundance, a C++ finite element toolkit for solution of variational problems developed by Kevin Long at Sandia. The blending of ideas from level set/phasefield surface representation, fictitious domain enforcement of boundary conditions, and full-space Newton-Krylov optimization solvers leads to a purely Eulerian method that avoid dynamic mesh (re)generation and shape (re)parameterization. The tradeoff is that the convergence rate of the numerical approximation is suboptimal, but we believe this is a small price to pay for avoiding the significant geometry and parallelism difficulties of Lagrangian methods.

Conservation Laws with a Flux Function Discontinuous in Space

G. D. Veerappa Gowda **Thu 13:45**

TIFR Centre, Bangalore, India, eMail: sidmisra@math.iisc.ernet.in

We study scalar conservation law:

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(k(x), u) = 0 \text{ for } x \in I\!R,\ t > 0 \\ u(x,0) = u_0(x),\ x \in I\!R \end{cases} \tag{1}$$

where the function $k(x)$ is discontinuous. This type of problem appears for example in modelling of two phase flow in porous media, in sedimentation problem and in traffic flow. Corresponding Hamilton-Jacobi equation appears in Shape from Shading. Because of the discontinuity of the flux in space, the Kruzkov method does not guarantee existence of a weak solution and even if the solution exists, it may not be unique. Here we propose a Godunov type numerical method for which we prove the convergence.

At the interface we introduce interface entropy condition and very simple formula is given for the interface flux. A numerical comparison between our method and the upstream mobility flux is given for two phase flow in porous media. A consequence of the convergence theorem is an existence theorem for the solution of the conservation law 1. Furthermore this solution satisy Lax-Oleinik entropy condition across the discontinuities of $k(x)$. This ensures the uniqueness of the limit solution.

Computation of Dilute Two-Phase Flow in a Pump

S. B. Hazra, Konrad Steiner **Fri 17:00**

Fraunhofer Institut für Techno- und Wirtschaftsmathematik, Germany, eMail: steiner@itwm.fhg.de

Present work is concerned with computation of dilute two-phase flow through a pump in turbulent condition. The flow field for the continuous phase is computed using the Reynolds averaged Navier-Stokes equations together with mixing length turbulence modeling. The dispersed phase is treated using the Lagrangian approach by tracking it's trajectory along which the information is passed. It is found that the bubbles and small solid particles flow out of the chamber (between the rotating impeller and the casing wall) with the conveying fluid. The solid particles of relatively bigger sizes accumulate at the low pressure zones near the cashing wall or the rotating shaft.

Interior Point Methods in Shape Optimization

Roland H. W. Hoppe, C. Linsenmann, Svetozara Petrova **Fri 09:45**

University of Augsburg, Germany, eMail: hoppe@math.uni-augsburg.de

For the numerical solution of shape optimization problems in continuum mechanics we consider an “all-at-once” approach featuring the numerical solution of the state equations as an integral part of the optimization routine. In particular, we rely on primal-dual Newton interior-point methods with special emphasis on both the efficient iterative solution of the primal-dual Hessian system and convergence monitoring by means of a hierarchy of merit functions.
Applications include the structural optimization of microcellular biomorphic ceramics in biomimetics by homogenization modeling and the optimization of the inflow and outflow of electrorheological shock absorbers based on an extended Bingham-type fluid model.

Computational Modelling of Slug Flow in a Capillary Millireactor

Madhvanand Kashid **Wed 11:50**

University of Dortmund, Germany, eMail: kashid@math.uni-dortmund.de

Liquid-liquid slug flow capillary millireactor has been suggested to carry out mass transfer limited and strongly exothermic reactions. The benefits include the ability to adjust the individual transport mechanisms i.e. convection inside the slug and diffusion between two slugs. The mass transfer rate is enhanced by internal circulation which arises due to the shear between slug axis and continuous phase or capillary wall. State-of-the-art assumes that there is no significance of the presence of film on the internal circulations within the slugs. During these studies, it had been assumed that there was no distortion in slug geometry at same average flow velocity and no significant shear stress between two fluids. The computational fluid dynamics (CFD) simulations were carried out considering each slug as single phase domain and solved for decoupled individual slugs. These circulation patterns were visualised with the help of virtual particle tracing methods in post processing.

More detailed studies on liquid-liquid slug flow revealed that more viscous slug exerts a considerable shear on the film. As a result, it moves with a slightly higher rate than the less viscous fluid and thereby yields an asymmetric geometry of the slug at the same average liquid flow velocity. To examine this phenomenon, we are developing a two-phase CFD methodology. Volume of Fluid (VOF) and levelset are two of the best possible interface reconstruction methods. As a first approach, VOF methodology is considered because it is relatively simple and naturally conservative. The flow of each fluid is governed by the incompressible Navier Stokes equations. It was assumed that there is no interphase mass transfer between the fluids. The equations are discretized with a Finite Element method and realised in the CFD package FEATFLOW. The interfacial force (surface tension) is also implemented in these equations. In order to simplify the problem a single slug was considered rather than the train of slugs.

The obtained results give qualitative information about the slug flow behaviour at different operating conditions. Future work will address the mass transfer between the two fluids. The aim is to obtain a fundamental understanding of the hydrodynamics and mass-transfer mechanisms to design an appropriate reactor concept exhibiting best possible conversion and selectivity for a given liquid-liquid reaction.

The Mathematics of Cellular Behaviour

Markus Kirkilionis **Wed 13:45**

University of Warwick, United Kingdom, eMail: mak@maths.warwick.ac.uk

The talk will give an overview to model aspects of cellular behaviour. Cells have an immense complexity, and even intracelluar regulation of problems like protein transport, signalling and sorting have only just started to be understood. Many problems in biotechnology, medicine and developmental biology have even to deal with cellular

interactions and differentiation. We will present some models of cellular transport and cell growth in fermenters and tissues. The mathematics to describe these phenomena ranges from Dynamical Systems defined on Networks, Partial Differential Equations to Integral Equations. There are both interesting challenges with respect to Mathematical Analysis as well for Numerical Methods which we will explore during the talk.

Flow Simulation and Shape Optimization for Aircraft Design

Norbert Kroll **Thu 09:00**

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Aerospace industry is increasingly relying on advanced numerical flow simulation tools in the early aircraft design phase. Today's flow solvers based on the solution of the Euler and Navier-Stokes equations are able to predict aerodynamic behavior of aircraft components under different flow conditions quite well. Due to the high computational expense required for flow simulations around realistic 3D configurations, in industry computational fluid dynamics tools are rather used for analysis and assessment of given geometries than for shape design and optimization. However, within the next few years numerical shape optimization will play a strategic role for future aircraft design. It offers the possibility of designing or improving aircraft components with respect to a prespecified figure of merit subject to geometrical and physical constraints. Consequently, recently large research effort is devoted to develop efficient optimization strategies for industrial aerodynamic aircraft design.
Over the last years, the development of numerical flow simulation and shape optimization is one of the major issues of the Institute of Aerodynamics and Flow Technology at DLR. Under the leadership of DLR the national CFD project MEGAFLOW was initiated in Germany, which combines many of the CFD development activities from DLR, universities and aircraft industry. Its goal is the development and validation of a dependable and efficient numerical tool for the aerodynamic simulation of complete aircraft. The MEGAFLOW software system includes the block-structured Navier-Stokes code FLOWer and the unstructured Navier-Stokes code TAU. Due to advanced algorithms and physical models, a quality controlled software development process and a comprehensive validation effort, both flow solvers have reached a high level of maturity and reliability. The MEGAFLOW software is routinely used in German aeronautic industry and research organizations for a wide range of applications. It is constantly updated to meet the requirements of industrial implementations. Due to the use of common software, the process of transferring latest research and technology results into production codes has been considerably accelerated. Current focus of the German CFD network is devoted to improve the capability for numerical shape optimization (national project MEGADESIGN).
The presentation will highlight the major elements of the national flow solver software MEGAFLOW and will demonstrate its capability to predict viscous flows around complex industrial applications. Main emphasis will be devoted to recent developments and improvements concerning numerical shape optimization including parametrization issues, meshing aspects and adjoint based optimization strategies.

Finite Pointset Method (FPM) for Two-phase and Low Mach Number Flows

Jörg Kuhnert, Sudarshan Tiwari **Fri 11:50**

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Finite Pointset Method (FPM) is a particle method for solving fluid dynamic equations. It is a Lagrangian and mesh free method. In this method, the spatial derivatives at an arbitrary point are approximated from the clouds of neighboring points with the help of weighted least squares method. A flow domain is filled by finite number of particles. Each phase of the flow is separeted by assigning the different color of particles. On each phase, we assigned the different densities and viscosities and they remain constant during the simulation. We consider two-phase flow as one phase by taking the weighted average of the densities and the viscosities on the interface and in its surrounding. The flow is computed by the incompressible Navier-Stokes equations using Chorin's projection approach. Furthermore, the low Mach number flow is computed by using compressible Navier-Stokes equations with consideration of large sound speed in the equation of state. The compressible Navier-Stokes equations are also solved by Chorin's projection approach, where we get Helmoltz type of equation for pressure. In general, we derive the general second order partial differential equations and which are solved by the classical iteration method in the least squares framework. The solutions of the PDEs can be obtained accurately and has second order convergence. The interface boundary can be exactly detected and the normal and curvature on the interface can be effectively computed. We present the numerical results with the densities varrying between 1 to 1000 and the viscosities varrying between 1 to 100.

Stability of Fluid Flow in Tubes and Channels with Flexible Walls

V. Kumaran **Thu 09:45**

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The nature of the flow in a channel or a tube (laminar or turbulent flow) is of importance in chemical engineering applications, because the drag force and transport coefficients in turbulent flows are orders of magnitude higher than those in laminar flows. It is well known that the transition from a laminar to a turbulent flow in a rigid tube takes place at a Reynolds number of about 2100. This lecture will examine the nature of the transition in channels and tubes with flexible walls, such as those encountered in biological and biotechnological applications.

Our theoretical studies show that in a flexible tube or channel, there are at least four different types of instabilities which could result in a transition from a laminar to a more complicated flow profile. Two of these are in the low Reynolds number regime, while the other two are in the high Reynolds number regime. All of these are qualitatively different from the instability in rigid tubes and channels. Experimental confirmation of the low Reynolds number instability will also be presented. Some implications for the possibility of enhanced transport coefficients due to the destabilisation of the laminar flow in micro tubes and channels will be discussed.

Cost-Optimal Static Super-Replication: Concept and Applications

JAN MARUHN **Wed 17:00**

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Static hedging of barrier options has been studied intensively during the past years. Exact hedging results are usually based on unrealistic assumptions like the availability of an infinite number of standard options. If these assumptions are dropped, static hedges may perform very poor for some low probability events.
To avoid this, we analyze the well known concept of super-replication in the context of static hedging both theoretically and numerically from an optimization point of view. Afterwards the obtained results are applied to the case of hedging barrier options in a stochastic volatility market. Numerical results show, that we can identify very attractive static superhedges by combining the theoretical results of barrier option hedging from the last decade with the approach of cost-optimal static super-replication. In particular the computed static superhedge is only marginally more expensive than the barrier option itself.

Asymptotic and Numerical Analysis of a Simple Model for the Ramdas Layer

A. S. V. MURTHY **Wed 14:55**

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A partial integro-differential equation (PIDE) of parabolic type that was proposed in 1991 as a model for the nocturnal temperature distribution near the ground is simplified (by localizing and linearizing) to a simple linear singularly perturbed non-homogenous heat equation (SPHE). An approximate analytical solution (AAS) to the SPHE is obtained using the boundary function method. The AAS shows good agreement with the numerical solution of the PIDE thus providing insight into the formation of the Ramdas layer.

Interaction of the Numerical Solution of Hyperbolic Equations with an Obstacle in the Flow Direction

Manouchehr Parsaei **Fri 15:45**

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When solving the following two dimensional conservation laws

$$u_t + au_x + bu_y = 0$$

$$u(x, y, o) = u_0,\ t > 0$$

the analytical solution will be a traveling wave with the phase speeds (a) and (b) in the x and y directions and there will be no changes in the waves amplitudes as it moves. The numerical solution to this problem requires some non-physical boundaries which should be transparent to the waves if the outcome has to agree with the analytical solution (open boundaries). Although this is the case for a large group of wave lengths in the system, but usually the numerical approximations are dispersive and the wave speeds and the wave directions are dependents of the wave lengths, this means that some wave lengths can move freely in the system and will be reflected when blocked by the boundaries (walls), In this paper we examine these waves and find out what happens if half of their path is blocked by the walls or if there is a wall with a slit in their path. When examining the area behind the walls any disturbance there is due to the part that has passed through the opening area since we have assumed that the waves do not pass through the walls. A careful examination of the numerical results indicates that in fact some disturbances can be seen in these areas. According to the wave propagation theorem every time a wave passes through an opening a diffraction appears behind the blocked area. The above mentioned numerical disturbances behind the walls are similar to these diffraction effects. We will see that these disturbances depend on the approximation method we have used, for example if we use high order elements in the finite element methods or high order differencing when finite difference methods are used the interrelation between the neighboring nodes results in a wide interdependencies and when these dependencies are disturbed by blocking the path the wave fronts in the undisturbed section of the solutions pass through and continue to play their parts in the neighboring nodes while the rest are stopped and reflected back and cannot play their rule in the neighborhood behind the walls.

A Fuzzy Soft Set Theoretic Approach to Decision Making Problems

A. R. Roy **Fri 11:25**

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A number of real life problems in many practical fields viz., engineering, social and medical sciences, economics etc., involve imprecise data and their solution involves the use of mathematical principles based on uncertainty and imprecision. Some of these

problems are essentially humanistic and thus subjective in nature (e.g., human understanding and vision systems) while others are objective, yet they are firmly embedded in an imprecise environment. To deal with such systems in an effective way we have so far, in the literature, various theories viz., theory of Probability, Fuzzy set theory, Intuitionistic Fuzzy sets, Vague sets, Rough sets etc. These are being utilized as effective tools for dealing with diverse types of uncertainties and imprecision embedded in the system. All these theories, however, are associated with an inherent limitation viz., the limitation of inadequacy of the parametrization tool.
Dimitri Molodtsov, in 1999, initiated a novel concept viz, the concept of Fuzzy soft set theory as a new mathematical tool for dealing with uncertainties and this theory is seen to be free from the above limitations. This theory has been applied by him in several directions.
The present talk is based on some of our recent work wherein we have used the concept of Soft set and Fuzzy Soft Set Theory to some decision making problems.
In particular we would like to present the problem of Object Recognition by using the Fuzzy soft set concept. As is well known the problem of object recognition has received paramount importance. The recognition problem may be viewed as a multi observer decision making problem, where the final identification of the object is based on the set of inputs from different observers who provide the overall object characterization in terms of diverse set of parameters.
In our approach towards this problem we have constructed a comparison table from a fuzzy soft set in a parametric sense for decision making.
The necessary algebra in formulating the fuzzy soft set concept used in this problems have been developed by us and will also be presented.

Solving Non-linear ODE and PDE via Feedforward Neural Networks

Ch. V. V. Mohan Sarma **Fri 14:55**

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We presented a method for solving initial and boundary value problems using feedforward neural networks. First we started with a trail solution of the differential equation, can be written as sum of two parts. The first part satisfies initial/boundary conditions without neural network parameters and second part is constructed so as not to affect the initial/boundary conditions. This part contains a feedforward neural network allowing adjustable parameters, weights and bias of the networks. Hence by construction of trail neural solution, network is trained to satisfy the differential equation. The applicability of this model ranges from single ordinary differentail equation to a system of coupled ODEs and PDEs. In this paper we illustrate the method, solved a variety of model problems and presented the comparisons with known analytic solutions. Considering other case of complex boundary geometry, where the boundary is determined by a number of points that belong to it and are closely located, so as to offer a reasonable representation. Two networks are employed: a multilayer perceptron and a radial basis function network. The latter is used to account for the exact satisfaction of the boundary condition. The method has been successfully tested on two-dimensional and three-dimensional PDEs and has yielded accurate results.

Scalable Implementation of the Finite-Volume Dynamical Core in the Community Atmospheric Model

William Sawyer **Thu 11:00**

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A distributed memory message-passing parallel implementation of a finite-volume discretization of the primitive equations in the Community Atmospheric Model is presented. Due to the data dependencies resulting from the polar singularity of the latitude-longitude coordinate system, it is necessary to employ two separate domain decompositions within the dynamical core. Data must be periodically redistributed between these two decompositions. In addition, the domains contain halo regions that cover the nearest neighbour data dependencies. These data movements are optimized through one-sided communication primitives and multithreading. The resulting algorithm is shown to scale to very large machine configurations, even for relatively coarse resolutions.

Multigrid Newton-Krylov Method for Radiation-Conduction in Semitransparent Media

Mohammed Seaid **Thu 16:10**

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Developing efficient and accurate techniques to solve radiative heat transfer attracts many researches from several applications as, radiation hydrodynamics, combustion, or glass manufacturing. In many applications, diffusion approximation could be the cheapest (as far as the efficiency is concerned) solution for such equations. However, this approximation fails to resolve accurately the boundary layers in the conduction processes. In non diffusive limits (optically thin material) only the solution of the full radiative heat transfer can provide high quality results.

In our contribution, we present a new algorithm to approximate the full radiative heat transfer problem. The algorithm consists of linear and nonlinear multigrid techniques. Thus using same mesh hierarchy for both radiative transfer and heat conduction, the linear system arising from the discretization of radiative transfer is solved by multilevel method using the Atkinson-Brakhage approximate inverse as a preconditioner. On the other hand a multilevel solver, using Newton-Krylov as a smoother, is used for the discretized heat conduction. In both methods linear systems are solved only on the coarse mesh.

Numerical investigations (robustness, efficiency and convergence rates) are carried out in three-dimensional problem. Special attention is given to an eight frequency bands model kindly provided by ITWM in Kaiserslautern for glass cooling. Comparisons to other methods and the sensibility of the algorithm on ordinate and space discretizations are also discussed in our contribution.

An ODE Traffic Network Model

ANITA KUMARI SINGH, MICHAEL HERTY, AXEL KLAR **Thu 11:25**

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Macroscopic modelling of vehicular traffic flows had started with the work of Lighthill & Witham. Simulation and optimization of traffic flow in networks lead to efficient traffic management. In [1] traffic models for the networks based on PDE's have been considered. Suitable conditions for the flow at junctions are given by [2, 3]. Based on averaged density evolution of traffic, we obtain an ODE model by using spatial approximations. One advantage of this model over [1] is that it can handle traffic jams. The PDE model supports traffic jam situations. However, from a computational point of view the ODE model is simple and needs less variables to be solved. We formulate optimization problem on the networks. We have derived adjoint calculus for the ODE model to compute the gradients efficiently. We use the adjoint gradient in different optimization algorithms and present numerical results.

[1] M. Herty, A. Klar, *Simplified Dynamics and Optimization of Large Scale Traffic Networks*, M^3AS, vol.14(4), April 2004.

[2] G. Coclite, B. Piccoli, *Traffic Flow on a Road Network*, preprint SISSA (2002).

[3] H. Holden, N. Risebro, *A Mathematical Model of Traffic Flow on a Network of Unidirectional Road*, SIAM J. Math. Anal. 26(4), (1995), pp. 999-1017.

Semi-smooth Newton Methods for Contact Problems with Friction in Linear Elasticity

GEORG STADLER **Fri 11:00**

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Second-order algorithms for an efficient solution of the Signorini contact problem in linear elasticity are discussed and analyzed in 2D as well as 3D. The contact problem with given friction (Tresca friction) leads to a constraint non-differentiable minimization problem. By means of the Fenchel duality theorem this problem can be transformed into a constrained minimization involving a smooth functional. A regularization technique for the dual problem motivated by augmented Lagrangians allows to apply an

infinite-dimensional semi-smooth Newton method for the solution of the probem with given friction. The resulting algorithms converge locally at a superlinear rate and can be interpreted as active set strategies. Comprehensive numerical tests discuss, among others, the dependence of the algorithmś performance on material and regularization parameters and show that a continuation procedure for the regularization parameter increases the speed of convergence. The remarkable efficiency of the methods carry over to the Signorini problem with Coulomb friction by means of fixed point ideals.

On PDE Solution in Gas Networks

Marc Steinbach **Thu 14:30**

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Operative planning in gas distribution networks leads to large-scale mixed-integer optimization problems involving, among other restrictions, a hyperbolic PDE defined on a graph. The lecture focuses on the modeling and numerical solution of the problem under prescribed combinatorial decisions, addressing in particular the hyperbolic gas flow equations with underlying network topology. We analyze the NLP resulting from a full discretization in space and time, discuss alternative numerical solution approaches, and present computational results.

Conservation of Cosymmetry in PDE Discretization

Vyacheslav Tsybulin **Wed 15:45**

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We consider the discretization for the PDE systems with unusual families of steady states when the stability property varies over the family. It was shown by V. Yudovich that these families caused by cosymmetry phenomenon not symmetry. We displayed in the previous works (CASC2́001; Computing, 2002) that the family of equilibria degenerates if an inappropriate approximation is used for its computation. The finite-difference and combined spectral-finite-difference discretizations are presented for Darcy model of viscous fluid convection in a porous medium and population kinetics model.

Weak Regularization for Signorini Problems with Friction

Tim Voetmann **Thu 17:00**

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The talk is devoted to the numerical solution of variational inequalities with set-valued operators in Hilbert space.
When dealing with ill-posed problems the classical proximal point method is a well-known regularization method employing Euclidean distances as a regularizing term in order to stabilize the arising auxiliary problems.
In contrast to that we investigate the use of Bregman-type generalized distances that additionally keep the iterates in the interior of the feasible domain yielding thus an interior point method for variational inqualities.
While in finite dimensions a wide variety of Bregman distances are well-known, this class of functions is harder to construct in arbitrary Hilbert spaces. We present conditions allowing us to incorporate the idea of weak regularization providing a significant acceleration of computations without losing the favorable convergence properties of the classical proximal method.
We present a scheme coupling a successive discretization of the variational inequality by means of the finite element method with regularization by the generalized proximal point method. Conditions on the exactness of the approximation and a smoothing procedure for the operators based on the epsilon-enlargement are discussed.
The practical efficiency of this scheme is demonstrated by application to contact problems from structural mechanics.

BaF_2 for Microlithography Applications: Modeling, Simulation and Optimization of the Growth Process

Axel Voigt **Wed 11:00**

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High quality Fluoride crystals for lenses in microlithography steppers are grown by Bridgman or Vertical Gradient Freece techniques. A major drawback of these techniques is that the growth process can not be controlled optically. So the quality of the produced crystal can not be monitored during growth. In order to understand and improve the processing, numerical simulation is nowadays a well established tool in the crystal growth community. To calculate the temperature distribution the different mechanisms of heat transfer have to be taken into account: conduction, convection and radiation. If the developed models are used to optimize running processes a high accuraccy of the predictions are needed. Unfortunately the physical properties of the involved materials are often not well known and might change in time. Therefore in a first stage parameters have to be adjusted to available experimental data. If the required accuracy is achieved, in a second stage process optimization can be performed. Quasi-Newton methods are applied for both optimization loops. The partial derivatives are calculated numerically on a PC-Cluster. We demonstrate how such an approach can be used to optimize the crystal quality of BaF_2 on an industrial scale.

Efficient Multigrid-FEM Method for Simulation of Liquid-Solid Flows with Large Number of Moving Particles

Decheng Wan **Fri 14:30**

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Liquid-solid flows with large number of moving particle are frequently found in technical and industrial processes. Examples are pneumatic conveying, fluidised beds, vertical risers, particle separation in cyclones, mixing devices, foods containing particles, slurry flows, mining extraction, etc.

From the numerical point of view, particulate flows are quite hard to simulate, since both the fluid velocity field and the domain in which it is defined are unknown, it can require a huge amount of time for the generation or deformation of the computational grid, as well as dealing with collision between particles for the case with huge number particles (greater than 10,000).

In this paper, we develop a simple and efficient 'fictitious boundary method' for the detailed simulation of particulate flows based on multigrid-FEM. It starts with a coarse mesh which contains already many of geometrical fine-scale details, and employs a (rough) boundary parametrization which sufficiently describes all large-scale structures with regard to the boundary conditions. Then, treat all fine-scale features as interior objects such that the corresponding components in all matrices and vectors are unknown degrees of freedom which are implicitely incorporated into all iterative solution steps. The motion of the solid particle is modeled by the Newton-Euler equations. No-slip boundary conditions are applied at the interface between the particles and the fluid. For handling collision between particles, the knowledge of locations of neigbouring partciles is required. In this paper, based on the multigrid-FEM, we proposed some special techniques to reduce the time consuming for searching collision partners in order to improve the particle collision calculations.

Numerical tests of 6400 particle flows in a tank show the present techniques can decreased greatly CPU time, and makes it possible that the present method can be used to simulate liquid-solid flows with large number of particles.

Wick-Stochastic Finite Element Solution of Reaction-Diffusion Problems

H. Manouzi, M. Sea, Mostafa Zahri **Wed 16:35**

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Many physical phenomena in real life are characterized by their inherent or externally induced uncertainties in the design parameters. Mathematically, these problems are modelled by stochastic partial differential equations. In our talk we consider the following stochastic reaction-diffusion equation:

$$\frac{\partial C}{\partial t} - \nabla \cdot \Big(D(\mathbf{x}, \omega) \nabla C \Big) = R(t, \mathbf{x}, \omega, C), \quad (t, \mathbf{x}, \omega) \in [0, T] \times \mathcal{D} \times \Omega, \tag{2}$$

where $C(t, \mathbf{x}, \omega)$ is the stochastic concentration of a chemical specie, $D(\mathbf{x}, \omega)$ is the stochastic diffusion coefficient and $R(t, \mathbf{x}, \omega, C)$ is the stochastic reaction term. In (2), $[0, T]$ denotes the time interval, $\mathcal{D}$ the spatial domain and Ω the probability sample of elements ω. We assume the stochastic functions $D(\mathbf{x}, \omega)$ and $R(t, \mathbf{x}, \omega, C)$ are independent white Gaussian noises with bounded and continuous expectations.
Introducing the notion of wick multiplication to regularize the product of generalized variables and discretizing the time variable by a semi-implicit integrator, the variational formulation of (2) is developed using a finite element method. Problem data and solution variables are expanded using the Wiener-Itô chaos system. The approach leads to a set of deterministic fully-discrete reaction-diffusion equations for which the numerical solution can be computed using the standard techniques.
Existence, uniqueness and convergence estimations are also discussed with details in our talk. Computational results in both one and two dimensions are presented.

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(Status: August 2004)

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