Abstracts

The order is alphabetical after the first author's last name.

A stable and Conservative Hybrid Scheme for Problems Involving Shocks

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It is well known that high order numerical schemes exhibit oscillations around shocks but are very efficient for smooth solutions. In flow fields where both shocks and weak features exist, both the shock capturing capability and high order accuracy are required.
We develop a hybrid scheme consisting of a combination of a second order MUSCL scheme and a high order finite difference scheme. The hybrid scheme is constructed in such a way that we can prove that it is stable. We can also show that it is high order accurate in smooth domains and oscillatory free close to the shock. The order of accuracy is measured locally to see its appropriate size. Numerical experiments will be done for simple linear problems, the Burger's equation, and for the Euler equations with high Mach numbers.

Numerical stabilization of the melt front for laser beam cutting

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The Finite Difference Element Method (FDEM) is a black-box solver that solves by a finite difference method arbitrary nonlinear systems of elliptic and parabolic partial differential equations (PDEs) on an unstructured FEM grid in 2D or 3D. For each node we generate difference formulas of consistency order q with a sophisticated algorithm. An unprecedented feature for such a general black-box is the error estimate that is computed together with the solution.
In this paper we present the numerical simulation of the laser beam cutting of a metal sheet. This is a free boundary problem where we compute the temperature and the form of the melt front in the metal sheet. During the cutting process, the numerical stabilization of the melt front is a great challenge.

A posteriori error estimators and metric tensors for generation of optimal meshes

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I consider optimal meshes that minimize the error of the piecewiselinear interpolation over all simplicial meshes with a fixed numberof cells. Theoretical results on asymptoticdependences of L_p-norms of the errors on the number of mesh cells arepresented.Both the interpolation error and the gradient of interpolation error areanalyzed. In practice, the conventional adaptive procedures produce meshes close to optimal. Such meshes are called quasi-optimal. They givea slightly higher errors but the same asymptotic rate of error reduction. Quasi-optimal meshes are uniform or quasi-uniform in an appropriate continuous tensor metric.Metric recovery is the cornerstone of the mesh adaptation. It is usually based on either a discrete Hessian recovery or a posteriori error estimators. I discuss difficulties related to both approaches and propose possible solutions. It is known that the accuracy of the Hessian recovery is very low although the method exhibits surprisingly good behavior in practice. A posteriori error estimators may provide a reliable alternative for metric recovery. I present a new method of metric recovery targeted to the minimization of L_p-norms of the interpolation error or the gradient error of interpolation. The core of the method is robust and reliable edge-based a posteriori error estimator. The method is analyzed for conformal simplicial meshes in spaces of arbitrary dimension.

Voltage and current excitation for time-harmonic eddy-current problems.

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We present a review of different formulations of the voltage and current intensity excitation problem for the time-harmonic eddy current model in electromagnetism. We consider both the case of a conductor with electric ports and the case of a conductor internal to the computational domain. We present formulations based on the magnetic or the electric field and potential formulations. We enlighten the influence of the boundary conditions on the proposed formulations and the difficulties arising in the case of an internal conductor. We also give a short description of some numerical approximation schemes based on finite elements.

Generalized multi-stage Variational Iteration method

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Many problems of science are represented by a system of linear or nonlinear differential equations. It is in general difficult to solve such type of systems and, hence, finding approximate or, if possible, closed-form solutions has been the subject of many researchers. The Variational Iteration Method (VIM) is an alternative to numerically solving those equations and has proven its applicability. We study the multi-stage version of the method, M-VIM, however, on the generalisation of the classical variational iterations. To illustrate the method we apply M-VIM to some chemical reaction equations that emerge as describing different phenomena in chemical and physical sciences. We compare the results with classical VIM.

Numerical optimization of a bioreactor for the treatment of eutrophicated water

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Eutrophication is a process of nutrient enrichment (usually by nitrogen and/or phosphorus) in large waterbodies such that the productivity of the system ceases to be limited by the availability of nutrients. It occurs naturally over geological time, but may be accelerated by human activities (e.g. sewage or land drainage). In this work we deal with a model governing eutrophication processes (based on a system of nonlinear parabolic partial differential equations with a great complexity) where a complete set of five species is analyzed: nutrient, phytoplankton, zooplankton, organic detritus and dissolved oxygen. For this complete model, several results of existence-uniqueness-regularity have been recently obtained by the authors.
The fundamental idea of a bioreactor consists of holding up water (rich, for instance, in nitrogen) in large tanks where we add a certain quantity of phytoplankton, that we let grow in order to absorb nitrogen and purify water. This problem can be formulated as an optimal control problem with state constraints, where the control can be the quantity of phytoplankton added at each tank or the permanence times, the state variables are the concentrations of the five species, the objective function to be minimized is the phytoplankton concentration of water leaving the bioreactor, and the state constraints stand for the thresholds required for the nitrogen and detritus concentrations in each tank. We prove that this optimal control problem admits a (non necessarily unique) solution, which can be characterized by a first order optimality condition, involving an adjoint system to be adequately defined.
After discretizing the control problem, we present a structured algorithm for solving the resulting nonlinear constrained optimization problem. Finally, we also present numerical results for a real-world example. (This work has been supported by Project MTM2006-01177 of M.E.C. of Spain.)

High order numerical method for Piecewise Deterministic Processes with ENO scheme

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We deal with a type of piecewise deterministic process, that results from the action of a semi-Markov process on an ordinary differential equation. We consider the Chapman-Kolmogorov equation, here named Liouville-Master Equation (LME), for the time dependent probability density distribution functions of the process, in absence of memory. Such that LME is a system of coupled hyperbolic PDE. For the numerical method we use the ENO scheme jointly to forward Euler, in order to obtain an high order numerical solution. We show some convergence result tests on applied models, and possible extensions to processes with memory.
References:
M. Annunziato, Comp. Meth. Appl. Math. Vol. 8 (2008) No. 1, pp. 3-20.
M. Annunziato, Math. Model. and Analysis, 12 (2007) 157-178.

Generalized combined field integral equations for the iterative solution of the three-dimensional Helmholtz equation at high-frequency

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This talk addresses the derivation of new second-kind Fredholm Combined Field Integral Equations for the Krylov iterative solution of three-dimensional acoustic scattering problems by a smooth closed surface. Existence and uniqueness occur for these formulations. These integral equations can be interpreted as generalizations of the well-known Brakhage-Werner and Combined Field Integral Equations (CFIE). One of their important property, and most particularly for high-frequency problems, is that their spectrum is characterized by a large cluster of eigenvalues. This provides a fast convergence rate of a Krylov iterative solver which is independent of the wavenumber and density of discretization points per wavelength. We will present some numerical experiments to test their efficiency.

A compact high-order embedded boundary method for the wave equation.

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Embedded boundary methods are highly efficient both in terms of operations and required memory per degree of freedom. They are also well suited for massively parallel computers. Here we focus on the wave equation and outline a high-order-accurate embedded boundary method based on compact finite-differences. Traditionally boundary values are assigned by extrapolation to ghost points outside the boundary, we impose the boundary conditions by assigning values via interpolation to ghost points just inside the boundary. Our new approach is more accurate and removes the small cell stiffness problem for the Dirichlet problem. For the Neumann problem we mitigate the small cell problem by adding a regularizing term to the interpolant before taking the normal derivative of the interpolant.

Multigrid methods for structured matrices and Anti-Reflective boundary conditions

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Anti-Reflective boundary conditions (AR-BC) have been introduced in 2003 and studied later on, in connection with good and fast deblurring algorithms. When applied to the problem of deblurring and denoising an image, the quality of the restored data using AR-BC is usually better or equal, according to the noise level, if compared with the data obtained by imposing other classical BC.
While imposing AR-BC to the above-mentioned problem, one has to solve a structured linear system. If the blurring is symmetric, the matrix of the system is strongly related to the 2-level tau algebra (it is 2-level tau with rank 2 correction at each level). For this reason, we first review some results on multigrid methods for structured matrices and then we investigate the special case of AR linear systems.

On Convergence of a Discontinuous Galerkin Finite Element Method for the Vlasov-Poisson-Fokker-Planck System

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In this paper we investigate the basic ingredients for global superconvergence strategy used for the mixed discontinuous Galerkin finite element approximations, in H^{1} and $W^{1,\infty}$-norms, for the solution of the Vlasov--Poisson--Fokker--Planck system. This study is an extension of the previous results by the author to finite element schemes including discretizations of thePoisson term, where we also introduce results of an extension of the h-versions of the streamline diffusion (SD) and the discontinuous Galerkin (DG) methods to the corresponding hp-versions. Optimal convergence results presented in the paper relay on the estimates for the regularized Green's functions with memory terms where some interpolation postprocessing techniques play important roles.

Modeling Aspects of Softening Hysteresis in Soft Biological Tissues

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This contribution deals with the modeling of soft biological tissues in the physiological as well as in the supra-physiological (overstretched) domain. In order to capture the softening hysteresis as observed in cyclic uniaxial tension tests, we introduce a scalar-valued damage variable into the strain-energy function for the embedded fibers such that remnant strains are obtained in the fibers for the natural state after unloading the material. This can be reasonably included by assuming an additively decoupled energy function into an undamaged isotropic part, for the ground substance, and superimposed transversely isotropic parts, for the embedded fiber families. A saturation function is considered accounting for converging stress-strain curves in cyclic tension tests at fixed load levels. As a numerical example we consider a circumferentially overstretched atherosclerotic arterial wall.

Adaptive Discretization in Deterministic Uncertainty Quantification for Compressible Flow Calculations

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We consider the deterministic propagation of statistical model parameter uncertainties in numerical approximations of nonlinear conservation laws. Example sources of parameter uncertainty include empirical equations of state, initial and boundary data, turbulence models, chemistry models, catalysis models, and many others. To deterministically calculate the propagation of model parameter uncertainty, stochastic independent dimensions are introduced and discretized. By employing a-posteriori error control via adaptive discretization, the high computational cost associated with treating multiple sources with statistical uncertainty is significantly reduced. Computational problems featured in this work include compressible Navier-Stokes flow with finite-rate chemistry and turbulence.

FEM for flow and pollution transport in a street canyon.

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We develop a mathematical model of air flow and pollution transport in 2D street canyon. The model is based on Navier-Stokes equations for viscous incompressible flow and convection-diffusion equation describing pollution transport. The solution is obtained by means of Finite Element Method (FEM). We use non-conforming Cruzeix Raviart elements for velocity, piecewise constant elements for pressure, and linear Lagrange elements for concentration. The resulting linear systems are solved alternatively by the Multigrid method and Krylov subspace methods. We treat two types of boundary conditions: Dirichlet and natural boundary condition. We present computational studies of the given problem.

Stabilized Finite Element Methods for Nonstationary and Nonlinear Convection-Diffusion-Reaction Equations

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Fluid flow problems with simultaneous reactive multicomponent transport of chemical species arise in many technical and environmental applications. The numerical solution of nonstationary convection-diffusion-reaction models is a challenge when convection is dominant and sharp layers of the concentrations arise. Here, the numerical approximation of scalar quasilinear convection-diffusion-reaction equations with stabilized finite element methods and shock capturing variants of such schemes as an additional stabilization is studied theoretically and numerically. Shock capturing may help to further reduce spurious oscillations and avoid negative concentrations. This is of importance for coupled systems of equations in which inaccuracies in one concentration affect all other ones.

Cubature on Wiener space in infinite dimensions with applications in finance

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We prove a stochastic Taylor expansion for stochastic partial differential equations and apply this result to obtain cubature methods, i.e., high order weak approximation schemes for SPDEs, in the spirit of T. Lyons and N. Victoir. We can prove a high-orderweak convergence for well-defined classes of test functions if the process starts at sufficiently regular points and for sufficiently regular driving vector fields. We apply these methods for high order weak approximation of Heath-Jarrow-Morton type interest rate models.

Finite element discretization of the Giesukus model for polymer flows

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We are interested in the numerical simulation of polymer flows. In order to capture the complex rheological behavior, we consider the Giesekus model which presents two main advantages. First, it yields a realistic behavior for shear, elongational and mixed flows. Second, only two material parameters are needed to describe the model. However, the nonlinear constitutive law involves, besides the objective derivative, a quadratic term in the stress tensor which is difficult to handle. Our numerical approach is based on the idea of preserving the positive-definiteness of the conformation tensor at the discrete level, in order to avoid numerical instabilities associated with large Weissenberg numbers. For this purpose, we use stabilized finite element and discontinuous Galerkin methods.

Numerical Simulation of Stratified Flows past a Body

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The article deals with the numerical simulation of 2D and 3D unsteady incompressible flows with stratifications. The mathematical model is based on the Boussinesq approximation of the Navier-Stokes equations. The flow field in the towing tank with a moving sphere is modelled for a wide range of Richardson numbers. The obstacle is modeled via source terms. The resulting set of equations is then solved by three different schemes. The first two schemes are based on the artificial compressibility method in dual time. For spatial discretization the fifth-order finite difference WENO scheme, or the second-order finite volume AUSM MUSCL scheme were used. The third scheme is based on the projection method combinated with the fifth-order finite difference WENO method in space and RK3 in time.

Numerical shape and topology optimization for loudspeakers and brass instruments

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We examine several design optimization problems for acoustical horns. The horn is used either as part of a loudspeaker or a brass instrument. In both cases, the acoustical properties turn out to be quite sensitive to the precise shape of the horn, which makes it reasonable to expect numerical design optimization to be effective for these applications. The objective is to find a tapering of the bell so that the horn satisfies a prescribed set of acoustical properties (which differ for loudspeakers and brass instruments). The bell shape is computed using optimization techniques combined with numerical solutions of the Helmholtz equation. For the brass instrument, the objective is to control the generation of standing waves inside the instrument so that they form, as closely as possible, a harmonic sequence. The results show that by allowing non-traditional shapes, we can obtain a more fine-grained control over the standing waves. The objective of horn loudspeakers is to enhance the efficiency of sound transmission and to direct the sound energy to regions in front of the horn. Instead of only considering the horn's tapering in the optimization, a larger class of admissible shapes can be conceived by applying so-called topology optimization, where an arbitrary distribution of material within a given region is subject to design. The combination of topology optimization and optimization of the horn's tapering enables the design of a horn/acoustic-lens combination that exhibits high transmission efficiency as well as an even angular distribution of sound energy in the far field.

Numerical solution of quasilinear elliptic PDEs with the RBF method

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Meshless schemes based on collocation of radial basis functions (RBFs) are a new class of numerical methods for the solution of PDEs. In this work, we numerically study the behavior of the RBF method when applied to the solution of the less-visited nonlinear elliptic equations. Concretely, we focus on quasilinear PDEs whose diffusion coefficient is a function of the squared gradient.
Such equations are interesting both from a purely mathematical point of view as well as from the many applications that are modelled in terms of them. For instance, both the p-Laplace equation and Plateau's problem belong to this type. The former is often encountered in the modeling of non-Newtonian fluids, while the latter is an especial case of the minimal surface problem of interest in civil engineering.

Preconditioning and conditioning issues in some image restoration PDE models

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Image restoration, i.e. the recovery of images that have been degraded by blur and noise, is a challenging inverse problem. We propose the solution of the related discretized partial differential equation models by iterative linear system solvers accelerated by a simple but flexible framework for updating incomplete factorization preconditioners that presents a computational cost linear in the number of the image pixels.We demonstrate the efficiency of the strategy in application to denoising and deblurring of some images by solving a generalized Alvarez-Lions-Morel-like partial differential equation by semi implicit complementary volume scheme but the same arguments apply for other discretizations.

A relaxation scheme to simulate gravitational flows

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We present a numerical procedure to approximate the solutions of an Euler-Poisson model. Such a model arises when considering gravitational flows issuing from astrophysical experiments. A two step method is proposed. During the first step, the Euler equations are approximated with a fixed gravitational source term. Next, the second step is devoted to solve the Poisson equation in order to approximate the gravitation. The main purpose of the present work concerns the first step of the procedure where a particular attention is paid on the source term. To access such an issue, a relaxation scheme is involved, and its robustness is established. Several numerical experiments coming from gravitational flows for astrophysics highlight the numerical scheme.

Domain decomposition strategies with black box subdomain solvers

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Most domain decomposition methods imply the repeated solution of subdomain problems, that consitute the bulk of the computation. Since extremely efficient optimized monodomain solvers are available in commercial/academic codes, it is desirable to have the possibility of using them directly in the solution process. Though many non conforming domain decomposition methods allow to use independent subdomain solvers, most of the times the coupling condition implies some modification for the corresponding code (at least in terms of input and/or output). We will discuss a theoretical strategy treating the subdomain solvers as black boxes and allowing to replace the subdomain solver with a simple call to a standard monodomain code.

Stabilized Finite Element Method for Compressible-Incompressible Flows

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We present a numerical method devoted to the prediction of unsteady flow consisting of immiscible liquid and gas fluids separated by a moving interface. Especially we consider the gaz as compressible and the liquid as incompressible.
An important part of this work is dedicated to the construction of a unified numerical scheme which is valid for both types of flow. Using Navier Stokes equations formulated in primitive variables we propose a method that relies on
- a stabilized finite element method to solve Navier Stokes equations,
- a Level Set method to track the interface with a discontinuous Galerkin method to solve the associated transport equation.
An averaging approach is used to treat the interface.
Several simulations will illustrate the good behaviour of the method.

Asymptotics of spectral norms of some interesting matrix sequences

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The talk concerns the asymptotic behavior of the spectral norm (which is the largest eigenvalue in the case of positive definite matrices) of the n-by-n truncations of infinite matrices as n goes to infinity. As examples, we consider matrices arising in the analysis time series with long memory and matrices that emerge in connection with best constants ininequalities of the Markov and Wirtinger types. The message of the talk is that a very fertile strategy for tackling the problem is an old idea by Harold Widom and Lawrence Shampine: replace matrices by integral operators and try to prove that the latter, after appropriate scaling, converge uniformly to a limiting integral operator.

Geometrically Consistent Mesh Modifications

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Mesh adaptivity basic principle is to equidistribute the computational effort. It relies on the implicit assumption that the domain geometry is correctly described at the discrete level, namely that position and curvature satisfy a natural geometric constraint. This constraint may be difficult or impossible to satisfy, thereby leading to geometric inconsistencies and ensuing numerical artifacts.
A new paradigm in mesh adaptation is the execution of geometrically consistent modification (such as refinement, coarsening or smoothing) on manifolds with incomplete information about their geometry.
We discuss the concept of discrete geometric consistency, show the failure of naive approaches, propose and analyse a simple geometrically consistent algorithm.

An immersed interface technique for the numerical solution of a PDE on a moving domain.

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We present a finite difference scheme for a parabolic problem with mixed boundary conditions on a moving domain. This is an extension of a similar work on a domain which does not depend on time, where an immersed interface technique was used to discretize the Neumann condition.Since the domain moves, the unknowns are not defined at the same points for all time steps, in which case they need to be interpolated or extrapolated near the boundaries.A discrete maximum principle is proven as well as the convergence of the scheme. Numerical tests confirm the convergence, comparisons are made with similar recent works where different kind of discretizations are used (finite elements, finite volumes).

A new stability criterium for finite-element schemes of Oldroyd-like models and a new efficient variance reduction technique for micro-macro dumbbell-models

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We present *a new stability criterium* for the long-time simulation of the *Oldroyd-B* system of equations -- a prototypical macro-macro model for viscoelastic fluids -- using finite-element schemes, which is based on the preservation of a *free energy*. We also discuss micro-macro models for polymeric fluids, coupling a (macro) equation for the solvent with a (micro) equation for the polymers. More precisely, we present a *new variance reduction technique* for segregated schemes, which consists in applying *a Reduced-Basis approach* to the numerous control variates that correspond to the many output expectations of parametrized SDEs -- like the *Hookean* or *FENE* dumbbell models parametrized by the velocity gradient --.

The time-domain BEM solution of nonlinear reaction-diffusion equations

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A boundary element method (BEM) with time-dependent fundamental solution is presented for the solution of the coupled system of nonlinear reaction-diffusion equations. The numerical algorithm is based on the iteration between the two diffusion-type equations with nonlinear reaction terms, which are treated as nonhomogeneities and assumed to be known from the previous time level. The use of time-dependent fundamental solution allows one to apply BEM directly to the governing equations without the need of a time integration scheme. Also, it enables us to use remarkably large time increments in the iterative process. The numerical solutions are obtained for the Brusselator system in 2D at various time levels.

Local projection stabilization for time-dependent flow problems

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In this talk we present recent advances for local projection techniques (LPS) for time-dependent flow problems. The method preserves the favourable stability and approximation properties of classical residual-based stabilization (RBS) techniques but avoid the strong coupling of velocity and pressure in the stabilization terms. LPS-methods belong to the class of symmetric stabilization techniques and may be characterized as variational multiscale methods. We will discuss in particular numerical accuracy in comparison to other stabilization techniques, the aspect of stability and accuracy for small time steps and efficient preconditioning.

A modified numerical scheme for the cubic Schrödinger and the modified Burgers' equation

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A finite-difference scheme based on the use of fourth order rational approximants to the matrix-exponential term in a two-time level recurrence relation is applied to the cubic Schrödinger and the modified Burgers' equation. The resulting nonlinear system is solved using an already known modified predictor-corrector method (see A.G. Bratsos, A numerical method for the one-dimensional sine-Gordon equation, Numer Methods Partial Differential Eq 24 (2008) 833-844). The method, which is applied *once*, consists in considering the corrector component wise and using an updated component in the corrector vector as soon as it becomes available.The efficiency of the proposed method is examined by comparing the results arising from the experiments with the relevant ones known in the bibliography.

A multiresolution space-time adaptive scheme for the bidomain model in electrocardiology

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The bidomain model of electrocardiology consists of a possibly degenerate parabolic PDE coupled with an elliptic PDE for the transmembrane and extracellular potentials, plus a time-dependent ODE for the gating variable. Since typical solutions exhibit wavefronts with steep gradients, we propose a finite volume scheme enriched by a fully adaptive multiresolution method to concentrate computational effort on zones of strong variation. Time adaptivity is achieved by locally varying time stepping or a Runge-Kutta-Fehlberg adaptive time integration. Numerical examples demonstrate the efficiency and accuracy of the methods. In addition, the optimal choice of the threshold for discarding non-significant information in the multiresolution representation of the solution is addressed.

On the numerical approximation of the Laplace Transform function from real samples and its inversion

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Many applications of NMR (Nuclear Magnetic Resonance relaxometry) are tackled using the Laplace Transform (LT) known on a countable number of real values. The usual approach is to solve the inverse problem in a finite dimensional space (CONTIN, UPEN,...). We propose a fitting model s_{Lt} enjoying LT properties. We discuss the computational efforts to define the model and to prove its existence and uniqueness. Taking into account asymptotic behavior of Laplace function, we define s_{Lt} like a *generalized spline*; according to the magnitude of data error the model must be an interpolating or approximating one. Through a suitable error analysis we give *a priori* and *computational* approximation error bounds to confirm the reliability of our approach. Numerical results are presented.

Discontinuous Galerkin Methods for Reaction-Diffusion systems with Transmission Conditions

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We present the Interior Penalty Discontinuous Galerkin fem for reaction-diffusion systems on partitioned domains with Kadem-Katchalsky transmission conditions at the sub-domains interfaces.
We extend the optimal error analysis of the method by Suli and Lasis [SINUM '07] to semi-linear systems with transmission conditions.
The problem considered is relevant to the modeling of chemical species passing through thin biological membranes.
In this context, the use of continuous fem was proposed by Quarteroni et al. [SINUM '01] for the modeling of the dynamics of solutes in the arteries.
An advantage of the DG method is that the transmission conditions are simply imposed by the addition of appropriate elemental boundary terms in the bilinear form, and thus no iteration between domains is necessary.

Multiscale finite element method for pollutant transport in urban area

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This talk is about pollutant transport in urban area. In this context, coefficients may change rapidly. Indeed we are facing a multiscale problem that we must compute in real time. We may not obtain a decent accuracy on a real time calculations with classical methods. In order to find a compromise between accuracy and CPU time, we use the multiscale finite element method developed by Thomas Hou. Moreover, we add an absorption term to penalize pollutant to penetrate into the obstacles (penalisation method). However, boundary conditions which are enforced on calculation are not physical and may create numerical artefacts. We suggest several techniques to improve the treatment of these artificial boundary conditions and we will show some numerical results.

Computational Challenges in the Calculus of Variations

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The computational nonlinear PDEs involve minimisation problems with various striking challenges such as measure-valued solution concepts or ghost solutions.
The presentation introduces the Mania example for the Lavrentiev phenomena for singular minimisers and its remedy via a penalty FEM. The convergence of FEM for polyconvex energy densities and the lack of a Gamma convergence proof are discussed as well as one convergent FEM.
Computational microstructures and relaxation FEM are studied with adaptive mesh-refining and its convergence for a class of degenerate convex energy densities. Numerical relaxation requires concepts of semiconvexity as illustrated for single-slip finite plasticity.

A high order finite volume numerical scheme for shallow water system: An efficient implementation on GPUs and applications to real geophysical flows.

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Our goal is to design an efficient implementation of a Roe-type high order finite volume numerical scheme on GPUs to simulate some geophysical shallow flows that can be modeled by using the one layer 2D shallow-water system, formulated under the form of a conservation law with source terms. These models are useful for several applications such us: simulation of rivers, channels, dambreak problems, etc. In this work, we propose a strategy to design an efficient implementation on GPUs using OpenGL and Cg, by adapting the calculations and the data domain of the numerical algorithm to the graphics processing pipeline. Some applications to real geophysical flows will be presented.

Solution of incompressible flow equations by a high-order term-by-term stabilized method

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We introduce in this talk a stabilized method for the numerical solution of steady incompressible flow problems by the Finite Element method. The method is able to stabilize the discretization of the pressure, and also of any single operator term such as convection, curl, Coriolis force, etc., with high order of convergence: That of the interpolation on the velocity finite element space. It sets independent stabilization of each one of these terms.We prove stability and error estimates, for the solution of Oseen equations with this method. We follow the analysis technique introduced in Chacón [1], with specific adaptations.We present numerical tests that confirm the theoretical expectations, in particular the high order of the method, and the stabilization properties.[1] T. Chacón Rebollo. *An analysis technique for the numerical solution of incompressible flow problems*. M2AN, Vol. 10, 543--561, 1993.

Existence result for the coupling problem of two scalar conservation laws with Riemann initial data

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In this work, we are interested in the coupling problem of two scalar conservation laws through a fixed interface located for instance at x=0. Each scalar conservation law is associated with its own (smooth) flux function and is posed on a half-space, namely x<0 or x>0. At interface x=0 we impose a coupling condition whose objective is to enforce in a weak sense the continuity of a prescribed variable, which may differ from the conservative unknown (and the flux functions as well).
We prove existence of a solution to the coupled Riemann problem using a constructive approach. The latter allows in particular to highlight interesting features like non uniqueness of both continuous and discontinuous (at interface x=0) solutions. The behavior of some numerical schemes is also investigated.

Copula of the Characteristic Functions: An Innovative Use of Copula

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The copula formula was initially defined in terms of cumulative distribution functions. We show that the copula formula is invariant under the Fourier transform, which is equivalent to say that the copula formula can also take characteristic functions as variable. As a consequence of this finding, we obtain a interesting collection of multivariate distributions with flexible choice of marginal distributions and arbitrary dependence structure. The resulting characteristic function leads to the application of efficient FFT-based numerical techniques, e.g. CONV method and COS method, in pricing derivative instruments with multivariate payoffs. In this research, we illustrate the application of the concepts introduced above in the problem of spread option pricing.

Predictor-corrector iterative algorithms for solution of parabolic problems on graphs

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We consider a reaction-diffusion parabolic problem on branched structures. Two different flux conservation equations are considered at branch points. The fully implicit scheme is based on the backward Euler algorithm. In order to decouple the computations at each edge of the graph, the values of the solution at branch points are computed by using the predictor or predictor -- corrector techniques. The stability and convergence of the discrete solution is proved in the energy norm, this technique enables to improve the convergence estimates previously obtained by using the maximum principle. Results of numerical experiments are presented.

Unified stabilized finite element formulations for the Stokes and the Darcy problems

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In this paper we propose stabilized finite element methods for both Stokes' and Darcy's problems that accommodate any interpolation of velocities and pressures. Apart from the interest of this fact, the important issue is that we are able to deal with both problems at the same time, in a completely unified manner, in spite of the fact that the functional setting is different. Concerning the stabilization formulation, we discuss the effect of the choice of the length scale appearing in the expression of the stabilization parameters, both in what refers to stability and to accuracy. This choice is shown to be crucial in the case of Darcy's problem. As an additional feature of this work, we treat two types of stabilized formulations, showing that they have a very similar behavior.

Fast iterative solution of large nonsymmetric linear systems on Grid computers

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In this talk we describe an efficient iterative algorithm for solving large sparse linear systems on Grid computers and review some of its advantages and disadvantages. The algorithm uses an asynchronous iterative method as a preconditioner in a flexible iterative method, where the preconditioner is allowed to vary in each iteration step. By combining a slow but coarse-grain and asynchronous inner iteration with a fast but fine-grain and synchronous outer iteration, high convergence rates may be achieved on heterogeneous networks of computers. We present results of a complete implementation using mature Grid middleware, with application to a 3D convection-diffusion problem. Numerical experiments on heterogeneous computing hardware demonstrate the effectiveness of the proposed algorithm.

Anisotropic mesh adaptivity for FSI applications with large deformations

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When solving fluid-structure interaction problems, a common way to handle the displacements of the structural nodes inside the fluid domain is to reposition the fluid nodes and adopt an ALE formulation of the fluid equations. However, this method suffers from obvious limitations as nodes repositioning cannot always provide a valid mesh when significant displacements of the structure are considered. In a previous work, an algorithm based on local mesh modifications has been proposed to overcome the issues. Local mesh modifications have some advantages compared to global remeshing: local solution projection procedures can be easily set up that ensure the local conservation of conservative quantities, the mesh remains unchanged in most of the domain, allowing to adapt the mesh frequently, local mesh modifications can be performed in parallel, enabling transient adaptive simulation to run on parallel computers. Here, we extend this approach to anisotropic meshes. We consider an anisotropic mesh metric field that represents the desired size of the mesh. A mesh metric field is a smooth tensor valued field that allows one to compute an adimensional length for each edge. The aim of the procedure is to modify an existing mesh to make it a mesh in which every edge is close to the size 1. Recent works have shown that local mesh adaptation techniques can generate anisotropic meshes which are efficient in capturing boundary layers in fluid computations. In this work, we use the algorithm described in a previous paper to maintain such a mesh while the boundary undergoes large displacements or deformations, enabling FSI computations to handle both boundary layers and large deformations.

The sensitivity equation method for aninverse problem in a class of hyperbolic balance laws system

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This paper is concerned with the sensitivity analysis and the numerical solution of an inverse problemfor a class of one-dimensional nonlinear hyperbolic balance law system,where the shock formation is prevented by assuming a dissipative condition.The flux and source functions of the mathematical model are the unknowns of the inverse problemand are determined by minimization of the cost functional representedby the L_2 norm of the difference between the model and observed profile solutions. The direct problem is discretized by afinite volume methodand the numerical gradient of the cost function is calculated viathe sensitivity of discretized equations with respectto the parameters.We report some physical examples and some numerical experiments.

Anisotropic adaptivity by direct construction of node based metrics from the length distribution tensor

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Most of the metric driven anisotropic meshers are taking the metric data at the nodes of the mesh for efficiency reason. We propose here the construction a continuous metric field. First we introduce the approximation tensor of the length distribution defined from the length of the edges. The natural metric field is then the inverse of the proposed symmetric positive definite tensor. The interpolation error is evaluated along the edge direction using a 1D analysis in association with a local interpolant operator. A new edge length distribution is calculated and therefore a metric field is designed at the nodes. Our adaptive procedure works under the constraint of a number of nodes and the error balance is sufficient to optimise the mesh. Industrial applications of the proposed method will be shown, involving boundary layers, immersed surfaces, free surfaces and interfaces and Level Set both in 2D and in 3D

Some applications of asymptotic results on Toeplitz matrices to communications and signal processing.

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Since the seventies, Gray's work on Toeplitz matrices has allowed to the engineering community to address the Szegö theory on the asymptotic behavior of Toeplitz matrices with simple mathematical tools. In the present paper we extend Gray's work to block Toeplitz (BT) matrices maintaining his mathematical tools. Although stronger results on large BT matrices have already been proved, we will see that our results are sufficient to solve important problems in the field of communications and signal processing.

Scientific Computations on GPUs

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There is an increased interest in science and engineering for continuously expanding the capability of employing computational resources for solving larger mathematical problems effciently. With recent progress over the last few years in dedicated hardware for graphics rendering devices for personal computers, workstations and game consoles, modern Graphical Processing Units (GPUs) have become very efficient for especially computer graphics. The efficiency of GPUs relies on a parallel architecture which can be more efficient than traditional Central Processing Units (CPUs). Since the year 2000, the programmability of the GPUs have improved beyond the point where they also can be used for non-graphics applications. In this project, we investigate the possibilities to move existing algorithms and codes to a GPU based approach, both for compute intensive but also for large scale (data intensive) applications. Typical questions that arise are of the type "How is the GPU architecture different, compared to the CPU?", "How do we utilize the memory on the graphics adapter in the best possible way?", "Under what conditions is it advantageous to use the GPUs for scientific computations?" etc. Some of the goals of this project include the development of illustrative program examples where one or a few classical problems will be solved using a GPU, as well as comparison of the developed GPU codes with an equivalent parallel implementation for a multi-core CPU using OpenMP.

Algorithms for fluid-structure interaction problems: some comparisons and application to blood flow simulations.

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In this talk we review some recent algorithms for FSIproblems, including fully coupled, semi-implicit, monolothic,and segregated approaches.
At each time step, the fully coupled approach needs to glue thefluid domain to the structure and to balance velocities and normalstresses at the F-S interface; in contrast in the semi-implicit approachthe fluid computational domain is extrapolated.
The monolitic approach looks at all the state variables - fluidvelocity and pressure, structure displacement, and fluid domaindisplacement - indistinctly; in the segregated one, one of the statevariables is chosen as representative and the other onesas dependent on the first one. These choices lead to different solution strategies.We present a comparison on problems relative to hemodynamics.

High performance computing of free surface Phase Field simulations.

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Phase field method has the last decade demonstrated to be a promising framework for the simulation of problems involving free surfaces, phase change, wetting surface etc. Unfortunately, this method requires a high mesh resolution of its inherent, diffuse interface. This makes high performance computations a necessity for transient free surface problems.We present here a parallel and adaptive scheme for free surface phase field simulations. This scheme keeps the history of the mesh refinements is minimized and local to facilitate de-refinement on parallel processing. We will demonstrate the accuracy and the computational performance of this scheme and show three-dimensional simulation results of dendrite growth and droplet dynamics in a microfluidic bifurcation.

A space-time discretization for dynamic contact problems with cohesive forces

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Standard time-stepping schemes applied to dynamic contact problems are well-known to trigger spurious oscillations and/or behave poorly in long-time simulation. These difficulties can be overcome by a modification of the mass matrix: the mass associated with the nodes of the contact boundary is set to zero. We extend this approach to cohesive zones. Cohesive zones are interface models with unilateral contact and softening cohesive forces. The potential energy of the problem is possibly nonconvex and inertial terms at the interface are necessary to convexify the problem. We propose a way to combine these two contradictory requirements. We analyze the well-posedness and the convergence of the method and perform some numerical simulations.

An accurate approximate Riemann solver for the radiative transfer equation.

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In the frame of atmospheric re-entry, the M1 model is used for the resolution of the Radiative Transfer Equation (RTE). This moment model comes from integrations of the RTE over directions and frequencies. For simulations of physical interest the well-known HLL scheme is rather viscous. To avoid such a loss of accuracy a relevant HLLC scheme is derived. Particular attention is paid on the energy positiveness, flux limitation and total energy conservation. Accurate numerical solutions are obtained with this robust scheme. Moreover, asymptotic regimes as radiative transfer into opaque middles are properly dealt with and a second order MUSCL scheme extension is performed. Scattering effects are also accounted for. Numerical results illustrate the interest of the presented numerical procedure.

Perfectly Matched Layer for 1-D and 2-D Schrodinger Wave Equations

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We present strongly well-posed and strongly stable perfectly matched layers for the 1-D and 2-D time-dependent Schrodinger wave equations. The layer consists of the Hamiltonian perturbed by a complex absorbing potential, and the equations are corrected by carefully chosen auxiliary variables that ensure a zero reflection coefficient at the interface between the physical domain and the layer. Energy estimates are derived, showing that the solutions in the layer decay exponentially in the direction of increasing damping and in time. Numerical experiments are presented showing the efficiency of our new model. We develop and implement second and fourth order stable difference approximations in 1-D and 2-D respectively. The numerical scheme couples the standard Crank-Nicolson scheme for the modified wave equation to an explicit scheme of the Runge-Kutta type for the auxiliary differential equations.

Iterative Solvers and their Control in Fluid-Structure Interaction

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In fluid-structure interaction (FSI), one faces an interface coupling of two non-linear fields: a flexible structure and an incompressible fluid with an Arbitrary Lagrangian-Eulerian grid. Applications in life science, such as hemodynamical flow, require strongly coupled solution methods and are thus numerically challenging. It is therefore essential to control the convergence criterias in the different levels of the linear and non-linear solvers to reduce the computational costs.
In the presentation, a framework for FSI problems is introduced with a focus on the usage of inexact Newton methods for the field problems and their mutual control. As an example we consider the blood flow through an artery.

Source Localization in the Human Brain Based on Finite Element Methods

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Epilepsy is one of the most common neurological diseases and about 0.5 to 1% of the population suffers from it. Correct and anatomically precise localization of the epileptic focus is mandatory to decide if resection of brain tissue is possible. The most important non-invasive diagnosis tool used at epilepsy surgery centers is electroencephalography (EEG). To find the brain sources, which are usually modeled as current dipoles, that are responsible for the measured potentials at the EEG electrodes at the scalp is an inverse problem. A major limitation in EEG-based source reconstruction has been the poor spatial accuracy, which is attributed to low resolution of previous EEG systems and to the use of simplified spherical head models for solving the inverse problem. This paper will discuss finite-element based methods to solve the forward problem on realistic head models as well as techniques to solve the inverse problem.

Stretched Grids as Buffer Zones in Aero-acoustic Simulations

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Non-reflecting boundary conditions are of vital importance in aero-acoustic simulations. There are several techniques such as Engquist-Majda non-reflecting boundary conditions,buffer zones and Perfectly Matched Layers. In a buffer zone the grid is simply stretched and the damping can be enhanced by a forcing function or a larger amount of artificial viscosity. The popularity of buffer zones lay in their simplicity. They are easy to implement and in most cases, the stability of the code is only marginally affected. The main difficulty with boundary zones is to determine how large grid stretching that should be applied and how many grid points in the boundary zone that should be used. Often the choice is based on rule of thumbs from previous knowledge of the particular code used.The objective of the work presented in this talk is to get a further understanding of the influence of grid-stretching and artificial viscosity, respectively, in a buffer zone. Discrete analysis for a hyperbolic model problem and a convection-diffusion problem, respectively, will be presented. In both cases, the frequency in time is kept fixed via periodic boundary data.From the analysis, a suitable number of grid points in a buffer zone can be estimated for a given the grid stretching.A further conclusion is that within the buffer zone, the influcene of the aritificial viscosity is small compared to the grid stretching. The analytical work is compared with numerical simulations of acoustic waves and a wave package with a non-linear Euler solver. The analytical and numerical results agree very well.

Time discretization of nonlinear evolution equations

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We give an overview of recent results on the convergence of time discretization methods for nonlinear evolution equations. Methods under consideration are the two-step backward differentiation formula on equidistant as well as variable time grids, the variable-step theta-scheme and a class of stiffly accurate Runge-Kutta methods. Without assuming any additional regularity of the exact solution, convergence of piecewise polynomial prolongations of the numerical solution towards a weak solution is shown. The equations studied are assumed to be governed by a time-dependent monotone and coercive operator that might be perturbed by a time-dependent strongly continuous operator.

On Efficient Methods for Pricing Options with and Without Early Exercise

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In this presentation we will discuss option pricing techniquesin the context of numerical integration. Based on a Fourier-cosineexpansion of the density function we can efficiently obtain Europeanoption prices and corresponding hedge parameters. Moreover a wholevector of strik prices can be valued in one computation. This techniquecan speed up calibration to plain vanilla options substantially.This pricing method, called the COS method, is generalized to pricingBermudan and barrier options. We explain this and present a calibrationstudy based on CDS spreads.

"Optimal" Scaling of Meshfree Kernel Methods

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Meshfree reproducing kernel methods are frequently used in the recovery of an unknown function given in terms of values of the function sampled at a (scattered) set of points in R^s. Even if we decide on a particular reproducing kernel Hilbert space as our approximation space we usually need to determine one or more *shape parameters* of the kernel - the variance of a Gaussian kernel may serve as a typical example. We will report on recent studies performed in our group at IIT on determining such shape parameters in an "optimal" way. Extensions to the collocation and RBF-pseudospectral solution of PDEs will also be included.

Space-time DG method for nonstationary convection-diffusion problems

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The paper is concerned with analysis of the space-time discontinuous Galerkin finite element method applied to the numerical solution of convection-diffusion problems. First we consider a linear problem with diffusion which can degenerate to zero. In this case uniform error estimates are derived. Then the method is applied to a nonlinear convection-diffusion problem. It is necessary to use a special technique in order to overcome difficulties caused by the nonlinearity. The theoretical results are demonstrated by numerical experiments.

Finite element methods with symmetric stabilization for the transient convection--diffusion--reaction equation

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We consider implicit and semi-implicit time-stepping methods for finite element approximations of singularly perturbed parabolic problems or hyperbolic problems.
We are interested in problems where the advection dominates and stability is obtained using a symmetric, weakly consistent stabilization operator in the finite element method. Several $\mathcal{A}-$stable time discretizations are analyzed and shown to lead to unconditionally stable and optimally convergent schemes. In particular, we show that the contribution from the stabilization leading to an extended matrix pattern may be extrapolated from previous time steps, and hence handled explicitly without loss of stability and accuracy. A fully explicit treatment of the stabilization term is obtained under a CFL condition.

Adaptive wavelet methods for gene models

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The stochastic description of reaction kinetics require the numerical solution of the chemical master equation. At present, the chemical master equation is almost exclusively treated by Monte-Carlo methods due to the large number of degrees of freedom. On the other hand wavelets allow to obtain a sparse representation of functions and it enables to reduce the size of the problem. The adaptivity in the context of wavelet discretization insists in establishing which wavelet coefficients to keep and which to discard. We propose a strategy how to predict significant wavelet coefficients of the solution at the next time step from the current approximation. Numerical examples are presented.

Simulation and Optimal control of the hydration of concrete for avoiding cracks

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After mixing of concrete, the hardening starts by an exothermic chemical reaction known as hydration. As the reaction rate depends on the temperature *y(t,x)*, the time in the description of the hydration is replaced by the maturity $\int_0^t g(y(\tau ,x)) d \tau$. The temperature *y* is governed by the heat equation with a right hand side depending on the maturity and *y* itself. The goal is to produce cheap concrete without cracks. Simple crack criterions use only temperature differences, more involved ones are based on thermal stresses. Control is possible by the mixture of the concrete, the initial temperature and the use of cooling pipes. In this talk the modelling of the heat distribution in concrete, related optimal control problems and their numerical treatment are discussed.

3-D Fluid Dynamics Modeling with Radial Basis Functions

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Radial basis functions (RBF) have the advantage of being spectrally accurate for arbitrary node layouts in multi-dimensions with extreme algorithmic simplicity, and naturally permit local node refinement. We will show the first ever RBF method for a system of nonlinear coupled PDEs in 3-D spherical geometries. The application, pertinent to geophysicists, is mantle convection in the earth's interior at high Rayleigh numbers. Comparison to other codes in the community is done at low Rayleigh numbers, where the physics is known.

A Computer--assisted Proof of the Existence of Solutions to the Euler Equations

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We show existence of solutions to the Euler equations with some given parameters. It is a nonlinear system of three ordinary differential equations describing fluid flow. Following Yamamoto's idea, we integrate the equations to get a fixed-point problem. We analyse both Dirichlet boundary conditions and a mixture between Dirichlet boundary conditions and an integral boundary condition. The computer-assisted proof is computed with the free MATLAB package INTLAB.

Some algorithms for stable calculations with near-flat RBFs

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Spectral methods expand data in terms of basis functions, typically with certain orthogonality properties. Conversions between data values and expansion coefficients are usually very well conditioned. This approach works well in 1-D, but leads to severe restrictions already in 2-D with regard to domain shapes and node distributions. Radial Basis Functions (RBFs) work in any number of dimensions, but abandon all aspects of orthogonality. It seems counterintuitive to decrease their independence even further by making them nearly flat. However, we recently discovered that such computations can be both highly accurate and perfectly stable.We will here focus on the key properties of such near-flat RBFs, and on the numerical algorithms that now are available for this situation.

Local Projection Stabilization for convection-diffusion problems with characteristic layers

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We consider a singularly perturbed convection-diffusion problems with exponential and characteristic layers on the unit square. The discretisation is based on layer-adapted meshes. The standard Galerkin method and the local projection scheme are analysed for bilinear and higher order finite elements where in the latter case enriched spaces were used.For bilinears, first order convergence and second order supercloseness is shown for both the methods.For the enriched $\mathcal{Q}_p$-elements, which already contains the space $\mathcal{P}_{p+1}$, a convergence order $p+1$ in the $\eps$-weighted energy norm is proved for both the Galerkin method and the local projection scheme. Furthermore, the local projection methods provides a supercloseness result of order $p+1$ in local projection norm.

A numerical method for a nonlinear spatial population model with a continuous delay

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A numerical method for a time-dependent nonlinear partial integro-differential equation (PIDE) is considered. This PIDE describes a spatial population model. This model of the population density includes a given carrying capacity and the memory effect of this environment.
One problem concerning partial integro-differential equations is the data storage. To deal with this problem an adaptive method of third order in time is considered to save storage data at smooth parts of the solution. Beyond this a post-processing step adaptively thins out the history data.

High Order Finite Volume Schemes for Numerical Solution of Stationary and Non-Stationary Flows

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The aim of this work is the numerical solution of stationary and non-stationary compressible transonic inviscid flows by the finite volume method. The emphasis is laid on investigation of the flow field behaviour in the case of forced oscillatory motion of a wing. Chosen methods are based on total variation diminishing cell-centered form of the MacCormack scheme and on weighted least square reconstruction. Non-Stationary effects are simulated with the use of small distubance theory (3D) and arbitrary Lagrangian-Eulerian method (both 2D and 3D). Validation of the obtained results is done using standard test cases - non-stationary flow over the NACA 0012 profile (in 2D) and stationary flow over the Onera M6 wing (3D).

A comparison of semi-Lagrangian and Lagrange-Galerkin methods with high order finite elements

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We study the behaviour, in terms of CPU time and accuracy, of semi-Lagrangian versus Lagrange-Galerkin methods with high order finite elements in convection-dominated-diffusion equations and Navier-Stokes equations.

We use nodal and modal polynomials for semi-Lagrangian methods, whereas we use modal polynomials for the conventional and p-adaptive Lagrange-Galerkin methods.

Our conclusions are the following. (1) In terms of CPU time, semi-Lagrangian methods perform better with modal interpolation than with nodal interpolation; as for the accuracy, both interpolations are the same. (2) Lagrange-Galerkin methods are more accurate than semi-Lagrangian methods; but with respect to CPU time, they are comparable with semi-Lagrangian modal interpolation methods.

High-order finite volume methods for nonconservative hyperbolic systems

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In recent years, there have been increasing interest in the development of high-order numerical methods for nonlinear hyperbolic systems with source terms and/or nonconservative products. Part of this interest has been motivated by applications to the simulation of complex geophysical flows, e.g., shallow water flows, sediment transport, submarine avalanches, turbidity currents, etc. We give an overview on recently developed high-order finite volume schemes for hyperbolic systems written in nonconservative form, based on reconstructions of states. We also analyze some of their relevant properties, in particular, those related to the well-balanced character of the schemes. Finally, we test the performance of the methods by showing some applications to the simulation of geophysical flows.

The finite element immersed boundary method: model, stability, and numerical results

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The Immersed Boundary Method (IBM) has been designed by Peskin for the modelingand the numerical approximation of fluid-structure interaction problems.Recently, a finite element version of the IBM has been developed which offersinteresting features for both the analysis of the problem, the robustness andflexibility of the numerical scheme.In this talk we shall review our model and present a stability analysisshowing that the time step size and the discretization parameteralong the immersed boundary are linked by a CFL condition. This conditionis confirmed by our numerical experiments.

An A Posteriori Analysis of Operator Decomposition for Multiscale ODEs

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We analyze an operator decomposition time integration method for systems of ordinary differential equations that present significantly different scales within the components of the model. With this formulation we derive both an a priori error analysis and a hybrid a priori-a posteriori error analysis. The hybrid analysis has the form of a computable a posteriori leading order expression and a provably-higher order a priori expression. Both analyses distinguish the effects of the discretization of each component from the effects of operator decomposition. The effects on stability arising from the decomposition are reflected in perturbations to certain associated adjoint operators.

On the numerical simulation of some visco-plastic flows

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The main goal of this presentation is to address some of the issues associated with the numerical simulation of visco-plastic flows. Among these issues let us mention:
1) The fact that due to yield stress most viscoplastic models involve non-smooth operators.
2) Thermal dependance and thixotropy.
3) Compressibility.
The methods to be discussed will be validated by the results of numerical experiments.

Multiscale radial basis approximations for the numerical solution of PDE

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We consider meshfree schemes for partial differential equations, where the approximating spaces are formed by linear combinations of radial basis functions (RBF). The motivation for using RBF approximations comes from the possibility of achieving high accuracy with low complexity algorithms, for arbitrary choice of node locations, and, consequently, suitable for multi-dimensional irregular geometries. The new contributions of this work are two fold. Firstly, instead of the common formulation by collocation, we adopt a least squares scheme. Secondly, for solutions which features change in time, effort is directed to the study of a multi-level approach for radial basis functions. Numerical simulations are presented for the Black-Sholes model for European basket call option.

Goal-oriented error estimation and hp-adaptivity for discontinuous Galerkin finite element method applied to biharmonic equation.

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A posteriori goal-oriented error estimation for the discontinuous Galerkin finite element method is considered for the biharmonic equation. It is based on approximate solutions of the dual problem associated to the target functional. Using our estimation, we design and implement an error indicator, and the corresponding hp-adaptive algorithm. The resulting approximation spaces ensure an efficient error control of the prescribed functional. We present numerical experiments to illustrate the performance of the error indicator and of the resulting hp-adaptive algorithm. The results are comparated with uniform h-refinement and with other hp-adaptive refinament strategies.

Adaptive Two-Step Peer Methods for Incompressible Navier-Stokes Equations

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The paper presents a numerical study of two-step peer methods up to order five, applied to the nonstationary incompressible Navier-Stokes equations. These linearly implicit methods show good stability properties, but the main advantage over one-step methods lies in the fact that even for PDEs no order reduction is observed. To investigate whether the higher order of convergence of the two-step peer methods equipped with variable time steps pays off in practically relevant CFD computations, we consider typical benchmark problems. A higher accuracy and better efficiency of the new methods compared to third-order linearly implicit one-step methods of Rosenbrock-type can be observed. Therefore, they are good candidates for CFD computations that demand for high resolution.

Local Fourier analysis on triangular grids for quadratic finite elements

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To approximate solutions of mathematical physics problems defined on irregular domains it is very common to apply regular refinement to an unstructured input grid. Assuming that the coarsest grid is rough enough in order to fit the geometry of the domain, a hierarchy of globally unstructured grids is generated. This kind of meshes are suitable for use with geometric multigrid and this method is implemented using stencil-based operations to remove the limitations on the size of the problem that can be solved by using this process of refinement. In this framework, we are interested in the design of efficient geometric multigrid methods on hierarchical triangular grids using quadratic finite element methods.
To design these geometric multigrid methods, a Local Fourier Analysis is necessary. This analysis is based on an expression of the Fourier transform in new coordinate systems for space variables and for frequencies. This tool permits to study different components of the multigrid method in a very similar way to the rectangular grids case. Different smoothers are studied depending on the shape of the triangles. Numerical test calculations validate the theoretical predictions.

Tensor Approximation on Fibre-Crosses

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In order to treat problems with tensors efficiently, one has to keep all data in a low rank format. The most efficient lowrank format in terms of arithmetic complexity and storage requirements is the representation by elementary tensor sums. In this talk we will focus on the task to approximate a given high-dimensional tensor A by a low rank tensor X. Our goal is to find a good approximation X by sampling only very few entries of the tensor A. However, for tensors the construction of a low rank approximation by sampling only few points of A is a challenging task, both in terms of approximation quality and in terms of computational complexity. We present the state of the art and some numerical examples.

On the Convergence of Non-linear Additively Preconditioned Trust-Region Strategies and Applications to Non-linear Elasticity

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A new class of nonlinear additive preconditioning algorithms for the solution of non-linear and non-convex pointwise constrained minimization problems is formulated. We introduce a novel subdomain objective function which is minimized employing a Trust-Region strategy yielding a subdomain correction. In combination with a new a posteriori descent control for these additively computed corrections, the strategy becomes a non-linearly preconditioned globalization strategy. The mayor advantage of the new approach is the application of a local step-length criterion and, thus, a better resolution of local nonlinearities. Moreover, while computing local corrections, no parallel communication takes place, which, in turn, reduces the overall communication time. Alltogether, this opens new perspectives for the parallel solution of strongly nonlinear problems. In this talk, we also present numerical results from the field of non-linear elasticity in a Finite Element framework in 3d, illustrating the reliability and efficiency of the new strategy.

Entropy viscosity for nonlinear conservation laws

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We introduce a shock-capturing technique for solving nonlinear conservation laws. The method consists of adding a nonlinear viscosity to the Galerkin formulation of the nonlinear equation. The nonlinear viscosity is proportional to the residual of the entropy equation and limited by first-order dissipation. The method is very simple to implement on arbitrary finite elements meshes and is proved to be convergent in some simple cases. We illustrate the method numerically on various two-dimensional benchmark problems for scalar conservation laws and the Euler equations.

An implementation framework for solving high-dimensional PDEs on massively parallel computers

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Accurate solution of time-dependent, high-dimensional PDEs requires massive-scale parallel computing. We describe an implementation framework for multi-block cartesian grids and discuss techniques for optimization on clusters where the nodes have one or more multi-core processors. In particular, tools and methods for cache-performance analysis and control of process/thread locality are presented. We show some examples where the time-dependent Schrödinger equation is solved.

Adaptive numerical methods for the valuation of basket options and its Greeks

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We present an efficient approach for the numerical valuation of basket European and American options and some of its Greeks. After discretization in terms of adaptive finite elements in space and finite differences in time, the inequality constraints for the American options are reformulated as semismooth equations which are solved in terms of a primal-dual active set strategy.

To estimate the Greeks, we construct a piecewise multilinear interpolant of the pricing function with respect to the market parameters and compute its partial derivatives. The number of function evaluations necessary for the interpolation is reduced by using dimension-adaptive sparse grids.

Several numerical examples illustrate the robustness and applicability of the schemes.

Discontinuous Galerkin Methods for Bifurcation Phenomena in Fluid Flow through Open Systems

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In the past, studies of bifurcation phenomena of flow in a cylindrical pipe with a sudden expansion have proven inconclusive. In a new study we seek to exploit the O(2)-symmetric properties of the problem, thus making it tractable by reducing a 3-dimensional problem to a series of 2-dimensional ones. For the numerical solution of the incompressible Navier-Stokes equations we advocate the use of a Discontinuous Galerkin method and, in addition, develop goal-oriented error estimation techniques and an adaptive strategy to ensure the accurate location of any bifurcation points. We then apply the methods to a number of well documented cases, as well as the matter at hand.

Discrete maximum principles on prismatic finite element meshes

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In this talk, we discuss sufficient geometric conditions, which guarantee availability of the discrete maximum principles (DMPs) for finite element solutions of linear elliptic and parabolic problems on prismatic partitions. These conditions give two-sided bounds for the angles and heigths of prismatic finite elements. The sharpness of the obtained bounds is studied in numerical examples, where we demonstrate that the derived conditions are quite sharp, but room for improvement still exists.

Nitsche XFEM for the approximation of interface three field Stokes problems.

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In this talk we will discuss recent advances in the unfitted finite element method for incompressible flow. We will show how a Stokes problem with discontinuous shear viscosity can be discretized in an optimal way, even in the case where the interface is not fitted to the mesh, using Nitsche-type mortaring in the interior of the elements. In particular we show that the discrete inf-sup condition is satisfied thanks to a specially designed penalty term. The extension to the case of the three-field Stokes problem, relevant for free surface viscoelastic flows will then be discussed. Some numerical examples will be proposed to illustrate the theoretical results.

Discontinuous finite element methods for elasto-plasticity

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A new interior penalty discontinuous finite element method for small strain elasto-plasticity, using piecewise linear approximations, is introduced. The method allows for the scale corresponding to inter-element slip to be represented, unlike standard finite element methods that only allow for element interiors to exhibit plastic behavior.

A finite element method for PDEs with stochastic input data

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We compute the expectation and the two-point correlationof the solution to elliptic boundary value problems withstochastic input data. Besides stochastic loadings, viaperturbation theory, our approach covers also ellipticproblems on stochastic domains or with stochastic coefficients.The solution's two-point correlation satisfies a deterministicboundary value problem with the two-fold tensor productoperator on the two-fold tensor tensor product domain. Forits numerical solution we apply a sparse tensor productapproximation by multilevel frames. This way standardfinite element techniques can be used. Numerical examplesillustrate feasibility and scope of the method.

On Robust Parallel Preconditioning for Incompressible Flow Problems

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We consider time-dependent, incompressible flow problems discretized via higher order finite element methods. Applying a fully implicit time discretization and a linearization by a Newton or fixed point method leads to a saddle point system. This linear system is solved using a preconditioned Krylow method, which is fully parallelized on a distributed memory parallel computer.
We introduce a robust block-triangular preconditioner which is able to adapt to situations of dominant diffusion, reaction or advection. The key ingredients for our preconditioner are good approximations of the Schur complement and the velocity block. Beside numerical results of the parallel performance we explain and evaluate the main building blocks of the parallel implementation.

Monte Carlo simulation of biochemical reaction networks on the Cell Broadband Engine

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In computational systems biology, cellular reaction networks are frequently simulated by the stochastic simulation algorithm (SSA). Being a Monte Carlo method, it is computationally intensive due to the slow convergence but well suited for parallelization.

We have implemented SSA on the Cell broadband engine (Cell/BE), and we use it to simulate a few different models from the systems biology literature on a single Sony Playstation 3 (PS3), a cluster of PS3s and on the IBM BladeCenter QS22. The performance is compared to an efficient SIMD-ized and parallelized implementation on a multi-core PC workstation.

We also introduce CellMC, a multi-platform XSLT-based SBML compiler producing executables for multi-core PCs and for the Cell/BE from models expressed in the SBML markup language.

Adaptive local radial basis function method for interpolation and collocation problems

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We construct an adaptive algorithm for radial basis function (RBF) method based on residual subsampling technique and local RBF method known as RBF in finite difference mode. Residual subsampling technique is a simple strategy to decide whether nodes can be added or removed based on residuals evaluated at a finer point set. Local RBF method can be seen as the generalization of finite difference method without specific stencils. The use of variable shape parameters of RBFs based on the nodes spacings to slow down the growth of condition number is substansial in some numerical experiments. Numerical examples with localized features will be shown.

Numerical Simulation of Epitaxial Growth by Phase-Field Method

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In the contribution we consider the problem of epitaxial crystal growth. This problem is described by a phase-field model based on the Burton-Cabrera-Frank theory, see [Karma, Emmerich]. For numerical simulations performed in three dimensions, we develop a numerical scheme based on the finite difference method. We investigate the influence of numerical parameters on the growth patterns. We present computational studies related to the pattern formation and to the dependence on model parameters. The next step in modelling is incorporation of elastic effects generated by the misfit strain between the substrate and the epitaxial layer.
[Karma] A. Karma , and M. Plapp, Phys. Rev. Lett. 81, 20 (1998), pp. 4444–4447.
[Emmerich] H. Emmerich, Continuum Mech. Thermodyn., 15 (2003), pp. 197-215.

Adaptive Multi Level Monte Carlo Simulation

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We describe generalizations of a multilevel Forward Euler Monte Carlo Method (FEMCM) introduced by M. Giles for the approximation of expected values depending on the solution to an Itô SDE. Giles proposed a multilevel FEMCM based on a hierarchy of uniform time discretizations and control variates to reduce the Computational Cost (CC) required by a standard, single level FEMCM. This work introduces a hierarchy of non uniform time discretizations generated by adaptive algorithms which are based on a posteriori error expansions.
Under sufficient regularity conditions, both our analysis and numerical results, which include one case with singular drift and one with stopped diffusion, exhibit savings in the CC to achieve an accuracy of O(tau) from O(tau^{-3}) to O(tau^{-2}\log^2(tau)).

Adaptive Finite Element Methods for Turbulent Flow

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We present recent advances on adaptive computation of turbulent flow based on General Galerkin (G2) finite element methods, with kinetic energy dissipation directly proportional to the residual of the Navier-Stokes equations. The adaptive method is based on a posteriori error estimation, and the mathematical foundation is weak solutions and well-posedness of mean value output. Full resolution of turbulent boundary layers is impossible, instead we use skin friction boundary conditions with skin friction treated as data. G2 opens new possibilities for high Reynolds number flow simulation for industrial problems with complex geometry, of which we present several examples. All methods are implemented in the open source software Unicorn, freely available at the FEniCS project.

Hybrid modeling of plasmas

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Space plasmas are often modeled as fluids. However, many observed phenomena cannot be captured by fluid models. Therefore kinetic models are used, where also the velocity space is resolved. Particle in cell (PIC) methods represent the charges as discrete particles, and the electromagnetic fields are stored on a spatial grid. For the study of global problems in space physics, hybrid model are often used, where ions are represented as particles, and electrons are modeled as a fluid.
Here we present the mathematical and numerical details of a general hybrid model for plasmas. The implementation uses adaptive grid refinement and is parallel. We show examples of classical test problems, and we show results from applications for the Moon and Mars.

A priori error estimates for DGFEM applied to nonstationary nonlinear convection-diffusion equation

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We deal with a numerical solution of a scalar nonstationary convection-diffusion equation with nonlinear convective as well as diffusive terms which represents a model problem for the solution of the system of the compressible Navier-Stokes equations. We present a discretization of this model equation by the discontinuous Galerkin finite element method (DGFEM) with several variants of the interior penalty, namely NIPG, SIPG and IIPG types of stabilizations of diffusion terms. Moreover, under some assumptions on the nonlinear terms, domain partitions and the regularity of the exact solution, we introduce a priori error estimates in the L^{\infty}(0,T; L^2(\Omega))-norm and in the L^{2}(0,T; H^1(\Omega))-semi-norm. A sketch of the proof and numerical verifications are presented.

Monolithic FEM techniques for nonlinear flow with temperature, pressure and shear-dependent viscosity

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We present special numerical simulation methods for non-isothermal incompressible viscous fluids which are based on LBB-stable FEM discretization techniques together with monolithic multigrid solvers. For time discretization, we apply the fully implicit Crank-Nicolson scheme of 2nd order accuracy while we utilize the high order Q_2 P_1 finite element pair for discretization in space which can be applied on general meshes together with local grid refinement strategies including hanging nodes. To treat the nonlinearities in each time step as well as for direct steady approaches, the resulting discrete systems are solved via a Newton method based on divided differences to calculate explicitly the Jacobian matrices. In each nonlinear step, the coupled linear subproblems are solved simultaneously for all quantities by means of a monolithic multigrid method with local multilevel pressure Schur complement smoothers of Vanka type. For validation and evaluation of the presented methodology, we perform the MIT benchmark 2001 of natural convection flow in enclosures to compare our results w.r.t. accuracy and efficiency. Additionally, we simulate problems with temperature and shear dependent viscosity and analyze the effect of an additional dissipation term inside the energy equation. Moreover, we discuss how these FEM multigrid techniques can be extended to monolithic approaches for viscoelastic flow problems.

Dynamics of Bose-Einstein Condensate with Dipolar interaction

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We study the numerical simulation of time-dependent Gross-Pitaevskii equation describing Bose-Einstein condensation of trapped dipolar quantum gases. We mainly simulate the symmetry breaking, the blow-up of solutions, the dynamics of the vortices, etc, under the Dipolar interaction and the external potential.

Auto-regularization for ill-posed inverse problems

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We consider two different approaches for regularization. The common goal is to solve the given ill-posed problem with matrix A on the signal subspace restraining the noise subspace. The first method is a generalization of Tykhonov regularization with a weight function depending on the original matrix A. Here the Tykhonov correction is modelled as a polynomial coinciding with A for large eigenvalues and vanishing for near zero eigenvalues. In the second approach we use a preconditioned iterative solver based on the MSPAI preconditioner. Here the main task is to design a preconditioner that coincides with A, resp. $inv(A)$, on the signal subspace and vanishes for the noise subspace. The preconditioner should lead to a better reconstruction of the original information in less iterations than the unpreconditioned solver. For both methods we present numerical examples.

ADI finite difference schemes for the Heston PDE with correlation term

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This talk deals with numerical methods for solving time-dependent multi-dimensional PDEs arising in financial option pricing theory. For the numerical solution we consider the well known method-of-lines approach, whereby the PDE is first discretized in the spatial variables, yielding a large system of ordinary differential equations (ODEs), which is subsequently solved by applying a suitable numerical time-discretization method. In general, the obtained systems of ODEs are very large and stiff, and standard time-discretization methods are not effective anymore. Accordingly, tailored numerical time-stepping methods are required. In the past decades, operator splitting schemes of the Alternating Direction Implicit (ADI) type have proven to be a successful tool for efficiently dealing with many of such systems. However, PDEs modelling option prices often contain mixed-derivative terms, stemming from correlations between the underlying Brownian motions, and ADI schemes were not originally developed to deal with such terms. In this talk we shall consider the popular Heston stochastic volatility model, which is a time-dependent two-dimensional convection-diffusion equation containing a mixed derivative term. After describing its semi-discretization by finite differences, we show how various ADI schemes can be adapted to the numerical solution of the obtained ODE systems. We subsequently discuss several recent theoretical results on the stability of these schemes. Next, numerical experiments are presented for realistic examples from the literature. Finally, we discuss extensions and future research directions.

Adaptive ADER Schemes for Scalar Conservation Laws using Kernel-Based WENO Reconstructions

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ADER schemes are recent finite volume methods for scalar hyperbolic conservation laws, which can be viewed as generalizations of the classical first order Godunov method to arbitrary high orders. In this talk, we combine high order flux evaluations of ADER with kernel-based WENO reconstructions, yielding finite volume discretizations of arbitrary high order, where the control volumes are adaptively modified during the simulation. The utilized kernel-based WENO reconstruction is, unlike previous WENO schemes, numerically stable and very flexible. This talk first explains the key ingredients of the ADER method, before important theoretical and computational aspects of kernel-based WENO reconstructions are addressed. Finally, supporting numerical examples are presented for illustration, showing the good performance and the enhanced robustness of the proposed ADER method.

Multi-objective Optimization of MIMO Antenna Systems

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The performance of MIMO antenna systems is highly dependent on the received signal levels and also on the correlation between the signals. Also, from a radio-engineering point of view, there are limitations on the S-parameters of the design. Further, the antennas also need to share space with other devices on the platform, which adds requirements on the size of the antennas. All these aspects often lead to conflicting requirements, which traditionally are dealt with by weighting the different requirements into a single requirement. The trial-and-error approach of setting those weights has many disadvantages, and multi-objective optimization provides a better insight in possible tradeoffs. The optimization algorithm is a novel response surface method based on approximation with radial basis functions. It is combined with CAD software, mesh generation software, electromagnetic solvers and a decision support system.

Numerical Methods for 3D Advection-Diffusion-Reaction Models

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We present numerical methods for 3D advection-diffusion-reaction models governed by the following system of equations $c_t + \nabla \cdot (vc) - \nabla \cdot (D \nabla c) = R(c)$. Several phenomena of relevant interest can be studied by using these models, such as: chemotaxis model, the pollutant transport in the atmosphere, the mucilage dynamics, the ash-fall from vulcano etc. One of the simplest numerical approaches for the solution of model is the so-called operator-splitting, in which the solution procedure is split up into independent steps corresponding to the advection, diffusion, and reaction processes, and each step is handled independently. By using the Strang splitting, we obtain second order accuracy, provided each subproblem is solved with a second order accurate method.

Analysis of a variant of the fractional-step timestepping-scheme: Comparison to other schemes and application to fluid flow

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In the context of fluid flow stable and non-dissipative time-stepping schemes are required. In this talk a new variant of the fractional-step time-stepping scheme which was proposed by Glowinski is analyzed. The numerical stability, dissipation, and damping properties are considered and compared to other well known time-stepping schemes. These criteria are discussed for choosing appropriate time-stepping schemes for long time computations in fluid flow. The various schemes were considered by the means of numerical examples.

Unified continuum modeling of 3D fluid-structure interaction

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We propose a Unified Continuum (UC) model of incompressible fluid-structure interaction in Euler (laboratory) coordinates with a moving mesh for tracking the fluid-structure interface as part of the General Galerkin (G2) discretization, allowing simple and general formulation and efficient computation. The model consists of conservation equations for mass and momentum, a phase convection equation and a Cauchy stress and phase variable as data for defining material properties and constitutive laws. We present recent advances in mesh motion methods based on mesh adaptation (split, collapse and swap) combined with elastic smoothing. A 2D benchmark as well as a 3D turbulent flexible flag test are computed. The Unicorn implementation is published as part of the FEniCS Free Software project.

A Parallel Mesh Adaption Method for Massively Parallel Architectures

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To obtain good parallel speedup, one often needs to design algorithms with minimal communication and synchronization. For massively parallel computations, the large amount of processors increase the demand on concurrent and load balanced algorithms. We present a parallel mesh adaption method suitable for large scale finite element computations. The refinement is based on recursive edge bisection, where both propagation and synchronization problems are solved within a highly concurrent communication pattern. To obtain good parallel efficiency a dynamic load balancer, based on a remapping scheme, redistributes the mesh prior to any adaption. Here, we present a performance study, comparing scaling and complexity of different imbalance models and edge bisection algorithms.

Discontinuous Galerkin Methods for Miscible Displacement Problems

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Miscible displacement methods are increasingly used in oil recovery to enhance the production. A model is presented which models incompressible, miscible displacement in porous media. The discretisation in the spatial variables consists of a discontinuous Galerkin method, which is combined with a mixed FE method.
Under minimal assumptions on the regularity of the problem, it is shown that subsequences of numerical solutions converge to weak solutions of the problem. Novel features are:
(i) The scheme does not require stabilisation or regularisation of the advection term.
(ii) Convergence does not rely on uniqueness of the exact solutions or on convexity or smoothness of the domain.
(iii) The dG spaces are embedded to facilitate an analysis which is in form of a conforming method.

A posteriori error estimates and stopping criteria for iterative solvers

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We consider the finite volume and the lowest-order mixed finite element discretizations of a second-order elliptic pure diffusion model problem. We derive guaranteed and fully computable a posteriori error estimates which take into account an inexact solution of the associated linear algebraic system and hence gather the information about both discretization and algebraic errors. We claim that the discretization error, implied by the given numerical method, and the algebraic one should be in balance, i.e., that it is enough to solve the linear algebraic system to the accuracy which guarantees that the algebraic part of the error does not contribute significantly to the overall error. Our estimates allow a reliable and cheap comparison of the discretization and algebraic errors. One can thus use them to stop the iterative algebraic solver at the desired accuracy level, without performing an excessive number of unnecessary additional iterations. Several numerical experiments illustrate our theoretical results.

A new DG method for the Stokes problem with a priori and a posteriori error analysis

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We present a discontinuous Galerkin method for the velocity-pressure formulation of the 2D Stokes problem, based on (P_k^2, P_{k-1}) discontinuous elements for k = 1, 2 or 3. The new feature of this method is its stabilization term, which yields the robustness with respect to large values of the stabilization parameter : our solution then tends to the one of the (P_k^2, P_{k-1}) nonconforming approximation of the Stokes problem. We show the well-posedness of the discrete formulation and we derive optimal *a priori* error estimates. Our choice of the stabilization allows us to define a reliable and efficient *a posteriori* error estimator, based on a locally conservative tensor of H(div) constructed from the discrete solution. Numerical tests and comparisons with another DG method are carried out.

Bechmarking finite element methods for the Brinkman problem

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Various finite element families for the Brinkman flow (or Stokes-Darcy flow) are tested numerically. Especially the effect of small viscosity is studied. In this case the equations are best described as singularly perturbed Darcy equation.
The tested finite elements are the MINI element, Taylor-Hood P2-P1 element, and stabilized P1-P1 and P2-P2 methods. The benchmark problem is the physically correct Poiseuille flow profile. The emphasis of the numerical tests is on the a posteriori and adaptive methods. Also the effect of boundary conditions is tested using both the traditional boundary conditions and Nitsche's method.

Numerical and Practical Method for Statistical Quality Control Using Local Fractal Dimension in Discrete Time Series

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In order to monitor numerical quality fluctuation or unstable quality time series in general information systems, a numerical method using local fractal dimension has been proposed. Based on numerical experiments, it has been observed that the moving LFDs on both of the uniform and normal random processes belong to almost the same normal distribution. The obtained results can be easily applied to general numerical quality systems using the 95% confidence interval. As advanced applications, the proposed method can be also applied to the difference time series between altitudinal seawater temperatures. That is, the prediction of abnormal phenomena such as warnings of phase transitions in monitoring systems may be possible, in case a moving LFD falls outside the 95% confidence interval.

Integrating forms and functionals: towards efficient and reusable structures.

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Whether it is in Newton-like methods, time-stepping schemes or the evaluation of errors and estimates, the integration of forms and functionals is ubiquitous in finite element codes. It is also a part of the code, where the outer structure, the loop over the mesh cells and faces, is generic, while the innermost part, the integration over a single cell or face is problem dependent. Modern multicore architectures mandate the use of a sophisticated parallel outer loop which should be part of a finite element library without requiring to be recoded for every application. This in turn poses the question of an interface to the cell integrator, which is versatile and efficient, without necessitating the generation of data not required by a particular problem.

Numerical modelling of steady and unsteady Newtonian and non-Newtonian fluids flow

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This paper deals with the numerical solutions of laminar incompressible flows for generalized Newtonian (Newtonian and non-Newtonian) fluids in 2D and 3D branching channel. The mathematical model is the incompressible system of Navier-Stokes equations. The right hand side of this system is defined by power-law model. The unsteady system modified by artificial compressibility method in continuity equation is solved by multistage Runge-Kutta finite volume method. Steady solution is achieved with using steady boundary conditions. Two numerical approaches are used for unsteady computation. The artificial compressibility method and dual-time stepping method. Numerical results for Newtonian and non-Newtonian in 2D and 3D branching channel are presented and compared.

Homogenization Theory for Transport of Particles in a Strong Mean Flow with Periodic Fluctuations

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The transport of passive scalars has been well studied using the advection diffusion equation in the case of periodic fluctuations with a weak mean flow or a mean flow of equal strength through homogenization techniques. However in the regime of strong mean flow homogenization seems to breakdown.We study the transport of passive scalars using Monte Carlo simulations for tracer trajectories and obtain the enhancement in diffusivity. We also compute the enhancement in diffusivity by extrapolating the homogenization code for the equal strength case. Comparing the two we note that homogenization theory does in fact seem to work in this case as well.We then develop a mathematical framework of non-standard homogenization theory to explain the numerical result.

Tensor product approximation of operators and functions in the Hartree-Fock equation

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We discuss newly developed algorithms for the efficient computation of the Coulomb and Exchange matrices in the Hartree-Fock equation. The discrete tensor product approximation on n x n x n Cartesian grids, allows to compute the corresponding multi-dimensional convolution integrals with linear cost O(n log n). Rank reduction by the multigrid accelerated Tucker tensor decomposition proposed recently enables the computation of the Hartree potential by the 3D tensor product convolution on large spacial grids, which are necessary to resolve multiple strong cusps in electron density. Efficient numerical evaluation of the Exchange operator is one of the bottleneck problems in the computational quantum chemistry. Fast multi-linear algebra operations in low-rank tensor formats make feasible the direct computation of the nonlocal Exchange operator with almost linear cost in the univariate grid size n.
We illustrate the efficiency of our methods by electronic structure calculations for the molecules CH4, C2H6, H2O and CH3OH. In particular, the accuracy of order 10^(-5) in max-norm for the Hartree potential is achieved on large 3D Cartesian grids with the univariate grid size up to n ~ 10^4, in the time scale of several minutes in Matlab.

Tensor-structured numerical methods for elliptic boundary-value/spectral problems in high dimensional applications

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Modern methods of low rank tensor-product approximation allow an efficient data-sparse representation of functions and operators in R^d. The main tool is the robust and fast nonlinear (multigrid based) tensor approximation using the Tucker/canonical formats in high dimension. This allow to perform various tensor operations with linear scaling in d. In particular, we mean the convolution transform, FFT, the tensor-tensor contracted product or inversion of tensor-structured matrices. We focus on the construction of low tensor rank spectrally close preconditioners for elliptic operators in R^d and then dicsuss the concept of rank structured truncated iteration for solving related BVP/EVPs in higher dimension. The asymptotic complexity of the considered approach is estimated by O(d n log^{*}n), where n is the univariate discrete problem size. Numerical illustrations demonstrate the efficiency of tensor methods in computational quantum chemistry and in the stochastic PDEs.

Towards a micro-scale simulation of convective gel drying

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A 3D mathematical model for the process of convective drying of gels at the micro-scale is presented. Drying is the last step in the production of gels from colloidal suspensions. Convective drying is an inexpensive process, but because of the presence of a liquid phase, capillary forces usually destroy the solid structure. Since these effects cannot be quantified yet, a numerical simulation of the process shall give more insight into the stress and the damage in the solid phase. Simulation results for the fluid part of the process are presented, which involve convective and diffusive transport as well as phase transition phenomena. A stationary, uniform grid is chosen for the discretization and the liquid-gas interface is tracked with the volume-of-fluid method in a time-stepping scheme.

Lagrangian discretization of hyperelastic systems, and introduction of plasticity

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Firstly, we extend the Lagrangian Finite Volumes hydrodynamic schemes to hyperelasticity. Doing this, one of the crucial point is the discretization of the jacobian matrix of the motion. We suggest a discretization which guarantees some geometric requirements and the exact degeneracy of the extended scheme to the chosen hydrodynamic one. The extended scheme is conservative and satisfies an entropy criterion.Secondly, we present a model of finite plasticity for which we obtain analytic solutions for flyer-plate experiment. This model is discretized by the preceding scheme. The model and the scheme are validated by comparison with analytic solutions and experimental datas.

Stability of finite element discretizations of convection-diffusion equations

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We discuss the application of the finite element method to the numerical solution of scalar convection-diffusion or convection-diffusion-reaction equations. We are interested in the singularly perturbed case when the diffusivity is significantly smaller than the convection. The numerical solution of such problems is still a challenge, despite the fact that it has been the subject of an extensive research during several decades.

In the presentation we shall review various finite element discretizations currently used for the numerical solution of convection dominated problems. Our main aim is to discuss the stability of these methods with respect to various norms and to compare these theoretical results with the actual quality of numerical solutions obtained for model problems.

Finite difference method for solution of tidal wave equations

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For a system of the shallow water equations type, describing propagation of tidal waves, a finite difference scheme on an unstructured grid is constructed. Its properties are studied; in particular,it is shown that after elimination of a part of the unknowns from the finite difference scheme the matrix of the obtained system is an M-matrix.

Numerical solution of Volterra integral equations with weakly singular kernels which may have a boundary singularity

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We propose a piecewise polynomial collocation method for solving linear Volterra integral equations of the second kind with kernels which, in addition to a weak diagonal singularity, may have different boundary singularities. To avoid problems associated with the use of strongly graded grids we first perform in the integral equation a change of variables so that the singularities of the derivatives of the solution will be milder or disappear. After that we solve the transformed equation by a collocation method on a mildly graded or uniform grid. Global convergence estimates are derived and a collection of numerical results is given.

Global error control for the simulation of the time-dependent Schrödinger equation

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A posteriori error estimation theory is used to derive a relation between local and global errors in the temporal propagation for the time-dependent Schrödinger equation (TDSE). This enables us to design an *h,p*-adaptive Magnus–Lanczos propagator capable of controling the global error of the time-marching. The step size control can be performed locally, implying that the Schrödinger equation has to be solved only once. The TDSE can be used to model the interaction of a molecule with time-dependent fields. We present results for molecules including bounded and dissociative states, illustrating the performance of the method. Moreover, we describe how our evolution method can be combined with an adaptive finite element discretization in space allowing for error control in both space and time.

Efficient solution of an optimal control problem in quantum chemistry

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We consider an optimal control problem for the time-dependent Schrödinger equation modeling molecular dynamics. Given a molecule in its ground state, the interaction with a tuned laser pulse can result in an excitation to a state of interest. We use a reformulation to Fourier space for reducing the dimensionality of the problem of how to optimally choose the shape of the laser pulse, and then apply the BFGS algorithm for solving the optimization problem. By exploiting the self-adjointness of the Schrödinger equation, we devise an efficient scheme for computing the gradient. We show computational results for some relevant problems and relate the computational procedure to experimental settings.

Hierarchical error estimates for non-smooth problems

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Hierarchical error estimates are based on a finite dimensional extension of the given finite element space S by a (sufficiently large) incremental space V. A posteriori error estimates consisting of local error indicators are then obtained from local defect problems as resulting from a suitable decoupling of V. The theoretical analysis of this concept is well-understood for self-adjoint linear problems but much less developed for nonlinear problems. Nevertheless, hierarchical error indicators have been applied successfully even to non-smooth problems like contact problems in elasticity, phase transition or phase separation. In this talk, we will report on some of these applications and comment on recent theoretical results.

Geometric topics in reliable finite element modeling

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Nowadays, it is becoming more and more obvious that various reliability aspects in the FE modeling are closely related to the quality and geometric properties of the underlying finite element (FE) meshes, which naturally poses the following basic questions: meshes with which characteristics are really needed, and how to construct (and further suitably adapt/refine) such meshes? Various subjects in the mesh generation are relatively well studied (and implemented in most of existing software) in the two-dimensional case, but already in 3D, the mesh generation processes meet many serious algorithmic and implementation obstacles. Moreover, mesh generation in higher dimensions is, in fact, studied extremely weakly. However, the capacity of modern computers (and the nature of FEM) already allows simulations of higher-dimensional models, which are used more and more often in modern sciences and engineering. We are planning to report on own progress in this direction and also describe several open areas/subjects for further research.

A Convergent Adaptive Uzawa Finite Element Method for the Nonlinear Stokes Problem

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Solving the steady state Stokes equation is equivalent to minimizing a functional with respect to the pressure. In the linear case the Uzawa algorithm can be deduced by the method of steepest descent direction applied to this functional. We generalize this technique to nonlinear problems using quasi-norm techniques induced by the nonlinear nature of the problem.
The adaptive Uzawa algorithm (AUA) is based on an Uzawa outer iteration to update the pressure and an inner iteration using an adaptive Galerkin finite element method for velocity. The sequence of pressures and velocities produced by AUA is shown to converge to the solution of the nonlinear Stokes problem.

On a bisection algorithm that produces conforming locally refined simplicial meshes

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We examine the longest-edge bisection algorithm that chooses for bisection the longest edge in a given face-to-face simplicial partition of a bounded polytopic domain in R^d. Dividing this edge at its midpoint, we define a locally refined partition of all simplices that surround this edge. Repeating this process, we obtain a family of nested face-to-face simplicial partitions [1]. Then we generalize this algorithm using the so-called mesh density function. We prove convergence of the generalized algorithm. Numerical examples will be presented.
[1] S. Korotov, M. Krizek, A. Kropac: Strong regularity of a family of face-to-face partitions generated by the longest-edge bisection algorithm, Comput. Math. Math. Phys. 48 (2008), 1687-1698.

A conservative level–set model for two-phase flow with Cahn–Hilliard contact line dynamics

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The level–set method provides an accurate and efficient mathematical model for PDE-based two-phase flow simulations. However, the plain model fails in moving contact lines where the interface between the two fluids touches solid walls. The phase field model, an alternative approach based on the Cahn–Hilliard equation, accurately models the physics of contact lines, but is often too expensive for large simulations. The Cahn–Hilliard equation can be mathematically interpreted as an extension of a conservative level–set formulation by a fourth and second order diffusion term. This enables us to use a level–set-based model with Cahn–Hilliard information added close to boundaries. We provide mathematical and numerical evidence for consistency of the switch between the two models.

Study of Moving Mesh Strategies for Hyperbolic Conservation Laws

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The paper deals with an adaptive numerical solution of the time dependent partial differential equations such as the Euler equations in the fluid dynamics. The subject-matter of this paper is the comparative study of moving mesh strategies we have developed for problems with moving discontinuity. The proposed vertex quality parameter moving mesh method (VQPMM) is numerically tested and compared with a moving mesh method based on the moving mesh partial differential equations (MMPDEs). The ability of both types of methods is tested on two dimensional problems. The special attention is paid to the conservative solution interpolation which satisfies the so called geometric mass conservation law. The mesh adaptations is applied in the framework of the high-order ADER finite volume method.

The discontinuous Galerkin method for convection-diffusion problems in time-dependent domains

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This paper is concerned with the numerical treatment of convection-diffusion problems in time-dependent domains. A suitable formulation of the governing equations is derived using the Arbitrary Lagrangian-Eulerian (ALE) method. The equations are then discretised in space using the discontinuous Galerkin method. The resulting space-semidiscretisation scheme is numerically tested on the compressible Navier-Stokes equations describing the flow of compressible viscous gases. The particular form of these equations allows the use of a semi-implicit time discretization, which has already been extensively studied in the case of stationary computational domains.

An Embedded Boundary Method for Compressible Navier-Stokes/LES Equations

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A second order accurate Embedded Boundary method to set boundary conditions for the compressible Navier-Stokes equations in two- and three dimensions is presented. The explicit Runge-Kutta time-stepping scheme is stable with a time step determined by the grid size away from the boundary, i.e. the method does not suffer from small-cell stiffness. To mitigate the effects of unresolved flows using the embedded boundary method in boundary layers, we have used local mesh refinement, LES and relaxed the no-slip condition at walls to using so called wall-conditions. We show that for resolved flows the results are excellent. When the flow and/or geometry are very unresolved we observe 'numerical rougness' which can to some extenent be mitigated by the use of LES and wall-model.

The issue of arbitrary level hanging nodes in 3D

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This contribution deals with the hp version of the finite element method in three dimensions. This method is very succesfull thanks to its ability to use appropriate type of elements in different parts of a computational domain. In order to avoid unnecessary refinements in the mesh, we use arbitrary level hanging nodes. That reduces number of degrees of freedom and also simplifies the adaptivity algorithm. On the other hand, construction of conforming basis functions in highly unstructured hexahedral mesh becomes rather complicated. We focus on geometrical aspects of mesh refinement and basis functions construction.

Analysis of the Brinkman problem with H(div)-conforming finite elements

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We study the non-conforming finite element approximations of the Brinkman problem with H(div)-conforming elements. The Brinkman problem is a combination of the Stokes and Darcy equations. Nitsche's method is applied to achieve consistency and stability in the mesh-dependent energy norms introduced. Furthermore, we present a local postprocessing scheme for the pressure. Using the postprocessed pressure we are able to derive both efficient and reliable a posteriori error estimators for the problem. All the results are parameter independent, and hold true even for the limiting Darcy problem.

A monolithic space-time multigrid solver for distributed control of the time-dependent Navier-Stokes system

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We present a hierarchical space-time solution concept for optimization problems governed by the time-dependent Navier-Stokes system. Discretization is carried out with finite elements in space and a one-step-scheme in time. By combining a Newton solver for the treatment of the nonlinearity with a monolithic space-time multigrid solver for the linear subproblems, we obtain a robust solver with a convergence behaviour which is independent of the number of unknowns of the discrete problem and robust with regard to the considered flow configuration. Several numerical examples demonstrate the efficiency of this approach.

A posteriori error control for discontinuous Galerkin methods in time-dependent problems

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I will address the derivation of a posteriori error bounds for time-dependent problems where the spatial variable is discretized using discontinuous Galerkin methods. Most of the talk is about a recent paper, joint with E. Georgoulis, for linear parabolic problems, we derive energy-norm a posteriori error bounds for an Euler timestepping method combined with various spatial discontinuous Galerkin schemes for linear parabolic problems. For accessibility, we address first the spatially semidiscrete case, and then move to the fully discrete scheme by introducing the implicit Euler timestepping. All results are presented in an abstract setting and then illustrated with particular applications. Time allowing, I'll talk about extensions, mainly work in progress on second order hyperbolic problems.

A Spectral Time-Domain Method for Computational Electrodynamics

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The finite-difference time-domain method has been a widely-used technique for solving the time-dependent Maxwell's equations. This talk presents an alternative approach to these equations in the case of spatially-varying permittivity and/or permeability, based on Krylov subspace spectral (KSS) methods. KSS methods for scalar time-dependent PDE are high-order explicit methods that compute each Fourier coefficient of the solution using techniques developed by Golub and Meurant for approximating elements of functions of matrices by Gaussian quadrature in the spectral domain. We show how they can be generalized to systems of equations, such as Maxwell's equations, by choosing appropriate basis functions. We also discuss the implementation of appropriate boundary conditions.

Domain decomposition and radial basis function approximation for PDE problems

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When using infinitely smooth radial basis functions (RBFs) to approximate the solution of a PDE, the resulting linear system of equations is dense. With direct solution methods this leads to high computational costs and memory requirements. Furthermore, the matrices become increasingly ill-conditioned both with size and as the shape parameter of the RBFs become small. In this talk, we explore how partition of unity methods can be used in this context to break up the global problem into smaller subproblems. We combine this with the recently developed RBF-QR method, which allows stable numerical solution for small shape parameter values. We hope to show that an unconstrained choice of shape parameter leads to improved convergence rates for the error as the density of node points increase.

High Order Difference Method for Fluid-Structure Interaction in Human Phonation

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The interaction between the vocal folds in the larynx and the air flow from the lungs constitutes the source of sound for our speech. Modeling that fluid-structure interaction can help to identify voice disorders and to provide a tool for surgeons to simulate larynx surgery in the future. In our 2D model, we simulate the air flow by solving the compressible Navier-Stokes equations based on the arbitrary Lagrangean-Eulerian formulation for the moving geometry using high order summation by parts operators. The vocal folds are modeled as a compressible neo-Hookean hyperelastic material. The corresponding Lagrangean field equations are solved with a high order difference method similar to our flow method. Fluid and structure are coupled by a partitioned explicit approach.

Finite element approximation of the linear stochastic Cahn-Hilliard equation

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We analyze spatially semidiscrete and completely discrete approximations of the linear stochastic Cahn-Hilliard equation. Strong convergence estimates are obtained. The proofs are based on precise error estimates of the corresponding deterministic finite element problem.

Some recent theoretical and numerical contributions to stochastic homogenization and related problems

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The talk will overview some recent contributions on several theoretical aspects and numerical approaches in stochastic homogenization.In particular, some variants of the theory of classical stochastic homogenization will be introduced. The relation between such homogenization problems and other multiscale problems in materials science will be emphasized. On the numerical front, some approaches will be presented, for acceleration of convergence in stochastic homogenization (representative volume element, variance reduction issues, etc) as well as for approximation of the stochastic problem when the random character is only a perturbation of a deterministic model. The talk is based upon a series of joint works with X. Blanc (CEA, Paris), PL. Lions (College de France, Paris), and F. Legoll, A. Anantharaman, R. Costaouec (ENPC, Paris).

RBF generated finite differences on scattered nodes for hyperbolic PDEs

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Finite differences combined with explicit time-stepping are attractive to use for hyperbolic PDEs. However, they require a structured mesh. For scattered data layouts or geometries that are not amenable to gridding, meshless methods may be an alternative. In this talk, we look at different ways of generating stencils over scattered nodes using radial basis functions (RBFs). The flexibility of the RBF method, for instance allowing adaptivity, is thus combined with the cost-efficiency of finite differences. Preliminary results show that it is not so easy to generate stencils that allow for explicit time-stepping for purely hyperbolic problems. We will investigate this further and see if we can find a viable approach.

Error estimation and anisotropic mesh refinement for aerodynamic flow simulations

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Aerodynamic flow fields are dominated by anisotropic features at both boundary layers and shocks. Solution-adaptive local mesh refinement can be improved considerably by respecting those anisotropic features. Two types of anisotropy indicators are presented. Whereas the first one is based on polynomial approximation properties and needs the evaluation of second and higher order derivatives of the solution the second one exploits the inter-element jumps arising in discontinuous Galerkin methods and can easily be used with higher order discretizations and even hp-refinement. Examples for sub-, trans- and supersonic flows combining these anisotropic indicators with reliable residual or adjoint based error estimation techniques demonstrate the potential and limitations of this approach.

A MHD problem on unbounded domains - Coupling of FEM and BEM

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We consider the magnetohydrodynamic (MHD) problem:

$$
\begin{aligned}
B_t &= -\operatorname{rot} E && \text{in } \Omega_c \\
\operatorname{rot}(m^{-1}B) &= s\,(E + u \times B + j^c) && \text{in } \Omega_c \\
\operatorname{rot}(m^{-1}B) &= 0 && \text{in } \Omega_v \\
\operatorname{div} B &= 0 && \text{in } \Omega.
\end{aligned}
$$

In the so-called direct problem, the magnetic induction B and the electric field E are unknown and u is a given incompressible flow field. The domain Ω consists of conducting and insulating regions (Ω_c and Ω_v). After semidisrectization in time with the implicit Euler-scheme, a Lagrange finite element approach is used in a bounded region and a boundary element approach in the unbounded insulating region. We present results on the well-posedness of the continuous and the semidiscrete problem, algorithmic aspects and first results of the numerical analysis.

Multiscale Mixed Finite Elements for the Stokes-Brinkman Equations

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We present a multiscale mixed finite-element method for solving the Stokes-Brinkman equations. This gives a unified and efficient approach to simulating flow in carbonate reservoirs that contain both free-flow and porous regions. The multiscale method uses a standard Darcy model to approximate pressures and fluxes on a coarse grid, but captures fine-scale effects through basis functions determined from local Stokes-Brinkman flow problems on an underlying fine-scale grid. For the special case of Darcy flow in a homogeneous medium, the multiscale elements reduce to the lowest-order Raviart-Thomas elements. We present a few illustrative numerical experiments and discuss various discretizations of the fine-scale problem to enable efficient solution of cases with multi-million cells in 3D.

Well-posedness and stability of a coupled fluid flow and heat transfer problem

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As a part of a microfluidic and heat transfer problem we study a coupled system of one dimensional partial differential equations. One equation is an incompletely parabolic system of equations which is considered a model of the Navier-Stokes equations, and the other is the heat equation. We couple these equation at an interface and study how heat is transfered from the flow part into the structural part. The long term goal is to study the linearized and symmetrized Navier-Stokes equations and couple it with the heat equation in two dimensions. In this paper we derive well-posed boundary and interface conditions as well as stability for the semi-discrete problem before implementing using high order finite difference methods.

Energy-law Preserving C0 Finite Element Methods for Simulation of Liquid Crystal and Multi-phase Flows

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The liquid crystal (LC) flow model is a coupling between orientation(director field) of LC molecules and a flow field. The model may probablybe one of simplest complex fluids and is very similar to an Allen-Cahnphase field model of multiphase flows if the orientation variable isreplaced by a phase function. We propose a C^0 finite element formulationin space and a modified midpoint scheme in time which accurately preservesthe inherent energy law of the model. We use C^0 elements because they aresimpler than existing C^1 element and mixed element methods. We emphasizethe energy law preservation because from the PDE analysis point of viewthe energy law is very important to correctly catch the evolution ofsingularities in the LC molecule orientation. In addition we will seenumerical examples that the energy law preserving scheme performs betterin the multiscale situation, for example, it works better for highReynolds number flow fields and allows coarser grids to qualitativelycatch the interface evolution of the two-phase flow. Finally we apply thesame idea to a Cahn-Hilliard phase field model where the biharmonicoperator is decomposed into two Laplacian operators. But we find thatunder a C^0 finite element setting non-physical oscillation near theinterface occurs. We find out the reason and provide a remedy. A number ofnumerical examples demonstrate the case.

Simulation of scattered waves on the base of low-reflection local temporal-spatial mesh refinement

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As scattered waves are getting of a high importance in geophysics, for example, in reservoir monitoring nowadays one needs to be able to simulate them properly. Due to the typical sizes of the problem it is convenient to use locally refined grids: fine ones at the vicinity of the scatters and coarse ones elsewhere. To construct stable and low-reflection algorithm we propose to apply refinement of temporal and spatial stepping consequently, instead of simultaneous ones. Refinement of the temporal stepping is free from interpolation and based only on finite difference approximation of the wave equation which makes it stable. According to theoretical study and series of numerical experiments the proposed approach possesses low enough artificial reflection.

DOLFIN: Automated Finite Element Computing

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DOLFIN is a library aimed at automating the solution of partial differential equations using the finite element method. By employing novel techniques for automated code generation, DOLFIN combines a high level of expressiveness with efficient computation. Finite element variational forms may be expressed in near mathematical notation, from which low-level code is automatically generated, compiled and seamlessly integrated with efficient implementations of computational meshes and high-performance linear algebra. Easy-to-use object-oriented interfaces to DOLFIN are provided in the form of a C++ library and a Python module. A number of examples are presented to demonstrate the use of DOLFIN in application code.

Immersed interface method for the propagation of transient mechanical waves

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The finite-difference schemes on cartesian grids are very efficient to simulate the wave propagation in homogeneous media. However, interfaces damage these qualities, for the following reasons. First, non-smoothness of solutions across interfaces decreases the order of convergence, and instabilities may be triggered. Second, a stair-step representation of interfaces on cartesian grid gives birth to spurious diffractions. Third and last, finite-difference schemes do not incorporate the jump conditions.
To solve these problems, we propose to apply an *immersed interface method*. Locally, some numerical values used for time-marching are modified, based on the jump conditions and on the geometrical features of the interface. This method is coupled straightforwardly to conservative schemes for hyperbolic systems. The additional cost is negligible compared to the cost of the scheme.
Various applications of the method will be presented, to cite a few: linear and non-linear jump conditions between solids, poroelastic media, free surface in seismology.

ReALE : an automatic reconnection ALE method via Voronoi tesselation

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In this work we propose to automatically perform mesh reconnection within an ALE framework. ALE framework is often defined as a three step process: a Lagrangian scheme step to update the physical quantities, a rezoning step to improve the current mesh, a conservative remap step to project the physical quantities onto the rezoned mesh.Rezone and remap phases are performed at fixed connectivity. Therefore specific motions like shear, vortex, slide line are difficult to solve with a moving mesh. In presence of these specific motions, the ALE code is run in its Eulerian configuration. ReALE mimics the ALE three step process. The difference resides in an automatic mesh reconnection based on the Voronoi tesselation of a set of moving generators. Generators are adaptively moving with the fluid, each being associated with one cell, defining a unique mesh. However while moving, a generator can change its local neighbor generators, and, as a consequence the resulting mesh connectivity.We will present numerical evidences of automatic mesh reconnection that ReALE authorizes in vortex and shear like test cases with comparisons with classical ALE and Lagrangian results.

Analysis of a Dynamical Low Rank Approximation for Tensors

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For the low rank approximation of time-dependent data tensors and of solutions to tensor differential equations, an increment based computational approach is proposed and analyzed. In this variational method, the derivative is projected onto the tangent space of the manifold of low rank tensors at the current approximation. The error analysis compares the result with a best approximation in the manifold of low rank tensors. It is proven that the approach gives locally quasi-optimal low rank approximations and under additional assumptions the error grows only linearly also over long time intervals. The implications for variational approximations in quantum dynamics are indicated. Numerical experiments illustrate the theoretical results.

RBF: The optimal choice for the shape parameter

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In the theory of radial basis functions multiquadrics are a very powerful tool. However there is a shape parameter c in such functions whose optimal value is unknown. This question has been perplexing for many years. The author tries to uncover its mystery and presents some criteria for its optimal choice. The theoretical ground is the exponential-type error bounds raised by Madych, Nelson and Luh.

On FC-AD PDE solvers for complex domains and boundary conditions with normal derivatives

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Through the combination of a Fourier Continuation and an Alternating Direction partial differential equation (PDE) splitting scheme, an class unconditionally stable FC-AD solvers for PDEs on complex domains were recently developed. High-order accuracy and memory/computational efficiency are among the unique properties of these FC-AD solvers. The alternating direction mechanism inhibits the use of FC-AD techniques on complex domains with Neumann boundary data. Recent efforts to extend the FC-AD techniques to cover this particular case are presented including a further splitting of the PDE and subsequent application of integral boundary element methods to a reduced linear equation to correct for the normal derivative boundary data.

Sonic log simulation in anisotropic media

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Based on the application of a finite-difference approximation of an initial boundary value problem for an elastic wave system, a numerical method and its algorithmic implementation have been developed to perform a computer simulation of sonic logging. A very general situation is dealt with – the surrounding medium is allowed to be an arbitrary 3D anisotropic heterogeneous medium, and the source can be located at any point inside or outside the well. In order to truncate the computational domain extension based on the so-called Spectrally Matched Grids are employed to ensure stability. Implementation of parallel computations is done via Domain Decomposition. Data exchange between Processor Units is performed with the help of the Message Passing Interface library.

Quantitative analysis of numerical solution for the Gray-Scott model

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This contribution deals with numerical solution of the Gray-Scott model [GS1983, GS1984]. We introduce two numerical schemes for this model based on the method of lines. To perform spatial discretization we use FDM and FEM, alternatively. Resulting systems of ODEs are solved using the modified Runge-Kutta method with adaptive time-stepping. We present some of our numerical simulations and perform comparison of both schemes from the qualitative point of view.
[GS1983] P. Gray and S. K. Scott, Chem. Eng. Sci. 38:29-43 (1983).
[GS1984] P. Gray and S. K. Scott, Chem. Eng. Sci. 39:1087-1097 (1984).

Stochastic modeling of T Cell Homeostasis for Two Competing Clonotypes via the Master Equation.

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Stochastic models for competing clonotypes of T cells by multivariate, continuous-time, discrete state, Markov processes have been proposed in the literature by Stirk, Molina-Paris and van den Berg (2008). We describe someefficient PDF approaches by directly solving the governing equations, known as the Master Equation. These computations are made very efficient through an approximation of the state space by the Finite State Projection and through the use of Krylov subspace methods when evolving the matrix exponential.Time-dependent propensities naturally arise in immunological processes due to, for example, age-dependent effects. Incorporating time-dependent propensities into the framework of the Master Equation can be done efficiently via Magnus formulas.

Cell-centered and staggered discretizations of the multi-dimensional Lagrangian hydrodynamics by means of sub-cell force formulation

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The main goal of this talk is to present recent developments and extensions concerning multi-dimensional schemes for solving the compressible gas dynamics equations written in the Lagrangian formalism. Using the sub-cell force framework, which is well known in the context of staggered discretization, we will derive an original cell-centereddiscretization that is compatible with the geometric conservation law. This scheme conserves momentum, total energy and satisfies a local entropy inequality. It is based on nodal solvers which can be viewed as multi-dimensional approximate Riemann solvers located at the nodes. We will describe the genuinely multi-dimensional high-order extension constructed using the generalized Riemann problem methodology in the acoustic approximation. We will also focus on the comparison between this cell-centered discretization and the more classical staggered one.

Ultrasound Image Sequence Segmentation via motion estimation

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We are concerned with the segmentation of the left ventricle (LV) during the cardiac cycle. The goal is to track the expansion of the LV chamber. Besides the elimination of speckle noise, the difficulty is to delineate the movement of the ventricle contour in the vicinity of the cardiac valve. We recover missing parts using the optic flow. The problem is described by nonlinear time-dependent PDEs: speckle reduction based on nonlinear coherent diffusion, segmentation based on geodesic active contours and the optic flow computation based on a nonlinear diffusion-reaction equation. The PDEs are discretized using semi-implicit schemes. At each scale step we solve a sparse linear system by using the GMRES method equipped with a multilevel preconditioner. Experiments on real data are discussed.

Simulation of Coating Processes in Automotive Industry

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Paint and surface treatment processes in the car paint shop are to a large extent automated and performed by robots. Having access to tools that incorporate the flexibility of robotic path planning with fast and efficient simulation of the processes is a major competitive advantage. The combination of high physical complexity, large moving geometries, and demands on near real time results constitutes a big challenge. We have developed an immersed boundary octree flow solver based on algorithms for coupled simulations of multiphase and free surface flows, electromagnetic fields, and particle tracing. The solver is included in an in-house package for automatic path planning. The major improvement of computational speed compared to other approaches is partly due to the use of grid-free methods which in addition simplifies preprocessing.

On stability issues for IMEX schemes applied to hyperbolic equations with stiff reaction terms

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Many physical problems are governed by hyperbolic conservation laws with non vanishing stiff source terms. In some problems the source terms depend only on the solution and yet the solution naturally develops structures in which the source terms are nonzero, and possibly large, only over very small regions in space.

With many numerical methods, taking a time step appropriate for the slower scale of interest can result in violent numerical instabilities. Moreover, a different type of numerical difficulty is encountered in numerical simulations that is the occurrence of fronts propagating at the wrong speeds.

The study for the fully explicit and fully implicit time marching schemes source that there is, in fact, a rather direct relation between the mesh spacing and the numerical delay.

Optimal control for river pollution remediation

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The main goal of this work is to use mathematical modelling and numerical optimization to obtain the optimal purification of a polluted section of a river. The most common strategy consists of the injection of clear water from a reservoir in a nearby point. Thus, we are interested in finding the minimum quantity of water which is needed to be injected into the river in order to purify it up to a fixed level. We formulate it as a hyperbolic optimal control problem with control constraints, deriving a first order optimality condition in order to characterize the optimal. Finally, we deal with the numerical resolution of a realistic problem, where a finite element/finite difference discretization is used, an optimization algorithm is proposed, and computational results are provided. (Research supported by Project MTM 2006-01177 of M.E.C.-Spain).

Generalized stochastic decomposition for large evolution problems

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We present an extension of the Generalized Stochastic Decomposition method for the resolution of large time-dependent uncertain problems. The approach essentially consists in approximating the solution as a series of unknown modes in the problem variables (time, space and uncertainty dimensions) and leads to very significant savings both in terms of computational time and memory requirement. Several strategies and functional forms for the decomposition are investigated and compared for numerical efficiency on the example of a 1-D convection-diffusion stochastic equation. In particular, an algorithm is proposed to construct a rank-1 decomposition of the solution. Strategies involving decompositions over time intervals and restart procedures are also considered to reduce the number of modes.

An anisotropic micro-sphere approach applied to the modelling of soft biological tissues

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A three-dimensional model for the simulation of anisotropic soft biological tissues is discussed. The underlying constitutive equations account for large strain deformations and are based on a hyper-elastic form. Its anisotropic part is determined by means of a so-called micro-sphere model, which allows to extend physically sound one-dimensional constitutive models to the three-dimensional case.Concerning the algorithmic implementation, the integration over the underlying micro-sphere is performed in terms of a finite number of integration directions together with corresponding integration factors. Anisotropy can conveniently be introduced by additionally weighting these integration factors with a so-called orientation distribution function.

Parallel anisotropic mesh adaptation for capturing multi-phase interfaces

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Anisotropic mesh adaptation is a key feature in many numerical simulations to capture the physical behaviour of a complex phenomenon at a reasonable computational cost. It is a challenging problem, especially when dealing with time dependent multi-phase flows and interface tracking problems. In this paper, we present an anisotropic parallel mesh adaptation technique. This is based on the definition of an anisotropic a posteriori error estimator and the search of the optimal mesh (metric) that minimizes the error estimator under the constraint of a given number of nodes. In addition, we use a serial mesh generator (MTC) in a parallel context. The parallelization strategy consists in balancing dynamically the work flow by repartitioning the mesh after each re-meshing stage. Numerical 2D and 3D applications are presented here to show that the proposed anisotropic error estimator gives an accurate representation of the exact error. We will show also, that the optimal adaptive mesh procedure provides a mesh refinement and element stretching which appropriately captures interfaces for practical application problems. The anisotropic adapted meshes provide highly accurate solutions that are shown to be unreachable with a globally-refined meshes.

On a sediment transport model in Shallow Water equations with gravity effects

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Sediment transport by a fluid over a sediment layer can be modeled by a coupled system with a hydrodynamical component, described by a shallow water system, and a morphodynamical component, given by a solid transport flux. Meyer-Peter&Müller developed one of the most known formuae for solid transport discharge, but it has the inconvinient of not including pressure forces. This makes numerical simulations not accurate in zones where gravity effects are relevant, e.g. advancing front of the sand layer.
Fowler proposed a generalization that takes into account gravity effects and length of the sediment layer.
We propose to solve this system by using a path-conservative scheme for the hydrodynamical part and a duality method based on Bermudez-Moreno algorithm for the morphodynamical component

Error Analysis for Gaussian Beam Superposition

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Gaussian beam superposition method is an asymptotic method for computing high frequency wave fields in smoothly varying inhomogeneous media. We study the accuracy of Gaussian beam superposition method and derive error estimates related to the discretization of the superposition integral and the Taylor expansion of the phase and amplitude off the center of the beam. We show that in the case of using odd order beams, the error is smaller than a simple analysis would indicate because of error cancellation effects between the beams. Since the cancellation happens only when odd order beams are used, there is no remarkable gain in using even order beams. Numerical examples verify the error estimates.

Convergence of path-conservative numerical schemes for hyperbolic systems of balance laws

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We are concerned with the numerical approximation of Cauchy problems for hyperbolic systems of balance laws, as a particular case of nonconservative hyperbolic systems. We consider the theory due to Dal Maso, LeFloch and Murat to define weak solutions of nonconservative systems, and path-conservative schemes (introduced by Pares) to numerically approximate them. In a previous work with P.G. Le Floch we have studied the appearance of a convergence error measure in the general case of noconservative hyperbolic systems. In this work we investigate the reasons why, for systems of balance laws, the experiments performed up to now show that this error is not observed if the correct choice of path-conservative scheme is done: the numerical solutions converge to the right weak solutions.

Adaptive variational multiscale methods

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We present a framework for multiscale approximation of elliptic problems on mixed form. The method is basedon a splitting into coarse and fine scales together with a systematic technique for approximation of the fine scale part basedon solution of decoupled localized subgrid problems. The fine scale approximation is then used to modify the coarse scale equations. A key feature of the method is the a posteriori error bound and the adaptive algorithm for automatic tuning of discretization parameters, based on this bound. We present numerical examples where we apply the framework to a problem in oil reservoir simulation.

Goal-oriented adaptivity for flux-limited Galerkin approximations to convection-diffusion problems

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Adaptive high-resolution finite element schemes for transport problems are presented. A new goal-oriented error estimator is obtained building on the duality argument. The error in the quantity of interest is expressed in terms of a linear target functional. The Galerkin orthogonality error caused by flux limiting is taken into account and provides a useful criterion for mesh adaptation. Gradient averaging is invoked to separate the element residual and diffusive flux errors without introducing jump terms. A decomposition of global errors into nodal (rather than element) contributions is shown to be essential. Practical aspects of mesh refinement and coarsening are discussed. Numerical results and adaptive meshes are presented for steady hyperbolic and elliptic problems in two dimensions.

A Shallow Water model for viscoelastic fluid from the kinetic theory for polymers solutions

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The aim of this work is to modelize the movement of a viscoelastic fluid. The idea is to use this model to simulate, for example, the movement of fuel by the ocean.
The hydrodynamic is given by the Navier-Stokes equations but the difficulty lies in the definition of the stress tensor for this non-Newtonian fluid.
In order to get an expression for it we focus on the microscopic properties of the fluid by considering a diluted solution of polymer liquids. A kinetic theory for these type of solutions gives us "constitutive equations" relating the stress tensor to the velocity. They are known as the Fokker-Planck equations.
Once the stress tensor is defined we shall derive the model by developing the asymptotic analysis of the joined system of equations to obtain a Shallow Water type model

An adaptive General Galerkin Finite Element Method for the Turbulent Compressible Flows

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We present an adaptive General Galerkin (G2) method for compressible Euler/Navier-Stokes equations. G2 is a finite element method with continuous piecewise linear approximation in space and time with componentwise streamline diffusion stabilization and shock-capturing terms. To capture and resolve features such as shocks, rarefaction waves, contact discontinuities and boundary layers, the mesh must be sufficiently refined. Hence, construction of adaptive algorithms are necessary for efficient simulations. Here, we present a duality based adaptive finite element method for turbulent compressible flow in three space dimensions. It will extend the earlier work on incompressible flows using G2 method.

Multi-dimensional optimization with a stochastic Lipschitz bound for problems in genetic analysis

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Techniques of branch-and-bounding for finding minima have been long known, based on techniques of defining local bounds of the function value on hypervolumes of varying sizes, progressively containing the possible minima in smaller volumes.Along this line, the Lipschitz-based optimization method DIRECT has earlier been applied to the problem of linear regression in the field of multidimensional optimization of searches for quantitative trait loci (QTL), identifying genetic locations that influence important traits, like body weight or propensity for diseases. We show how the use of a stochastic Lipschitz constant for a transformed objective function can improve performance by several orders of magnitude in the frequently used permutation-testing approaches exploited in QTL analysis.

On Stationary Viscous Incompressible Flow through Cascade of Profiles with the Modified Nonlinear Boundary Condition on the Outflow and Large Inflow

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The paper is concerned with the analysis of the model of incompressible, viscous, stationary flow through a plane cascade of profiles. The Navier-Stokes problem is formulated in a domain representing the exterior to an infinite row of profiles, periodically spaced in one direction and then reformulated in a bounded domain of the form of one space period and completed by the suitable boundary conditions. Let us recall that there is usually imposed the condition on smallness of the inflow velocity or the condition on the zero balance of fluid for each component of boundary in known theorems on existence of a weak solution of the boundary--value problem for the Navier--Stokes equation with the nonzero Dirichlet boundary condition. In this paper the case of a large inflow is considered.

Scalable Finite Element based sparse approximate inverses

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We discuss a construction of sparse approximate inverses (SPAI) of matricesand matrix blocks in the context of linear systems of equations arising from finite element discretizations of partial differential equations.The approximation is based on assembly of local, small-sized element matrix inverses, which are then assembled in the usual finite element manner and give raise to sparse matrix approximations.
The method is particularly useful to obtain a good idea of a suitable sparsity pattern of the approximate inverse, an issue which is one of the bottlenecks for other known methods to construct approximate inverses, for instance based on minimization of some weighted Frobenius norm. Once the nonzero pattern of the approximate inverse matrix has been obtained, then the quality of the approximated inverse can be improved using some of the already available methods.
An additional advantage of the method is that it processes a high degree of parallelism and is suitable for large scale numerical simulations.
In the talk, we explain the proposed method, discuss the properties of the obtained matrix approximations and give illustrations of the numerical and the computational efficiency of the above SPAI technique.

An optimized perfectly matched layer for the Schrödinger equation

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When using quantum chemical computations to simulate dissociation processes accurate absorbing boundary conditions are important. We solve the Schrödinger equation with a perfectly matched layer (PML) for accurate truncation of the computational domain. The PML equation is derived using a modal ansatz and finite difference methods of varying orders are used for spatial and temporal discretization. An Arnoldi time-stepping approach could also be used. We match the discretization error from the interior with the discretization error and the modelling error from the PML, respectively. This is done for numerical schemes of different orders. Numerical calculations in 1D and 2D show that the PML works efficiently and that it is possible to control and match errors at a prescribed error tolerance.

Multiscale and iterative subspace methods

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This talk discusses various relationships between multiscale methods, and their ancestors such as iterative subspace methods. We give the interpretation of the variational multiscale method as an instance of a heterogeneous multiscale method. Further, we show how the heterogeneous multiscale method itself can be presented as an accelerated iterative subspace method, strongly related to the additive Schwarz method with a coarse correction operator. Examples are given where these methods are applied to compressible two-phase flow problems in porous media, including gravity.

A priori model reduction technique for solving stochastic partial differential equations

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Galerkin spectral stochastic methods provide a general framework for the numerical simulation of physical models driven by stochastic partial differential equations (SPDEs). However, computing approximate solutions asks for the solution of very high dimensional problems. Recently, an a priori model reduction technique, named generalized spectral decomposition method, has been proposed in order to reduce computation costs. It takes part of the tensor product structure of function spaces and allows computing a quasi optimal separated representation of the solution for some classes of SPDEs. Here, we propose some modifications of the initial method in order to improve convergence properties of separated representations, especially for non self-adjoint stochastic operators.

Comparison study for Level set and Direct Lagrangian methods for computing Willmore flow of closed planar curves

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The main contribution of this presentation is a comparison of the level-set and the direct Lagrangian methods for computing evolution of the Willmore flow of embedded planar curves. We will present new numerical approximation schemes for both the Lagrangian as well as the level-set methods based on semi-implicit in time and finite/complementary volume in space discretisations. The Lagrangian method is stabilised by setting apropriate tangential velocity and for the level-set method redistancing of the level-set function is performed occasionaly.Both methods are experimentally second order accurate. Moreover, we show precise coincidence of both approaches in case of various elastic curve evolutions.

Using mesh adaptation and a new ALE-DGCL swap formulation for large-displacements moving domain simulations.

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Most of the industrial problems are unsteady and involve moving domains. Awidespread strategy for these problems consists in moving the mesh at fixed topology and constant number of vertices, remeshing when the mesh is too distorted, interpolate the solution on the new mesh and restart the ALE computation. The problem is that for large displacements, remeshings can be performed very often, which can be costly and can spoil the accuracy of the solution due to the effect of the interpolation.
As we want to introduce anisotropic mesh adaptation in ALE simulations, we would like to remesh only when we want to do it for adaptation purposes and not to be forced to do it due to our inability to move the mesh properly. Our strategy for this is twofold. On the one hand, we relaxed the fixed topology constraint by giving an ALE formulation of the edge flipping operation in 2D. On the other hand, we improved the existing moving mesh techniques and fit them for adaptation purposes.
All this is illustrated with the Euler equations on different cases: objects blown up by a propagating blast, various aerodynamic simulations.

An algebraic solver for variable viscosity Stokes equations with application to the Bingham fluid problem

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The talk concerns with an iterative technique for solving discretized Stokes type equations with varying viscosity coefficient and its application to numerical solution of incompressible non-Newtonian fluid equations. We build a special block preconditioner for the discrete system of linearized equations and perform an analysis revealing its properties. The method and the general analysis is applied to the regularized Bingham model of viscoplastic fluid.

How to use SVD in many dimensions

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A d-dimensional array with n points in each direction contains n^d elements,so special data structures are mandatory if we want to work with such arrays numerically.A ubiquitous canonical format of rank R contains dRn parameters, where $R=o(n)$or even does not depend on n. But, R still depends on d in the same exponential way,and for large values of d even 2^d parameters are regarded as unaffordable.Thus, we need a new data structure that can allow us to overcome the exponentialdependence on d (known as the curse of dimensionality). We present such a format whichwe call a tree-Tucker decomposition. It is based on a recursive reduction of the given tensorto a sequence of three-dimensional tensors. The number of representation parameters in thenew format does not exceed drn^2, where r is a number called the splitting rank.In many cases r is free from exponential dependence on d. Moreover, the newformat possesses nice stability properties of the SVD (as opposed to the canonical format)and is convenient for basic operations with tensors, in particular for fast evaluation of$d$-dimensional integrals.

FEM techniques for viscoelastic flow problems for high We numbers

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Similar to high Re number flows which require special discretization and solution techniques to treat the multiscale behaviour, viscoelastic fluids are very difficult to simulate for high Weissenberg (We) numbers ("elastic turbulence"). While many researchers believe that the key tools are appropriate stabilization techniques for the tensor-valued convection-reaction equation for the extra stress, we explain the concept of log conformation representation (LCR) which exploits the fact that the conformation tensor is positive definite shows an exponential behaviour. Together with appropriate FEM techniques and nonlinear Newton/linear multigrid solvers for the resulting fully implicit monolithic approaches, significantly higher We numbers seem to be reachable than compared with the standard formulation.

Numerical solution of mean curvature flow with topological changes

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This contribution deals with the numerical simulation of dislocation dynamics by means of parametric mean curvature flow. Dislocations are described as an evolving family of closed and open smooth curves driven by the normal velocity. Normal velocity is the function of curvature and the position vector. The equation is solved using direct approach by semi-discrete scheme based on finite difference method. Numerical stability is improved by tangential redistribution of curve points which allows long time computations and better accuracy. Our method contain an algorithm which allows topological changes. The results of dislocation dynamics simulation are presented (e.g. dislocations in channel, Frank-Read source, etc.).

Derivation of aggregation model of nanoscale particles including influence of electrostatic forces

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Nanoscale zerovalent iron particles are examined for remediation of soils and groundwater. Transport properties of nanoscale particles are influenced by process of nanoparticle aggregation. A mathematical model of aggregation is known for these factors causing the aggregation: heat fluctuations, drifting in water and sedimentation. The model determines a rate of aggregation that represents a probability of collision between two nanoparticles. The presentation will include derivation of an aggregation model with influence of electrostatic forces caused by electric layer on particle surface. Numerical analysis of influence of surface charge and application of the derived model for simulation of column experiments realized at Technical University at Liberec will be presented, too.

Recent advances on eigenvalue localization

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We present new localization results for the eigenvalues of a real matrix, either complementing or improving the information derived from the classical Gerschgorin disks. The results are applied to several subclasses of the class of P-matrices (matrices whose principal minors are all positive) important in applications, including nonsingular M-matrices (matrices whose off-diagonal entries are nonpsitive and with nonnegative inverse) and totally positive matrices (matrices whose minors are all nonnegative). Moreover, new lower bounds for the minimal positive eigenvalue of these matrices are presented and their application to several fields is illustrated.

Algebraic Multigrid Preconditioners for a Reaction-Diffusion System of Equations in Electrocardiology

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We deal with a nonlinear reaction-diffusion system of equations modeling the biolectric activity of the heart: the so called *Bidomain model*. We address the problem of efficiently solving the large linear system arising in the finite element discretization of the bidomain model when a semi-implicit method in time is employed. We analyze the use of structured algebraic multigrid preconditioners on two major formulations of the model, and report on our numerical experience under different discretization parameters and various discontinuity properties of the differential tensors. Our numerical results show that the less exercised formulation provides the best overall performance on a typical simulation of the myocardial excitation process.

Mesh adaptation driven by a metric-based optimization procedure

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The effectiveness of anisotropic grids is acknowledged in the numerical modelling of many real-life applications, due to the computational saving involved. The expertise gained in this area has been primarily addressed to mesh adaptation strategies driven by suitable error estimators, mainly of a posteriori type. The leading feature of our approach is the employment of a proper metric, stemming from the error estimator itself, to generate the adapted mesh. This procedure allows us to build optimal grids by minimizing the number of elements for an assigned accuracy. The model problems tackled so far comprise 2D elliptic problems, as well as Stokes and Navier-Stokes equations, up to unsteady problems (heat equation and advection-dominated problems).

Parallel Multistep Methods for the Wave Equation

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Discretizing the wave equation in time by a multistep method results in a discrete convolution equation. A simple trick transforms the discrete convolution into a decoupled system of Helmholtz equations. In the case of A-stable multistep methods, the corresponding wave numbers are strictly in the upper half of the complex plane. The transformation between the discrete convolution and the decoupled system can be performed efficiently by a scaled FFT.
In this talk we report on the efficient solution of the decoupled Helmholtz problems using finite element methods and multigrid-based preconditioning techniques. The presentation is supplemented by several numerical experiments.

Finite Element Approximation of a Quasi-3D Model for the River Flow

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Our purpose is to obtain a quasi-3D model, also called 2.5D model, for the hydrodynamical modeling and simulation of an estuarian river flow. The 3D model is based on the instationary Navier-Stokes equations from which simpler 2D models are derived, one in the vertical plane, the other one in the horizontal plane. We propose to search for an approximation in the sum of the spaces of these two 2D models. The new model takes into account the river's geometry and provides a three-dimensional velocity and the pressure. Since we can define suitable projection spaces, we are able to give a mixed weak formulation associated with the quasi-3D model. Then we compute the solution and validate the results with severals tests.

Multilevel predictor-corrector strategy for solving shape optimization problems

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We consider applications of multilevel methods for shape optimization of various composite materials structures. The objective functional depends on state variables describing the physical model and design parameters determining the shape. The general PDE constrained optimization problem gives rise to a large-scale nonlinear programming task. Additionally to the state equations as equality constraints we have inequality constraints which are technically or physically motivated. Adaptive multilevel path-following predictor-corrector methods with inexact Newton solvers are applied for the numerical solution of the optimization problem. Physical models described by specific PDEs for real-life problems and numerical experiments for multiscale applications are presented and discussed.

Local Least-Squares Reconstruction in Higher Order Schemes on Anisotropic Meshes.

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A method of local least-squares (LS) approximation has recently received a lot of attention in computational aerodynamics. Higher order finite-volume schemes are a class of discretization schemes where a LS method is frequently employed, as they require a local reconstruction of the solution gradient in the scheme. While a LS method provides accurate approximation on regular grids, in many practical applications it is required to reconstruct a function on highly anisotropic unstructured grids that are generated about an airfoil. In our talk we demonstrate that a higher order LS reconstruction can degrade to unacceptable accuracy on anisotropic meshes and weighting of distant stencil points does not result in a more accurate reconstruction. The concept of numerically distant points will be employed to explain the reasons behind the method's poor performance and to improve the results of a LS reconstruction on stretched meshes.

Shock capturing schemes for the stochastic Burgers' equation with time-dependent boundary conditions

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The stochastic Burgers' equation with uncertain initial and boundary conditions is approximated using a polynomial chaos expansion approach where the solution is represented as a series of stochastic, orthogonal polynomials. Even though the analytical solution is smooth, a number of discontinuities emerge in the truncated system. The solution is highly sensitive to the propagation speed of these discontinuities. High-resolution schemes, such as the MUSCL scheme, are needed to accurately capture the behavior of the solution. The different scales of the chaos modes require diversified model parameters for the dissipation operators to yield accurate solutions. We will compare the results using the MUSCL scheme with previously obtained results using conventional one-sided operators.

Anisotropic adaptive methods for geophysical applications in 3D

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Many application areas in geophysical fluid dynamics include massive variations in spatial scales that are important to resolve in a numerical simulation. An example is the global ocean where dynamics at spatial scales of thousands of kms has strong two-way coupling with important processes occurring at the km scale, e.g. boundary layers, eddies and buoyancy driven flows interacting with bathymetry. Adaptive methods represent an efficient means to simulate these systems. The smaller scale processes often have high aspect ratios and hence anisotropic methods should be used. In this talk our work applying anisotropic adaptive methods in these application areas will be summarised. Error measures, mesh to mesh interpolation and combined h and r adaptivity will be discussed.

Numerical solutions and bifurcations in a convection problem with temperature-dependent viscosity

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In this work we analyse the behaviour of the Chebyshev collocation method in a convection problem temperature-dependent viscosity in a 2D fluid layer. We apply bifurcation theory and branch continuation techniques to achieve a more comprehensive description of the nonlinear solutions. The variable viscosity is assumed to be exponentially dependent on temperature.
We benchmark the method and code to ensure the correctness of the results. Expansions of order 18 by 14 ensure sufficient accuracy within 1%.
This problem takes in features of mantle convection, since large viscosity variations are to be expected in the Earth's interior.

The Total Least Squares Problem and Reduction of Data

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It is proved that partial upper bidiagonalization of the extended matrix (b,A) determines a core approximation problem $A_{11}x_1 \sim b_1$, with the necessary and sufficient information for solving the original linear approximation problem $Ax \sim b$, Paige, Strakos, 2006. The transformed data b_1 and A_{11} can be computed Golub-Kahan algorithm. The core problem can be used in a simple and efficient way for solving the TLS formulation.

Our contribution concentrates on extension of core problem idea to problems $AX \sim B$ with multiple right-hand sides. The extension of the concept of a minimally dimensioned subproblem containing the necessary and sufficient information is not straightforward. We will survey results obtained during investigation of this problem and discuss some examples illustrating difficulties.

Solution strategies for stochastic Galerkin and stochastic collocation systems

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In this talk, we give an overview of solver and preconditioning strategies for the linear systems of equations that arise when the steady-state diffusion equation, with correlated random diffusion coefficients, is discretised via stochastic Galerkin and stochastic collocation techniques. The diffusion coefficient is modelled first as a Karhunen-Loeve expansion, a linear function of a finite set of random parameters, and then as the exponential of a such an expansion. We consider both the primal variational formulation, leading to positive definite systems of equations and mixed formulations, leading to saddle-point systems. For practical implementations, we focus on multigrid methods and exploit, wherever possible, existing solver techniques for the deterministic PDEs.

Domain Decomposition schemes for frictionless multibody contact problems of elasticity

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Parallel and sequential domain decomposition schemes which are based on the penalty variational formulation and iterative methods for variational equalities are proposed for the solution of unilateral frictionless multibody contact problems of elasticity. Numerical analysis is made for 2D contact problems using linear and quadratic finite element approximations on triangles and linear hybrid finite-boundary element approximations. The penalty parameter influence on the solution, the convergence rate of iterative schemes and its dependence from an iterative parameter, and the h-convergence are investigated. A generalization of the domain decomposition schemes for nonconforming finite element and boundary element meshes on the contact boundary is obtained by the mortar element method.

Lacunae Based Stabilization of PMLs

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PML are used for the numerical solution of wave propagation problems on unbounded regions. They attenuate and absorb the outgoing waves with no reflections from the interface between the domain and the layer. PML have also been found prone to instabilities that manifest themselves when the simulation time is long. We propose a modification that stabilizes PML applied to a hyperbolic partial differential equation/system that satisfies the Huygens' principle (such as Maxwell's equations in vacuum). We employ the lacunae of the solutions to establish a temporally uniform error bound for arbitrarily long-time intervals. The matching properties of the PML are fully preserved. The methodology can also be used to cure any other undesirable long-term computational phenomena.

Block preconditioners for the incompressible Stokes problem

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Our work is based on a block triangular preconditioner and a Schur method that use the scaled pressure mass matrix as preconditioner for the pressure part or as an approximation of the Schur complement. An important aspect of these two methods is that they scale with the increase in problem size and viscosity contrast. The Schur method that uses explicit construction of $BF^{-1}B^T$ seems expensive in isoviscous problem, however in problems having high viscosity contrast, performance is comparable with the block triangular preconditioner. To get a clear picture of the importance of scaling, we compare these two methods also with the LSC preconditioner that uses $BD^{-1}B^T$ factors in the Schur complement approximation, where D is the diagonal of the velocity matrix.

A posteriori estimates for variational inequalities

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In the talk, guaranteed and computable error bounds for variational inequalities and other nonlinear problems are discussed. The derivation of them is based either on variational techniques (a consequent exposition of this method can be found in [1]) or on transformations of integral identities and variational inequalities(see [2]).
Error indicators that follow from error majorants and computational aspects are also discussed.

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Iterative Substructuring in Biomechanics

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Domain decomposition methods of the FETI type are fast and robust solverssuitable for problems in structural mechanics and by design suited forparallelization. The biomechanics of soft tissues such as the mechanics ofarterial walls poses special challenges for solver convergence due toanisotropy, coefficient jumps and quasi incompressibility. In this talkseveral aspects of the solver environment are discussed.

Multiphase Modeling in Biomechanics for Growth and Remodeling

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Biological tissues like cartilage or organs are porous structures filled with fluid and show an overall anisotropic, viscoelastic and incompressible material behavior. The anisotropy is caused by heterogeneously distributed reinforcing textures like collagen fibers and the incompressibility is mostly generated by the intrinsic fluid. Finally, the viscoelasticity results from the frictionary fluid filter velocity. Tissue achieves the capability to react on outer loading changes by a simultaneous growth and degrading of the needed and unneeded structures. In this paper, an enhanced biphasic model is presented which predicts the behavior of biological tissues. The applicability will be shown with numerical example calculations on tissue behavior including remodeling and growth.

Longest-edge (nested) algorithms, applications and properties

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Longest edge (nested) algorithms for triangulation refinement in two dimensions are able to produce hierarchies of quality and nested irregular triangulations as needed both for adaptive finite element methods and for multigrid methods for PDEs. In addition, right-triangle bintree triangulations are multiresolution algorithms used for terrain modelling and real time visualization of terrain applications. These algorithms are based on the properties of the consecutive bisection of a triangle by the median of the longest edge, and can be formulated in terms of the longest edge propagation path (Lepp) and terminal edge concepts, which implies the use of very local refinement operations over fully conforming meshes (where the intersection of pairs of neighbor triangles is either a common edge or a common vertex). We review the Lepp-bisection algorithms, their properties and applications. We review recent simpler and stronger results on the complexity aspects of the bisection method and its geometrical properties. We discuss and analize the computational costs of the algorithms. The generalization of the algorithms to 3-dimensions is also discussed. Applications of these methods are presented: for serial and parallel view dependant level of detail terrain rendering, and for the parallel refinement of tetrahedral meshes.

Multigrid finite element method on semi-structured grids for the poroelasticity problem

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The classical quasi-static Biot model for soil consolidation, describes the time dependent interaction between the deformation of an elastic porous material and the fluid flow inside of it. This model can be formulated as a system of partial differential equations for the unknowns displacement and pressure. Here, we consider the case of a homogeneous, isotropic and incompressible medium.
A stabilized finite element scheme for the poroelasticity equations, based on the perturbation of the flow equation is considered. This allows us using continuous piecewise linear approximation spaces for both displacements and pressure, obtaining solutions without oscillations independently of the chosen discretization parameters. We present here an efficient geometric multigrid method for this discretization of the poroelasticity problem on semi-structured grids. Local Fourier Analysis on triangular grids has been applied to choose the suitable components of the algorithm.

Numerical Simulation of a Population Balance System with one internal coordinate

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The precipitation of particles during a chemical process is modeled by a population balance system describing an incompressible flow field, an isothermal chemical reaction and a population balance equation for the particle size distribution.
We will present simulations of the precipitation of calcium carbonate in a two- and a three-dimensional domain. The particle size distribution possesses the one internal coordinate, namely the diameter of the particles. For the particles, nucleation and growth are modeled.
The topics included into the talk are the discretization of the coupled system, approaches for the simulation of turbulent flowsand a comparison of the impact of the scheme for solving the higher-dimensional population balance equation.

A Fast Method for Solving the Helmholtz Equation Based on Wave-Splitting

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We present a fast method for computing a solution of the Helmholtz equation in a domain with varying speed of propagation. The method is based on a one-wave formulation of the Helmholtz equation. We solve approximate one-way wave equations (back and forward) with appropriate boundary conditions and source terms. For a p-th order method in 1D, we can show that the computational cost is just $O(\omega^{1/p})$ for fixed accuracy, where ω is the frequency. This is confirmed by numerical experiments.

A Multiscale Method for the Wave Equation in Heterogeneous Medium

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We consider the wave equation in a medium with a rapidly varying speed of propagation. We construct a multiscale scheme based on the heterogeneous multiscale method, which can compute the correct coarse behavior of wave pulses traveling in the medium, at a computational cost essentially independent of the size of the small scale variations. This is verified by theoretical results and numerical examples.

Performance analysis in the high frequency regime of local approximate DtN boundary conditions for prolate spheroidal-shaped boundaries

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We investigate analytically the performance of a new class of local approximate DtN boundary conditions when solving exterior Helmholtz problems. These absorbing boundary conditions have been designed to be applied on exterior artificial prolate spheroidal-shaped boundaries. We assess the efficiency of these conditions when employed for domain-based computation in the high frequency regime. Practical guidelines are suggested for the location of the artificial boundary for achieving a prescribed level of accuracy.

Finite element solution of the Primitive Equations of the Ocean by the Orthogonal Sub-scales method

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We introduce in this talk a stabilized method for the numerical solution of the steady Primitive equations of the Ocean. It is an adaptation of the Orthogonal Subscales Variational Multiscales method introduced by Codina. On one hand, this is a Stabilized Method, thus providing a stabilization of pressure and convection dominance effects with low requirements of degrees of freedom. On another hand, this method also provides a performing parameterization of the unresolved scales, and may be considered as a LES turbulence model.We use a reduced formulation of the Primitive equations, that only include as unknowns the horizontal velocity field and the "surface pressure", an ideal pressure that should be imposed on the surface to keep it flat.We prove stability and error estimates, for the solution of Primitive-Oseen equations and fully non-linear Primitive equations with this method. Our analysis follows a technique introduced by Chacon that is essentially based upon a re-formulation of the method as a stable mixed method.We present numerical tests that confirm the theoretical expectations, in particular the convergence order of the method, and the stabilization properties.

The Forward Euler method for Lipschitz differential inclusions converges with rate one

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When the Forward Euler scheme is applied to a non-convex differential inclusion, the error after only one time step is of the same order as the step length. The error is, however, of the same order as the step length also after long time. I will explain why this is so.

Domain Decomposition with DUNE

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DUNE is a set of C++ libraries for grid-based numerical methods. It offers an unseen amount of flexibility without compromising efficiency and usability. The core of DUNE is an abstract interface for grids, which allows to separate grid implementations from the algorithms that use them. Grid implementations can be changed at any moment in the development process without any impact on application code. Hence, for each application the perfect grid implementation can be chosen. Also, with this interface, it becomes straightforward to handle several different grid implementations at the same time. This can be convenient for domain decomposition methods involving subproblems on different grids or on grids of different dimensions. Generic coupling classes, for example, allow to easily assemble mortar transfer operators between any two grid implementations. We briefly describe the grid interface and then show several example applications, involving various kinds of mortar coupling and the coupling of grids of different dimensions.

Modeling of materials properties using high performance computation

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Ab-initio density functional calculations have been proved to be very successful in analyzing and predicting properties of materials with a reasonable accuracy. Here, we will show how large scale computations using density functional theory (DFT), we can understand the chemical and magnetic interactions of organic molecules on surfaces. Also, we will show how a combination of DFT and Monte-Carlo simulations can yield materials-specific properties to be compared with experiments. Finally, atomistic spin dynamics within the framework of DFT will be shown to demonstrate magnetization dynamics in diluted magnetic semiconductors.

Adaptive mesh procedures for viscoplastic and elastoviscoplastic fluid flows

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The constitutive equations for non-Newtonian viscoplastic fluids (Bingham model) is first presented in the introduction. Then, we present an finite element approximation by using the augmented Lagrangian method and an anisotropic adaptive mesh procedure. This approach is applied to practical computations in complex geometries (obstacles). The extension of this approach to the resolution of a flow with slip yield boundary condition at the wall is considered. Finally, a new elastoviscoplastic fluid flow model, that combines Bingham viscoplasticity and Oldroyd viscoelasticity, and is suitable for liquid foams, emulsions or blood flow, is considered.

Numerical Simulation of the Electrohydrodynamic Generation of Droplets by the Boundary Element Method

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A numerical simulation of the formation of droplets from an electrified capillary using the Boundary Element Method (BEM) is presented. An incompressible and perfectly conducting liquid is injected from a capillary into a dynamically inactive and insulating gas. Assuming an irrotational liquid flow, the problem consists in coupling the BEM resolution of two Laplace equations for the velocity potential inside the fluid domain and the electric potential in the capacitor gas gap. The motion of the free surface is determined by the Bernoulli's equation, resulting from the normal stress balance on the free surface, which injects the electric stress into the mechanical problem. The accuracy of the BEM simulation is demonstrated by showing good agreement with results of existing literature, obtained by the finite element method simulation. The work is in progress to apply the algorithm to the simulation of an electrospray nozzle used for laboratory mass spectrometry.

A two-level Newton-Krylov-Schwarz method for the Bidomain reaction-diffusion system

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A novel two-level Newton-Krylov-Schwarz (NKS) solver is constructed and analyzed for implicit time discretizations of the Bidomain reaction-diffusion system in three dimensions. This multiscale system describes the bioelectrical activity of the heart by coupling two degenerate parabolic equations with several ordinary differential equations. Together with a finite element discretization in space, the proposed NKS Bidomain solver employs an outer inexact Newton iteration to solve the nonlinear finite element system originating at each time step of the implicit discretization. The Jacobian update during the Newton iteration is solved by a Krylov method employing a two-level overlapping Schwarz preconditioner. A convergence rate estimate is proved for the resulting preconditioned operator, showing that its condition number is independent of the number of subdomains (scalability) and bounded by the ratio of the subdomains characteristic size and the overlap size. This theoretical result is confirmed by several parallel simulations employing up to more than 2000 processors for scaled and standard speedup numerical tests in three dimensions. The results show the scalability of the proposed NKS Bidomain solver in terms of both nonlinear and linear iterations, in both cartesian slabs and ellipsoidal cardiac domains.

Generalized Cayley maps and multistep Lie group methods

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Efficient numerical methods for integrating flows on a Lie group require a computationally fast map from the Lie algebra to the Lie group. For the common case of quadratic Lie groups the preferred map is the Cayley map, but constructing high order methods based on this is intricate. We introduce a family of generalized Cayley maps, and show how to use these to construct a family of multistep methods for flows on Lie groups (analogs of the Adams-Bashforth methods). These methods include explicit, A-stable methods of arbitrary order. The efficiency of these methods is comparable or better than existing Lie group methods, and the analysis of the order conditions is particularly simple. We illustrate use of the methods in the computation of distributions of finite time Lyapunov exponents.

Direct minimization with orthogonality constraints with applications in electronic structure computation

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In Density Functional Theory (DFT) the ground state energy of a nonrelativistic ensemble of N electrons together wit the electron density is computed by minimizing the Kohn Sham functional for N unknown functions subordinated to orthogonality constraints. This is a similar problem as finding the invariant subspaces corresponding to the N lowest eigenvalues of a symmetric operator. A preconditioned gradient method for minimzation of Stiefel and Grassmann manifolds is discussed

A pricing technique based on Theta-calculus and sparse grids covering different types of options

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When solving option pricing problems with PDEs numerically, problems usually have to be treated individually, depending on the type of the option. With the Theta-notation introduced by Dirnstorfer, financial products can be modeled by sequences of operators that describe for example transactions and stochastic processes.
We combined the idea of Theta-calculus with a sparse grid approach to realize a PDE-based option pricing technique that can handle different types of options by evaluating a sequence of operators. The application of the process operator corresponds for example to a time-step of the Black-Scholes PDE, a transaction can be considered as a shift of the grid axes.
This way we can easily deal with pricing of various types of multi-dimensional problems numerically with one general technique.

A posteriori error estimation in mixed finite element methods for Signorini's problem

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A posteriori finite element error estimates are presented for Signorini's problem which is discretized via a mixed finite element method of higher-order. The a posteriori error control relies on estimating the discretization error of an auxiliary problem which is given as a varational equation. The resulting error bounds capture the discretization error of the auxiliary problem, the geometrical error and the error given by the complementary condition. The estimates are applied within h- and hp-adaptive refinement and enrichment strategies. Furthermore, the approach is extended to a time-dependent Signorini contact problem. Numerical results confirm the applicability of the theoretical findings.

An epsilon-uniform method for singular perturbation problems on equidistant meshes without exact solution

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For a singularly-perturbed two-point boundary value problem, we propose an epsilon-uniform finite difference method on an equidistant mesh which requires no exact solution of a differential equation. We start with a fitted operator method reflecting the singular perturbation nature of the problem through a local boundary value problem. However, to solve the local boundary value problem, we employ an upwind method on a Shishkin mesh in local domain, instead of solving it exactly. We further study the convergence properties of the numerical method proposed and prove it nodally converges to the true solution for any epsilon.

Modelling complex dynamical systems in MVSTUDIUM

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MvStudium 6.0 – is a graphical environment with universal equation-–based and UML–based object-oriented modeling language, which graphical form based on B-charts and hierarchical functional diagrams. The environment supports technology of designing hierarchical models using oriented and non-oriented blocks, that behavior may be described by hierarchical B-Charts and it consists of Model Editor and Virtual Test-bench.
Model Editor has four user's interfaces that sequentially become more complex for different types of models: 1) an isolated classical dynamical system, 2) an isolated hybrid system, 3) a hierarchical model with components from multiple domains, 4) a model with predefined plan of computer experiment. User can build model using his own original blocks or imported blocks from other projects or libraries.
Virtual Test-bench uses numerical software for solving Non-Linear Algebraic Equations (NAE), ODE, DAE with elements of symbolic calculations.
A model may run under Virtual Test-bench, may be a standalone executable program, or may be realized as hidden or un-visual model in the form of DLL to use as a component of more complex model or for parameter optimization with the help of Virtual Test-bench toolbox.

Spectral features and asymptotic properties for alpha-circulants and alpha-Toeplitz sequences

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A matrix of size *n* is called *alpha*-Toeplitz if its entries obeys the rule $A=[a_{r\text{-}alpha\ s}]_{r,s=0}^{n-1}$. A matrix is called *alpha*-circulant if $A=[a_{(r\text{-}alpha\ s)mod\ n}]_{r,s=0}^{n-1}$. Such kind of matrices arises in wavelet analysis, subdivision algorithms and more generally when dealing with multigrid/multilevel methods for structured matrices and approximations of boundary value problems. In this talk we give an expression of the singular values and eigenvalues of *alpha*-circulants and we provide an asymptotic analysis of the distribution results for *alpha*-Toeplitz sequences in the case where the sequence of values $\{a_k\}$ are the Fourier coefficients of an integrable function *f* over the domain *(-pi,pi)*.

Numerical Calculations of Electron Optical Systems

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To develop an electron optical device with a high quality of an image on a screen it is necessary to calculate the electrostatic field in the device, trajectories of electrons emitted from a photocathode, and evaluate electron image quality characteristics.
Numerical algorithms for solving these mathematical problems for particular electron-optical systems are described in this work. Calculations of the potential distribution inside the device are based on the numerical solution of the partial differential equation of Laplace, and the electron trajectories are calculated using the Runge-Kutta method. Frequency-contrast characteristics are obtained using the trajectories of the electrons and the electron density function calculated here. Results of the numerical experiments are shown, and the electron optical system with optimized characteristics is developed.

Analysis of Conforming Adaptive Finite Elements for Nonlinear Problems

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Adaptive finite elements are successfully used since the 1970th. The typical adaptive iteration is a loop of the form
SOLVE --> ESTIMATE --> MARK --> REFINE.
Traditional a posteriori error analysis was mainly concerned with the step ESTIMATE by deriving computable error bounds for the true error. During the last years there is an increasing interest in proving convergence of the above iteration, this means that the sequence of discrete solutions converges to the exact solution.In this talk we extend the basic convergence result for linear problems in Morin, Siebert & Veeser and Siebert to convex non-linear problems.

Solution of an inverse problem for a 2-D turbulent flow around an airfoil

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The presented method is intended for a solution of an airfoil design inverse problem. It is capable of suggesting an airfoil shape corresponding to a given pressure distribution on its surface. The method is an extension of a method presented earlier. Using the k-omega turbulence model it can handle a turbulent boundary layer which improves its applicability. The method is aimed to a subsonic flow, the angle of attack is one of the results of the method. The method is based on the use of an approximate inverse operator coupled with the Navier-Stokes equations equipped with the turbulence model. The equations describing the flow are solved using an implicit finite volume method, the linearized system is solved by the GMRES method. Numerical results are also presented.

Convergence properties of preconditioned iterative solvers for saddle point linear systems

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In recently years there has been a significantly growing interest in the algebraic spectral analysis of matrices in the form $M = [\ A\ \ B^T\ ;\ B\ \ C\ ]$, and of their preconditioned versions $P^{-1}M$ with the nonsingular matrix P specifically chosen.These structured matrices often stem from saddle point problems in a variety of applications, that share some crucial algebraic properties.Under different hypotheses on A, B and C, most results aim at analyzing the spectrum of $P^{-1}M$when P has a block structure similar to that of M, and such that $P^{-1}M$ has favorable spectral properties.In this talk we review some of the recent results in the literature, with special focus on the influence of the spectral properties of $P^{-1}M$ and of the problem parameters on the convergence of Krylov subspace methods.

Adaptive high order finite element methods in H(div) and H(curl)

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Our purpose is to construct finite element spaces of H(div) and H(curl), based on bidimensional and tridimensional elements with constant Jacobians. Furthermore, the finite elemenst spaces are supposed to be of hierachical form to allow hp adaptivity. We show how to obtain such vectorial finite element spaces from a family of H1 scalar functions. For low order linear aproximation, the resulting H(div) spaces agree with the usual Raviart-Thomas elements, with constant normal components.

Curved elements in the DGFEM for nonlinear convection-diffusion problems in 2D

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Theoretical papers on the discontinuous Galerkin method for nonlinear convection-diffusion problems in 2D consider mostly problems on polygonal domains. However, in practice the boundaries of the domains are usually curved. In some cases the DGFEM does not give satisfactory results in the neighbourhood of curved parts of the boundary, if these parts are approximated by line segments. In our contribution we shall introduce one type of curved elements and we shall present the error estimate for the method employing these elements.

Numerical approximation for the fractional diffusion equation

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The use of the conventional diffusion equation in many physical situations has been questioned in recent years and alternative diffusion models have been proposed. Fractional space derivatives are used to model anomalous diffusion, where a particle plume spreads at a rate inconsistent with the classical Brownian motion model.
A one dimensional fractional diffusion model is considered, where the usual second-order derivative gives place to a fractional derivative of order alpha, $1 < \alpha < 2$. We consider the Caputo derivative as the space derivative, which is a form of representing the fractional derivative by an integral operator. The numerical solution is derived using Crank-Nicolson method in time combined with a spline approximation for the Caputo derivative in space. Consistency and convergence of the method are examined and a numerical test is presented.

Parallel MD simulations of ion solvation phenomena

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Many important chemical reactions take place at surfaces and/or interfaces. The distribution of particles on the surface can be very different from that in the bulk. Molecular Dynamics (MD) can be used to study the distribution of atoms. Compared to the bulk, a substantially larger number of particles are required in surface simulations to obtain converged properties. Parallelising MD simulations for small chemical systems is relatively trivial, but parallel scaling to many CPUs require domain decomposition algorithms to minimize the amount of communication between the processors. I will present some parallel algorithms used to parallelise MD, scaling results using these algorithms, as well as comparative results of ion solvation in the bulk and at liquid/vacuum surfaces.

Analysis of finite element methods for the Brinkman problem

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The Brinkman equation is a combination of the Stokes and Darcy equations. The natural mathematical framework for the analysis of the Brinkman equation is derived. It is capable of analysing accurately even the limiting Darcy equations.
A discrete extension of the framework is used to analyse various finite element method discretizations, such as the MINI element and stabilized P1-P1 and P2-P2 methods. All the methods are shown stable for both the Stokes and the Darcy equations. A priori and residual based a posteriori error estimates are also derived.

Adaptive wavelet methods for solving operator equations: An overview

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We describe the state of the art in the field of adaptive wavelet methods for solving operator equations that were introduced by Cohen, Dahmen and DeVore in 2000 and 2002. With an operator equation, we mean an equation of the form $Bu=f$, where B is a (linear) boundedly invertible mapping between ${\mathcal X}$ and ${\mathcal Y}'$ with ${\mathcal X}$ and ${\mathcal Y}$ being some Hilbert spaces. By equipping ${\mathcal X}$ and ${\mathcal Y}$ with Riesz bases, an equivalent formulation of the problem is given by a bi-infinite matrix vector equation ${\bf B}{\bf u}={\bf f}$. Examples include well-posed boundary value problems, integral equations or parabolic initial boundary value problems. Constructing these Riesz bases as wavelet bases, for a large class of problems the matrix ${\bf B}$ can be well approximated by sparse matrices. This allowed the design of adaptive schemes for solving the bi-infinite matrix vector equation that converge with the best possible rate in linear complexity. In particular, we will discuss the application of these schemes when tensor product wavelet bases are applied. In that case, the schemes have the unique feature thatthis best possible rate does not deteriorate as function of the space dimension. One promising application that we will discuss is that to the simultaneous space-time variational formulation of parabolic evolution equations, where, due to the tensor product structure, the additional time dimension does not increase the order of complexity to solve the system.

Analysis of the Parallel Finite Volume Solver for the Anisotropic Allen-Cahn Equation in 3D

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In this contribution, a parallel implementation of the finite volume solver is introduced, designated to numerically solve the initial boundary value problem for the Allen-Cahn equation with anisotropy. The steps of the theoretical convergence analysis are outlined, leading to an error estimate theorem. Furthermore, the experimental order of convergence is evaluated, based on extensive tests performed on high performance computing systems. The efficiency of the parallel algorithm is also investigated and the results are presented in the form of charts. The final part gives a brief overview of a magnetic resonance tractography (neural tract tracking and visualization) method consisting in the solution of the above problem.

Parameter identification in arterial models using clinical data

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The mechanical modelling of soft tissue has evolved over the last decades and models today include non-linear deformations, growth, remodelling etc. With increasing model complexity, the number of unknown parameters tend to grow. Whether a parameter describes the material or some other property, it must ultimately be identified from experiments. For clinical applications, these experiments are made within the body and typically give (mechanically) incomplete data. A large number of parameters in combination with incomplete data can be cumbersome from a parameter identification point of view and result in non-convexity and over-parameterisation. This talk will focus on ways to reduce these problems by using constraints in the parameter identification.

Numerical solution of the Helmholtz equation using the discretized boundary integral equation.

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The numerical solution of the Helmholtz equation with nonlocal radiation boundary conditions is considered. We model sound wave propagation in a multilayered piecewise homogeneous medium. A fourth-order accurate boundary integral (collocation) method is used, where the solution inside the domain is computed through a representation integral. The method is corroborated by comparison with a fourth-order accurate finite difference discretization of the partial differential equation.

On the numerical inverse problem of the detection of inhomogeneities for the Maxwell's equations

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We consider for the full time-dependent Maxwell's equations the inverse problem of identifying locationsand certain properties of small electromagnetic inhomogeneities in a homogeneous background medium from dynamic boundary measurements on the boundary for a finite time interval.

The ultimate objective of the work is to determine locations and certain properties of the shapes of smallelectromagnetic inhomogeneities in a homogeneous background medium from dynamic boundary measurements on part of the boundary and for finite interval in time. Using as weights particular background solutions constructed by a geometrical control method we develop an asymptotic method based on appropriate averaging of the partial dynamic boundary measurements.

Iterative substructuring method with balancing preconditioner for linear system with coercive matrix

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Iterative substructuring method with balancing preconditioner consists of Dirichlet solver for Schur complement in subdomain, Neumann solver for block-wise inverse in subdomain, and coarse grid solver for balancing procedure. Solvability of the coarse grid problem plays a key role. For incompressible fluid problems, some techniques are necessary for construction of the coarse space because solvabilities of indefinite system in subspaces are unknown. In case of coercive matrix, which is obtained from discretized equation with pressure stabilization, the coarse space can be constructed as the same way of the elasticity problems and Schur complement system is solved by Full Orthogonalization method (FOM) or GMRES.

Stabilized methods for nonlinear convection diffusion problems in fluid-structure interactions.

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This paper is devoted to the problem of numerical approximation of nonlinear convection-diffusion like problems by finite element method. Especially problems coming from the fluid-structure interactions are considered. We focus on interactions of two dimensional incompressible viscous flow and a vibrating structure. The structure is considered as a solid airfoil with two or three degrees of freedom. The numerical simulation consists of the finite element solution of the Reynolds Averaged Navier-Stokes equations coupled with the system of ordinary differential equations for description of the airfoil motion. The time dependent computational domain and stabilized finite elements are considered.

Adaptive variational multiscale methods: adaptivity and applications

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The adaptive variational multiscale method is constructed to solve partial differential equations with coefficients which varies over different scales in space. The method is based on a splitting into coarse and fine scales together with a systematic technique for approximation of the fine scale part based on solution of decoupled localized subgrid problems. The fine scale approximation is then used to modify the coarse scale equations. Key features are the a posteriori error estimation framework and the adaptive algorithm, for automatic tuning of discretization parameters, based on this error estimation framework. We will discuss implementation issues and show numerical examples in three spatial dimensions, in particular a problem in oil reservoir simulation.

A Mass-Conservative Characteristic Finite Element Scheme of Second Order in Time for Convection-Diffusion Problems

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It is well-known that the conventional Galerkin finite element scheme produces oscillating solutions for high Peclet number convection-diffusion problems. Elaborate numerical schemes such as upwind methods, Petrov-Galerkin methods and characteristic methods have been developed to perform stable computation. Among them we focus on the characteristic method, which leads to symmetric systems of linear equations.

An important property that the convection-diffusion problems possess is the mass balance. In the framework of characteristic methods it is not trivial to maintain this property. Recently we have developed a mass-conservative characteristic finite element scheme of first order in time for convection-diffusion problems [1] . In this talk we extend the scheme to that of second order in time. The mass balance is proved to be maintained for the numerical solution. We also prove the stability and convergence with second order in time increment and k-th order in element size when the P_k element is employed.

Reference

[1] Hongxing Rui and Masahisa Tabata, A mass-conservative characteristic finite element scheme for convection-diffusion problems, to appear in Journal of Scientific Computing.

Multigrid Methods for Elliptic Optimal Control Problems with Neumann Boundary Control

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In this talk we discuss multigrid methods for solving the discretized optimality system for elliptic optimal control problems. We concentrate on a model problem with Neumann boundary control.

The proposed approach is based on the optimality system, which, for the model problem, leads to a linear system for the state y, the control u and the adjoined state p. An Uzawa type smoother is used for the multigrid method. A rigorous multigrid convergence analysis is presented.

Moreover, we will compare this approach with standard smoothers, like Richardson and Jacobi iteration applied to the normal equation of the Kuhn-Tucker system. The numerical experiments also include a comparison with a completely different approach, based on a reduction to an equation in u only.

Analysis and implementation issues for the numerical approximation of parabolic equations with random coefficients

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We consider the numerical approximation of statistical moments of the solution of a linear parabolic PDE whose coefficients are random. We approximate the PDE coefficients in terms of a finite number of input random variables and restate the stochastic PDE as a deterministic parametric PDE, the dimension of the parameter set being the number of input random variables.We show that the solution of the parametric PDE problem is analytic with respect to the parameters. We consider global polynomial approximations based on tensor product, total degree or sparse polynomial spaces and constructed by either Stochastic Galerkin or Stochastic Collocation. We derive convergence rates and present numerical results that show how these approaches are a valid alternative to Monte Carlo Method.

Extension of the complete flux scheme to time-dependent conservation laws

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The complete flux scheme is a discretization method for the steady advection-diffusion-reaction equation, which is based on the solution of a local boundary value problem for the *entire* equation, including the source term. The integral representation of the flux therefore consists of a homogeneous and an inhomogeneous part, corresponding to the homogeneous and particular solution of the boundary value problem, respectively. Applying suitable quadrature rules to all integrals involved gives the complete flux scheme. To extend the scheme to time-dependent equations we apply the method of lines with the complete flux scheme as space discretization in combination with an efficient (stiff) ODE solver. We apply several (second order) time integration methods, such as the θ-method. A further extension is to include the time derivative in the inhomogeneous flux, resulting in an implicit semidiscrete ODE system having a matrix in front of the time derivative. This implicit system proves to have much smaller dissipation and dispersion errors than the standard semidiscrete system, obtained when the time derivative is not included in the inhomogeneous flux. Moreover, inclusion of the time derivative in the inhomogeneous flux significantly improves the accuracy of the fully discrete system. The final scheme displays second order convergence behaviour in the grid size and time step, uniformly in the (local) Peclet numbers, has only a three-point coupling in each spatial direction and does not generate spurious oscillations. We demonstrate the performance of the scheme for some test problems.

Solution of Navier-Stokes Equations Using FEM with Stabilizing Subgrid

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We consider the Galerkin finite element method (FEM) for solving the incompressible Navier-Stokes (NS) equations in 2D. The domain is discretized into a set of regular triangular elements and the finite-dimensional spaces employed consist of piecewise continuous linear interpolants enriched with the residual-free bubble functions. To find the bubble part of the solution, a two-level FEM with a stabilizing subgrid of a single node is described and its application to the NS equations is displayed. The results for backward facing step flow and flow through 2D channel with an obstruction on the lower wall show that the proper choice of the subgrid node is crucial to get stable and accurate solutions consistent with the physical configuration of the problems at a cheap computational cost.

Some variants of the local projection stabilization

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We consider the one-level and the two-level approach of local projection stabilization (LPS) applied to convection-diffusion equations. Stability and convergence for different choices of approximation and projection spaces will be discussed. Motivated by a careful analysis of the one-dimensional case, formulas for the stabilization parameter are derived which depend on the polynomial degree and the data of the problem.

Pricing American Options under the Bates Model

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A linear complementarity problem (LCP) is formulated for the price of an American option under the Bates model. The underlying partial integro-differential operator is discretized using a finite difference method and a simple quadrature. Time stepping is performed using a componentwise splitting method. It leads to the solution of sequence of one-dimensional LCPs which can be solved very efficiently using the Brennan and Schwartz algorithm. Numerical experiments demonstrate the componentwise splitting method to be fast and accurate.

Numerical Computation to Support Splitting and Merging Phenomena Caused by the Interaction between Diffusion and Absorption.

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Numerical experiments to nonlinear diffusion equations suggest several interesting phenomena. One of them is the occurrence of numerical support splitting phenomena caused by the absorption. The most remarkable property is that the interaction between diffusion and absorption causes numerically repeated support splitting and merging phenomena in a nonlinear model equation. From numerical computation it is difficult to justify whether such phenomena are true or not, because the space mesh and the time step are sufficiently small but not zero. In this talk we introduce the numerical support tracking method, and justify numerically repeated support splitting and merging phenomena from analytical points of view.

Model reduction for efficient simulation of fiber suspensions

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There is a strong anisotropy in the motion of slender rigidfibers. This anisotropy contributes to the very rich and complexdynamical behavior of fiber suspensions. The forming of "clusters" or"flocs" are purely three dimensional phenomena, and the directsimulation of these problems require simulations with many fibers forlong times.Earlier, we have developed a numerical algorithm to simulate thesedimentaion of fiber suspensions, considering a Stokes flow, forwhich boundary integral formulations are applicable. The algorithm isbased on a non-local slender body approximation that yields a systemof coupled integral equations, relating the forces exerted on thefibers to their velocities, which takes into account the hydrodynamicinteractions of the fluid and the fibers. Even though there is agreat gain in reducing a three-dimensional problem to a system ofone-dimensional integral equations, the simulations are stillcomputationally expensive, and the code has been parallelized and runon large computers to allow for more fibers and longer simulationtimes.In this talk, I will present a model where approximations have beenmade to reduce the computational cost. Modifications have mainly beenmade concerning computation of long range interactions of fibers. Thecost is substantially reduced by e.g. adaptively truncated forceexpansions and the use of multipole expansions combined with analyticalquadrature.I will present results from various simulations and discuss theaccuracy of the new model as I compare these results to results fromlarge parallel simulations with the full model. A substantialreduction of the computational effort is normally attained, and thecomputational cost may comprise only a small fraction ofthe cost of the full model. This is however affected by parametersof the problem, such as the geometry and the fiber concentration, aswill be discussed.

Multi-Resolution Scheme and Roe Solver for Stochastic Systems of Conservation Laws

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A spectral method for uncertainty propagation and quantification in hyperbolic systems of conservation laws is presented. We consider problems with uncertain initial conditions and model coefficients, whose solutions exhibit discontinuities in space and along stochastic dimensions. For the discretization, we rely on multi-resolution schemes with multi-wavelet bases at the stochastic level, and finite volume schemes in space. A Stochastic Galerkin projection is used to derive a system of deterministic equations for the stochastic modes. Hyperbolicity of the Galerkin system is discussed, and an efficient Roe solver with fast computation of approximated upwind matrixes is proposed. Simulation results for the Euler equation demonstrate the ability of the method to deal with discontinuities.

Construction of the Third Order of Accuracy Sequential Type Decomposition Scheme and Numerical Computation for Multidimensional Inhomogeneous Evolution Problem

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In the present work sequential type decomposition scheme with the third order of accuracy for the solution of multidimensional inhomogeneous evolution problem is constructedand investigated. Decomposition scheme is constructed on the basis of rational splitting of exponential operator function. Splitting of the third order is reached by introducing a complex parameter.The stability of the considered scheme is shown and explicit a priori estimations for the error of approximate solution are obtained. On the basis of the constructed decomposition scheme, numerical calculations for two and three dimensional inhomogeneous evolution problems are carried out. The stability and precision order of the scheme is shown basing on comparative analysis of results of numerical calculations for test problems.

FEM techniques for incompressible multiphase flow based on Level Set and Phase Field approaches

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We present our recent developments regarding modified problem formulations and special FEM techniques for an accurate handling of the unknown interface (w.r.t. interface position and mass conservation) and for an implicit treatment of surface tension. The corresponding discretizations and solvers are based on Level-Set and Phase Field models which have different numerical characteristics. Results from preliminary studies are presented and compared with results from the literature.

Spectral clusters and Toeplitz/rank structures for nonsymmetric multilevel matrices

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We overview the theory of spectral clusters proposed in [1] and extendedin [2] to the case of eigenvalue distribution for uni-level nonsymmetric Toeplitzmatrices. Then we show how this theory can be generalized to the caseof multilevel matrices. Moreover, we present a ``true version'' of distributiontheorems for some classes of nonsymmetric matrices.[1] E.E.Tyrtyshnikov, A unifying approach to some old and new theorems on distributionand clustering, Linear Algebra Appl. 232: 1-43 (1996).[2] E. Tyrtyshnikov and N. Zamarashkin, Thin structure of eigenvalue clusters fornon-Hermitian Toeplitz matrices, Linear Algebra Appl. 292: 297--310 (1999).

FEM Solution of Diffusion-Convection-Reaction Equations in Air Pollution

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We consider the numerical solution of the diffusion-convection-reaction (DCR) equation resulting in air pollution modeling. The finite element method (FEM) of Galerkin type with linear triangular elements is used for solving the DCR equations in 2D. The instabilities occuring in the solution when the Galerkin FEM is used, in convection or reaction dominated cases, are eliminated by using an adaptive stabilized FEM. The Crank-Nicolson scheme is used for the temporal discretization. The stabilization in FEM makes it possible to solve DCR problems for very small diffusivity constants. For transient DCR problems, the stabilization improves the solution for the case of reaction or convection dominance, but the improvement is not that pronounced as in the steady problems.

Adaptive wavelet-based approximation for the solution of the Chemical Master Equation

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In the stochastic formulation of reaction kinetics, the time evolution of the probability distribution for a system of interacting molecular species is governed by the Chemical Master Equation (CME). Using standard methods to solve this equation is usually impossible, as the number of degrees of freedom is far too large. In this talk, we propose the use of compactly supported orthogonal wavelets in order to avoid the "curse of dimensionality" that affects the CME. A thresholded wavelet basis is used to adaptively represent the solution and only the essential degrees of freedom are propagated in each step of the time integration. Several wavelet bases are investigated for their approximation properties and the performance of the method is illustrated by numerical experiments.

Software for Computing Acute and Non-obtuse Triangulations of Complex Geometric Domains

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A number of algorithms has been proposed in the literature for computing acute and non-obtuse triangulations of two-dimensional geometric domains. Generally, existing algorithms are limited in the complexity of geometric domains they can handle, or in their practicality. We present algorithms and software for computing triangulations of complex geometric domains where all angles are kept to be less than as low as 81 degrees. With this new software, one can compute nicely graded acute and non-obtuse meshes, while keeping all angles at least 35 degrees. We present experimental study to illustrate the premium quality meshing power of our software compared to existing triangulation (meshing) algorithms and software.

Formulation of Staggered Multidimensional Lagrangian Schemes by Means of Cell-centered Approximate Riemann Solver

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To satisfy the conservation laws in Lagrangian methods for compressible gas dynamics, the fluid equations should be discretized in a way compatible with the description of mesh motion.
In cell-centered schemes, conservation is naturally achieved but the issue arises how to translate velocity values from cells to nodes and thus consistently move the mesh. On the other hand staggered methods require some mechanism that dissipates the kinetic energy into internal energy across shock waves, which is usually provided by adding artificial viscosity.
We propose a new formulation of the staggered scheme by locating an approximate Riemann solver into the cell center. This description should provide deeper understanding of relations between cell-centered and staggered Lagrangian schemes.

Multigrid methods for control-constrained elliptic optimal control problems

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Multigrid schemes that solve control-constrained elliptic optimal control problems discretized by finite differences are presented. A gradient projection method is used to treat the constraints on the control variable. A comparison is made between two multigrid methods, the multigrid for optimization (MGOPT) method and the collective smoothing multigrid (CSMG) method. To illustrate both techniques, we focus on minimization problems governed by elliptic partial differential equations with constraints on the control variable.

Modeling Biogrout: a new ground improvement method based on microbial induced carbonate precipitation

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Biogrout is a new ground improvement method based on microbial induced carbonate precipitation. Bacteria and reagents are flushed through the soil, resulting in calcium carbonate precipitation and consequent soil reinforcement. A model was created that describes the process. The model contains the concentrations of the dissolved species that are present in the precipitation reaction. These concentrations can be solved from a convection-dispersion-reaction equation with a variable porosity. Other model equations involve the concentrations of the bacteria and the solid calcium carbonate, the decreasing porosity (due to precipitation) and the flow. The differential equations are solved by the Standard Galerkin Finite Element Method. Simulations are done for some 2D and 3D configurations.

Calderon-Zygmund singular integrals in continuous and discrete situations

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One considers certain points of Calderon-Zygmund singular integrals theory related to their digitization and description via special integral operators, which are one of multivariable analogues of well-known Hilbert transform. These last operators are closely related to some multivariable variant of classical boundary Riemann problem.

For the discrete Calderon-Zygmund operators particularly one observes an interesting phenomenon. It's shown the continual and discrete Calderon-Zygmund operators have the same specters, which don't depend on lattice parameter. It gives the base to construct and justify some approximate methods for solving equations with Calderon-Zygmund operators.

Introduction to adaptivity for non-linear and non-smooth problems

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The purpose of this presentation is to give a brief introduction to the a posteriori error analysis of finite element solutions and adaptive methods for non-linear and non-smooth problems, the subject of the minisymposium `Adaptivity for non-linear and non-smooth problems'. To this end, we shall consider model nonlinearities, discuss their relevant features, and survey some available results.

Angle Conditions for Discrete Maximum Principles in Higher-Order FEM

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This contribution addresses the question of nonnegativity of higher-order finite element solutions on triangular meshes. First we overview the theory of discrete maximum principles (DMP) for second order elliptic problems discretized by the finite element method. Then we recall the angle conditions guaranteeing the DMP for the standard piecewise linear finite elements. Finally, we present a series of numerical experiments, where we test nonnegativity of higher-order approximations at nodal points. The results reveal the dichotomy of the odd and even polynomial degrees and they indicate that the higher-order approximations allow for weaker angle conditions.

Mechanoenergetics of actomyosin interaction analyzed by cross-bridge model

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We present a mathematical model of actomyosin interaction, as a further development of an model that links mechanical contraction with energetics (Vendelin et al, Annals of Biomedical Engineering: 28, 2000). The new model is a three-state Huxley-type model for cross-bridge interaction and a model of calcium induced activation. The model is self-consistent and is based on T. Hill formalism linking the free energy profile of reactions and mechanical force. According to the experiments, the dependency between oxygen consumption and stress-strain area is linear and is the same for isometric and shortening contractions. In our simulations we replicated the linear dependence between oxygen consumption and stress-strain area together with other important mechanical properties of cardiac muscle.

An Adaptive Finite Element Method for Shape Optimization problems

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We examine shape optimization problems in the context of inexact sequential quadratic programming. Inexactness is a consequence of using adaptive finite element methods (AFEM) to approximate the state equation, update the boundary, and compute the geometric functional. We present a novel algorithm that equidistributes the errors due to shape optimization and discretization, thereby leading to coarse resolution in the early stages and fine resolution upon convergence. We discuss the ability of the algorithm to detect whether or not geometric singularities such as corners as genuine to the problem or simply due to lack of resolution - a new paradigm in adaptivity. We present some numerical examples.

A mathematical model for wound contraction and closure

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We construct a formalism for the simulation of dermal wound repair, taking into account proliferation of fibroblasts, myofibroblast, blood vessels, epidermal cells, growth factors and signaling agents. The model is formulated in terms of nonlinearly coupled visco-elastic equations and a set of diffusion-reaction equations for the biological constituents. Further, the visco-elasticity equations depend on the fibroblast density due theirpulling mechanism on the extra cellular matrix, which is produced by thefibroblasts.
The coupling between the partially overlapping processes is a novelty. Besides, the formalism of the model and some qualitative mathematical analysis of the problem, the finite element procedures for the coupling are discussed.

Unsteady High Order Residual Distribution Schemes with Applications to Linearised Euler Equations

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In this article we will present the latest development in the construction of higher order residual distribution schemes (RDS) for the solution of unsteady systems of conservation laws. The methodology used here considers time as a third dimension leading to prismatic space-time elements where we can reuse the steady methodology of RDS. To achieve high order we combine P^2 triangular finite elements with a quadratic discretization of the time. We subdivide these space-time elements in sub-elements and on each sub-element we compute the high order residual that is distributed to the space-time upwind nodes. The resulting scheme is 3rd order accurate in both space and time. We will show the improvement brought by the high order discretization on several testcases including the unsteady Euler equations and the Linearised Euler equations.

Analysis of semi-implicit time discontinuous Galerkin

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We deal with the general semilinear scalar convection-diffusion equation . We assume general discretization in space and obtain stiff system of ODE's.For time discretization we want to develop scheme of higher order of accuracy, without strong restriction on time step, which is suitablefor adaptation in time. Since standard multistep methods (like BDF) suffer from loss of stability for higher orders, we choose to employ time discontinuous Galerkin with suitable linearization which represents promising candidate for solving these problems. We show the most important pieces of the analysis, the resulting a priori asymptotic error estimates in L^\infty(L^2)-norm and L^2(H^1)-seminorm and several numerical examples verifying the theoretical results.

Stability of central finite difference schemes on non-uniform grids for the Black-Scholes equation

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We consider the well-known Black-Scholes equation from financial option pricing theory. The Black-Scholes equation is a time-dependent one-dimensional advection-diffusion-reaction equation and is supplemented with initial and boundary conditions.

A popular approach for the numerical solution of time-dependent partial differential equations is the method-of-lines. It consists of two steps: in the first step we perform a spatial discretization. This means that the partial derivatives w.r.t. the spatial variables are discretized on a finite spatial grid, yielding a (large) system of ordinary differential equations $U'(t)=AU(t)+b(t)$ $(t>0)$ with given fixed matrix A and vectors b(t). During the second step, the temporal discretization, the above system of ordinary differential equations is numerically integrated in time.

Our research focuses on the stability analysis of central second-order finite difference methods for the spatial discretization of the Black-Scholes equation. We first present practical upper bounds for $\|e^{tA}\|_2$ $(t>0)$ where $\|\bullet\|_2$ denotes a scaled version of the standard spectral norm. We subsequently present sufficient conditions for contractivity in the maximum-norm.

A virtue of our stability analysis is that it also applies to spatial grids that are not uniform. Such grids are often used in actual applications. Numerical experiments are provided which support our theoretical results.

Finally, we briefly discuss the stability of temporal discretization schemes.

Multigrid, adaptivity and finite differences in option pricing problems.

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We consider the numerical solution of the Black-Scholes equation using finite differences. To increase the efficiency of the method we employ adaptivity. The local truncation error is estimated and grid-points are placed in an optimal way to reduce this error. For high-dimensional problems (i.e. options on several underlying assets) this is of utmost importance in order to mitigate the curse of dimensionality.
In time we employ an implicit method yielding a linear system of equations to solve each time-step. This system of equations is solved using a Krylov subspace method. To reduce the number of iterations and the computational cost we employ multigrid as a preconditioner. We will present results both from a theoretical analysis as well as results from numerical experiments.

Machine learning approach to performance tuning of parallel power grid simulator

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Power grid simulation is an important stage of EDA design cycle. It requires use of parallel computations for simulating large PGs in adequate time. PG simulation is stated usually as solving ODE for time steps, where solution time is mostly spent on parallel solving of sparse linear equation systems. Selection of appropriate linear solver and tuning its parameters impacts on simulation performance. We propose method for automated selection and tuning solver. It is based on gathering simulation statistics and training nonlinear regression to approximate simulation complexity metric. Then, explicit complexity metric function that depends on power grid structure, solver and platform settings is created, then genetic algorithm is used to find its minimum on set of solver settings.

Scalable PCG Algorithms for Numerical Upscaling of Voxel Structures

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Numerical homogenization is applied for upscaling of the linear elasticity tensor of strongly heterogeneous microstructures. Rannacher-Turek finite elements are used for the discretization. The scalability of two parallel PCG solvers is studied. Both are based on displacement decomposition. The first one uses modified incomplete Cholesky factorization MIC(0) and the other - algebraic multigrid. The numerical homogenization scheme is based on the assumption of a periodic microstructure. This implies the use of periodic boundary conditions on the reference volume element. Numerical upscaling results are shown. The test problem represents a trabecular bone tissue. The voxel microstructure of the bone is extracted from a high resolution computer tomography image.

Computational estimation of fluid mechanical benefits from modifying the shape of artificial vascular grafts

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Intimal hyperplasia (IH) at the distal end of artificial vascular grafts is considered an important determinant of graft failure. The connection between IH and unhealthy hemodynamics motivates the use of CFD to search for improved graft designs. We simulate the blood flow using Navier-Stokes equations, where a shear-thinning viscosity model describes the non-Newtonian aspects of the blood. In the present study, we focus on IH at the suture line and illustrate benefits from the introduction of a fluid deflector to shield the suture line from an unhealthy high wall shear stress.

The Credit Channel and Asset Prices

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We study the implications of the credit channel for asset prices and economic growth. Specifically, we consider how resources are optimally allocated between a banking sector and a risky sector. To do so, we use a two trees framework with a risky and risk free sector, in which capital moves sluggishly between the two. We characterize equilibrium, and illustrate how financial flexibility affects the term structure and social welfare. We develop a pricing equation for the equilibrium term structure and characterize the steady state distribution of growth rates in the economy. In addition, we demonstrate by example how financial innovation may increase or decrease the growth rate of the economy, how the effectiveness of monetary policy depends on the current state of the economy, and how a central bank can reduce theprobability that the economy is in a low growth state.

An Appraisal of a Contour Integral Method for the Black-Scholes and Heston Equations

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Traditionally, semi-discretizations of linear parabolic PDEs have been integrated with Runge-Kutta or Multistep Methods (the method-of-lines). In the past two decades or so, however, new methods based on Laplace transformation and numerical contour integration have gained popularity. In previous work [1,2] contour parameters were optimised and convection-diffusion and fractional-diffusion equations were solved. In the present work we extend these ideas to some of the PDEs from mathematical finance. The pros and cons of these methods are examined, and numerical results are presented.

[1] JAC Weideman and LN Trefethen, "Parabolic and Hyperbolic Contours for Computing the Bromwich Integral", Math. Comp., Vol. 76, pp. 1341-1356 (2007)
[2] JAC Weideman, "Improved Contour Integral Methods for Parabolic PDEs", to appear in IMA J. of Numer. Anal.

Solving Differential Algebraic Equations with Singularities

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We study the convergence behaviour of collocation schemes applied to approximate solutions of BVPs in index 1 DAEs which exhibit a critical point at the left boundary. Such a critical point of the DAE causes a singularity within the inherent ODE system. We focus our attention on the case when the inherent ODE system is singular with a singularity of the first kind. We show that for a well-posed boundary value problem for DAEs having a sufficiently smooth solution the global error of the collocation scheme converges with the order s, where s is the number of collocation points. Superconvergence cannot be expected to hold in general, due to the singularity, not even for the differential components of the solution. The theoretical results are illustrated by numerical experiments.

Adaptive refinement for variational inequalities

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A posteriori error estimators for variational inequalities (obstacle or Signorini type) are considered. Our estimators are based on H(div)-conforming liftings from the equilibrated fluxes on the edges. In the case of a membran problem low order standard mixed finite elements can be used. The situation is more complex for an elasticity problem where a symmetric tensor is required. Upper and local lower bounds for the error are shown for a one-body contact problem without friction, and a AFEM result is provided. The constant in the upper bound is equal to one. Numerical examples illustrate the quality of the estimator. To show the flexibility, we also generalize our results to two-body contact problems with Coulomb friction on non-matching meshes and to obstacle problems with two membrans.

High Frequency Wave Propagation in Solid-State Laser Resonators

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Common simulation techniques for the optical wave in solid-state lasers either require certain approximations or are not applicable due to the large typical size of laser resonators, typically about 10.000-100.000 wavelengths. For this reason we present a new 3-dimensional, time-dependent finite element method to simulate the laser beam inside the resonator: The wave equation is transformed by a special ansatz and the resulting quasi-Schroedinger equation is solved by a robust GMRES solver in combination with a fast multigrid preconditioner. By this technique, several well-known numerical issues with high frequency oscillations are avoided. Yet, optical elements like lenses, curved interfaces, mirrors, and the dynamic interaction with the laser medium can still be described accurately.

RBF Approximation of vector functions and their derivatives on the sphere with applications

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Vector fields tangent to the surface of the sphere, S^2, appear in many applications. For example, in the atmospheric sciences the horizontal velocity of the air in the atmosphere is modeled as a tangent vector field. We present a new numerical technique based on radial basis functions (RBFs) for fitting tangent vector fields from samples of the field at "scattered" locations on S^2. The method is entirely free of any coordinate singularities, naturally provides a way to decompose the reconstructed field into its individual Helmholtz components (i.e. divergence- and curl-free parts), and can be used to approximate surface derivatives of the field. Examples for fitting and decomposing vector fields are given and applications for simulating PDEs are discussed.

On Challenges for Hypersonic Turbulent Simulations

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This talk discusses some of the challenges for design ofsuitable spatial numerical schemes for hypersonic turbulent flows,including combustion, and thermal and chemical nonequilibrium flows.Often, hypersonic turbulent flows around re-entry space vehicles andspace physics involve mixed steady strong shocks and turbulence withunsteady shocklets. Material mixing in combustion poses additionalcomputational challenges. Proper control of numerical dissipation innumerical methods beyond the standard shock-capturing dissipation atdiscontinuities is an essential element for accurate and stablesimulations of the subject physics. On the one hand, the physics ofstrong steady shocks and unsteady turbulence/shocklet interactionsunder the nonequilibrium environment is not well understood. On theother hand, standard and newly developed high order accurate(fourth-order or higher) schemes were developed for homogeneoushyperbolic conservation laws and mixed hyperbolic and parabolic partialdifferential equations (PDEs)(without source terms).

Approximating a delta function with support on a level set

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Many problems to which level set methods have been applied contain singular functions, and the approximation of Dirac delta measures concentrated on curves or surfaces is an important component in the discretization. A common approach to approximate such a delta function is to extend a regularized one-dimensional delta function to higher dimensions using a distance function. Precaution is needed since this approach may result in O(1) errors [J. Comput. Phys. 200, 462 (2004)]. We present a second order accurate approximation of the delta function which is easy to implement and suitable for level set methods. We prove the rate of convergence and present numerical experiments.

Breaking the curse of dimensionality in stochastic Galerkin methods using tensor product approximations

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In Stochastic Galerkin methods we are faced severly with the curse of dimensionality. The spectral approximations for the solution have the size of the product of spatial and stochastic dimensions. In using tensor product approximations of the solution already in the solution process, we try to break this curse. We show that this approach turns out to be equivalent to working with Karhunen-Loève approximations of the intermediate solutions. The size of those intermediate solutions is reduced to only the sum ofspatial and stochastic dimension times some small constant. Furthermore, the runtime is greatly decreased due to much fewer calls to the deterministic solver.

The Use of Principal Component Analysis for Reduction of Dimension of Reactive Transport Model

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One of the basic problems of real-world reactive transport simulation is too large dimension of the problem given by the number of simulated chemical species in solution. There is a possibility to solve this problem by using standard algebraic tools, such as Principal Component Analysis (PCA).
PCA helps to reduce dimension of the problem. The reason for using PCA is to speed up the transport simulation reducing the size of memory, which is taken by the information about chemical analyses. The reduction can be effeciently realized on linearly correlated data through transforming the data to the new system of coordinates, which has lower dimension.
In our presentation we are going to describe our approach and its specific application we realized.

Hierarchical error estimates for a Signorini problem

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In this talk, we presents hierarchical error estimates for the linear finite element approximation of Signorini problems in twoor three space dimensions. The main result is to show that the discretization error is equivalent to our hierarchical estimatorsup to some additional data oscillation terms. We perform several numerical experiments to verify our theoretical results.

Finite element tensor representations through automated modeling

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The solution of partial differential equations (PDEs) has motivated the development of automated modelling software such as the FEniCS project [1] for which the main goals are to achieve generality and efficiency of the modelling process. Recent developments of the FEniCS Form Compiler (FFC) has greatly increased the range of problems which can be handled in a generic fashion. However, for complicated variational problems, where automation is particularly desirable, efficiency can be elusive. We present here some recent advances in FFC that address the efficiency issue and thereby increases the range of problems to which the automated modelling paradigm can be applied in practise by restoring the balance between generality and efficiency.
[1] http://www.fenics.org

List of participants