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This was the first meeting in Oberwolfach on scientific computing with special emphasis on technical applications. This interdisciplinary conference organized by Franz Durst (Erlangen), Roland Glowinski (Houston), and Christoph Zenger (München) brought together applied mathematicians and engineers working in the field of numerical simulation of technical processes modelled by systems of partial differential equations. In a group of main lectures mathematical models from various fields of applications (compressible and incompressible flows, material sciences, electromagnetic fields, heat transfer, turbulence, stochastic phenomena, phase transition, structural analysis) were elaborated in some detail. In shorter contributions new numerical methods were presented (multilevel schemes, construction of adaptive grids, a priori and a posteriori error analysis and error control, discretization of partial differential equations etc.). Discussion was encouraged to get more insight which methods are or may be applicable to specific problems. One afternoon session was devoted to the situation of scientific computing in Germany including the problem of a sufficient funding of research projects and appropriate hardware equipment for high performance computing.

The participants agreed that the interdisciplinary selection of participants was advantageous and the initiatives encouraging the cooperation of numerical analysts, engineers, and computer scientists should be brought forth to bring the newest methods immediately to the applications and to get mathematicans interested in complex applications where mathematical models do not exist or are at least questionable. The quiet and stimulating atmosphere of the institute and the excellent service provided a good basis for the conference to go a successful step in this direction.

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Vortragsauszüge

Dietrich Braess

Efficient Smoothers for Multigrid Methods for the Stokes Problem or for Mortar Elements

We divide iterations for saddle point problems into those which are called u-dominant and those which are p-dominant.

It turns out that for the problems mentioned the u-dominant iterations provide better smoothers. In particular the matrix A from

$$\begin{pmatrix} A & B^T \\ B & O \end{pmatrix}$$

may be replaced by a multiple of the identity. The auxiliary problems require the solution of a Poisson equation, or a solution of a problem living on a small set. The smoothing property can be established by algebraic arguments since only a Lagrangian term is now added.

The approximation properties are obtained by using advanced techniques form finite element theory.

Michael Breuer

Large Eddy Simulation of Turbulent Flows

The lecture gives an introduction into the large eddy simulation (LES) technique. The fundaments of LES are presented starting with Kolmogoroff's energy cascade which leads to the basic concept of LES. The filtering approach is explained separating the large energy-carrying vortices which can be computed directly (grid-scale) from the nonresolvable subgrid-scale structures which have to be modeled by a subgrid-scale model. The governing equations for LES are given and the most widely used subgrid-scale models are explained. Furthermore, the problem of defining appropriate boundary conditions is addressed. Then an example for a LES computation is shown, namely the flow around a surface mounted cubical obstate placed inside plane channel flow at $Re = 40,000$. This test case demonstrates that LES is well suited for turbulent flows past bluff bodies which are in general very complicated, including complex phenomena such as separation, reattachment or vortex shedding. A second test case is the turbulent flow past a circular cylinder at a sub-critical Reynolds number ($Re = 3900$). The objective of this investigation was not to investigate the physical phenomena of this flow in detail but to study numerical and modeling aspects which influence the quality of

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LES solutions. Concerning the numerical method the most important component is the discretization of the non-linear convective fluxes. On the modeling side the influence of different subgrid scale models was studied in detail. The results were evaluated by comparison with experimental data available. Finally, the lecture will give a conclusion of the investigations mentioned above.

Hans-Joachim Bungartz

Towards Optimal Grid Pattern for Hierarchical Tensor Product Spaces

In this talk, we want to show ways to an optimal ε-complexity of the representation of functions of d variables living in spaces of bounded mixed derivatives. Here, the ε-complexity of a problem indicates the number of operations that are necessary to solve the problem up to an accuracy of ε.

For the setting of a tensor product based and piecewise linear hierarchical subspace splitting, we derive finite dimensional approximation spaces or grid patterns, respectively, that are optimal with respect to the ratio of invested unknowns (cost) vs. achieved accuracy (profit). The underlying optimization process can be formulated both as a restricted continuous optimization problem and as a restricted discrete optimization problem, a so-called binary knapsack problem. In our special situation, both problems can be solved explicitly via Lagrange multipliers or rational knapsack solvers, respectively. As the most important result, we get that the (*global*) process of finding optimal approximation spaces can be reduced to studying the (*local*) cost profit ratio of each hierarchical subspace. Due to the fact that a subspace's profit depends on the norm in which we measure its contribution to the overall interpolant, we get different optimal grids for different norms. For the L_∞- and the L_2-norm, standard sparse grids turn out to be the solution of this optimization process. Here, we get $O(h^{-1}|\log h|^{d-1})$ grid points and an accuracy of $O(h^{-1}|\log h|^{d-1})$. For the H^1-norm, we get even sparser optimal grids with $O(h^{-1})$ grid points and an $O(h)$ accuracy. In terms of the ε-complexity, this means that we can construct approximation spaces and grid patterns leading to an $O(\varepsilon^{-1})$ complexity of the problem of representing or interpolating functions of bounded mixed derivatives. It is even possible to construct a multilevel solver for Poisson's equation of the same complexity $O(\varepsilon^{-1})$, i.e., apart from constant factors, without dependence on the problem's dimensionality d.

Wolfgang Dahmen

Compression of Flux Computation in Finite Volume Discretizations

This talk is concerned with accelerating the computation of numerical fluxes in finite volume discretizations for conservation laws. The key ingredients are certain multiscale transformations by which the evolution of cell averages is turned

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into the evolution of multiscale coefficients which represent finer detail of the conservation variables when progressing to higher discretization levels. In particular, the size of these coefficients indicates where expensive accurate flux calculations are necessary or where unexpensive interpolation from coarser scales suffices. It is pointed out how to increase the compression effect by properly tuning the multiscale transfromations. Some numerical experiments for hypersonic blunt body flow are presented.

Jake Davis

Abstract

In this lecture we briefly discuss, first, a distributed Lagrange multiplier based, fictitious domain method for the numerical simulation of incompressible viscous flow, modelled by the Navier-Stokes equations, around moving rigid bodies. Then we apply the above method to simulate the sedimentation of densely and regularly packed solid particles, initially at rest and located on top of a lighter fluid. The simulation clearly shows that a Rayleigh-Taylor instability takes place at the beginning of the sedimentation phenomenon.

Peter Deuflhard

Modelling, Simulation, and Visualization in the Clinical Cancer Therapy Hyperthermia

The talk addresses regional hyperthermia, i. e. the local heating of a tumour (and *not* the sane tissue), typically in combination with chemo- or radio-therapy. In order to concentrate the heat in the region of interest, the numerical solution of Maxwell's equation in heterogeneous media (applicator with 8 radio frequeny antennas, water bolus, human body) and a bio-heat-transfer equation have to be solved fast — to be useful in the clinical environment. The generation of a 3D grid for the (individual) virtual patient and supporting visualization play an important role in this context.

Michael Griebel

Parallel Adaptive Multiscale Methods Using Hash–Tables and Space Filling Curves

The parallelization of adaptive multiscale methods is a problem in both molecular dynamic applications and the solution of PDEs. We propose to use hash–tables instead of the usally applied tree–like data structures. Furthermore, parallelization can be achieved in a simple manner by using the approach of space filling curves.

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We give the details of the method and report on the results of our numerical experiments on parallel computers.

Günther Grötzbach

Simulation of Turbulent Heat Transfer in Nuclear Reactor Safety

Detailed thermal and fluiddynamical investigations are performed in studying safety features of existing and new nuclear reactors. For cost and safety reasons it is often not possible to perform realistic full scale experiments. As a consequence, series of model experiments are performed at different scales and at about relevant dimensionless numbers. The results are used to validate the computer codes which are used to transfer the experimental findings to realistic reactor parameters. In this presentation, it will be shown how direct numerical simulations can be used to provide detailed information on the statistics of turbulence in natural convection at unusual conditions, e.g. for liquid sodium at $Pr = 0.006$ and for internally heated fluids at $Ra = 10^{10}$. For these cases there is no sufficient information from experiments to develop reliable turbulence models. The simulation results are used to study the convection and to gain the information to improve existing Reynolds models for those flows. The extended statistical models are then applied in engineering codes to analyse the natural convection in certain model experiments and will finally be used to study the behaviour in the reactor geometry. Typical CPU-times range with both kinds of codes from several tens to several hundreds of hours on high performance vector/parallel computers. Thus efficient solution methods are always required.

Currently we develop a new method to simulate two-phase flows, especially bubbly flow, by a large eddy simulation technique. In a first step we perform model experiments to study the velocity and turbulence field in the near area around bubbles. With other water-air experiments we investigate the augmentation and damping of turbulence by bubbles and the forces acting on bubbles in upward and downward flow. Basing on the experimental results we develop a code for the direct numerical simulation of turbulence surrounding a few bubbles. The results of experiments and simulations will finally form the information basis to develop subgrid scale models and subgrid scale inter-phase relations which shall be implemented in a commercial CFD code. The overall objective is to provide a code for engineering applications, that is for complex geometries and for complex physical phenomena; the code shall give detailed results on local phenomena in three-dimensional time-dependent turbulent two-phase flows, phenomena which are not accessible by the common two-fluid approach. The computational effort will be challenging for nowadays computer systems; thus, a careful selection of suitable solution methods is going on.

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Dieter Hänel

Adaptive Grid Methods for Conservation Laws of Fluid Dynamics

A survey is given about present developments of adaptive grid methods for CFD. The conservation equations of compressible fluids are discretized by Finite-Volume schemes with upwind flux formulations of second order. Explicit and implicit schemes are employed for integration in time.

Different adaptation concepts are considered. Concepts for structured grids are based either on the grid redistribution principle or on hierarchical grid refinement. The latter in form of AMR or DMR methods have shown to be well suited for simulation of complex wave pattern in reactive and non-reactive flows. A very high flexibility for adaptation offer unstructured, triangulated grids. An adaptation method for such grids is presented, based on local grid transformation according to a given adaptation criterion. This method is demonstrated by a number of different, steady and unsteady problems. Finally a new object-oriented solution concept is introduced, which shall enable adaptive solutions on grids of arbitrary element types.

Carlos Härtel

Direkte numerische Simulation von Intrusionsfronten

Die gravitationsgetriebene Ausbreitung von Intrusionsfronten in einem relativ leichteren Umgebungsfeld ist ein Strömungsphänomen, dem man vor allem in den Geowissenschaften häufig begegnet. In der Vergangenheit wurden solche Fronten experimentell intensiv untersucht, bis heute bestehen aber noch zahlreiche offene Fragen, insbesondere hinsichtlich der inneren Struktur der Fronten und ihrer Stabilitätseigenschaften. Direkte numerische Simulationen (DNS), bei denen alle relevanten physikalischen Skalen in Raum und Zeit numerisch aufgelöst werden, können hier nun einen wichtigen Beitrag leisten, um das Verständnis der Frontendynamik zu verbessern.

Im Vortrag werden Ergebnisse einer DNS Studie zur Ausbreitung von Industriefronten in einem ebenen Plattenkanal vorgestellt ("Lock-Exchange Flow"). Die durchgeführten Simulationen basieren auf den Boussinesq Gleichungen, die mit Hilfe eines gemischten Spektral-/Spektral-Elemente-Verfahrens diskretisiert werden. Neben der Darstellung der Simulationsergebnisse sollen im Vortrag auch Details des numerischen Verfahrens sowie die Validierung des Simulationsprogramms an Hand ausgewählter Testprobleme diskutiert werden.

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Ronald H.W. Hoppe

Numerical Simulation of Microelectronic Devices and Systems

The design and layout of microelectronic devices and systems based on semiconductor technology require a physically consistent mathematical modelling of the underlying physical phenomena and powerful numerical solution techniques for a cost-efficient and robust simulation of the operating conditions of such devices and systems. In my talk, I will focus on the second issue and present adaptive finite element methods whose characteristic features are multilevel based iterative solution processes on adaptively generated hierarchies of triangulations where the mesh adaption is founded on efficient and reliable a posteriori error estimators.

As applications, I will consider basic devices such as field effect transistors, reverse biased pn-junctions and insulated-gate bipolar transistors used in high power electronic systems as well as microelectromechanical systems whose functioning is based on the coupling of electrostatic and mechanical effects.

Graham Horton

Mixed Discrete-Continuous Stochastic Models: A Computer Science Application in Scientific Computing

Stochastic models play an important role in Computer Science as the basis for predicting performance and reliability measures of computer systems and networks. These models have been almost exclusively discrete in nature and are usually Markov chains, which lead to manageable numerical problems. The transient analysis of a Markov chain requires the solution of a linear initial value problem, and the steady-state analysis the solution of a linear system of equations.

For several reasons, an extension of the available modeling power to include continuous quantities seems desirable; one attempt to do so leads to the so-called *fluid stochastic Petri-nets (FSPN)*, a hybrid modeling paradigm. The underlying stochastic process of an FSPN is a (continuous) Markov process represented by a system of first order linear hyperbolic partial differential equations. An appropriate discretization of the continuous problem yields a Markov chain. The systems of equations thus generated can be extremely large, owing to the potential high-dimensionality of the continuous part of the state space, and to the combinatorial explosion in the discrete part.

We describe a multi-level method for the steady-state analysis of Markov chains that is based on intuitive probabilistic, as opposed to algebraic, arguments. However, it can be shown that the algorithm can be interpreted as a multi-grid method with a non-linear prolongation operator. Experimental results show that the scheme can be significantly faster than more traditional approaches, especially

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for stiff problems.

Bülent Karasözen

Structure-Preserving Numerical Methods for Volterra Lattice Equations

Numerical integrators which preserve the geometric features, such as time-reversal symmetry and symplectic structures for conservative nonlinear systems arising in simulations of celestial mechanics, rigid-body motion and molecular dynamics become important in recent years. The benefits of these geometric integrators are the improved energy conservation and stability in long-term simulations. But the question of practical importance of these integrators in numerical simulations has so far remained open. Especially for very large systems arising from the discretization of conservative nonlinear partial differential equations, the efficiency issues become very important. In this context, the problem of "integrable discretization" is crucial, i.e. how to discretize an evolutionary Hamiltonian system, like Korteweg de Vries, nonlinear Schrödinger und Landau-Lipschitz equation, such that the integrability of the resulting finite dimensional ordinary differential equation system in maintained.

Volterra equations arising in ecological systems turn out to be integrable discretizations of some PDEs like the inviscid Burger's equation and the Korteweg de Vries equation.

There are mainy three approaches for the time integration of these lattice equations:

- An implicit integrator; Kahan's reflexive splitting, which is equvalent to the implicit mid-point rule with one Newton iteration for Volterra equations.
- An explicit integrator based on vector field splitting and Lobatto IIIA-B pair.
- An explicit integrator based on Hamiltonian splitting and composition methods.

Horst Körner

Numerische Simulation der Aerodynamik von Flugzeugen

Neben der experimentellen Simulation der Aerodynamik von Flugzeugen im Windkanal und im Flugversuch hat die numerische Simulation eine große Bedeutung gewonnen. Wurden früher Flugzeuge im Windkanal optimiert, wird eine Optimierung heute numerisch durchgeführt, und Windkanal und Flugversuch dienen als Leistungsnachweis. In der Entwicklung befinden sich numerische Verfahren zur

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Lösung der Reynolds-gemittelten Navier-Stokes-Gleichungen (RANS) für komplette Flugzeugkonfigurationen.

Der Vortrag wird eingehen auf die Anforderungen an numerische Verfahren. Ein RANS-Verfahren, das im Rahmen eines Verbundprojektes zwischen Großforschung, Universitäten und Industrie derzeit entwickelt wird, wird beschrieben, wobei auf Netzgenerierung, Strömungslöser, Validierung, Qualitätssicherung und alternative Verfahren eingegangen wird.

Dietmar Kröner

A Posteriori Error Estimates for Time Dependent Conservation Laws

The most successful tools for accelerating numerical codes are higher order discretizations, multigrid methods, parallelization and in particular local adaption of the grid. For the last one, there is a well developed theory for elliptic and parabolic partial differential equations, but not for conservation laws. For the first ones, a posteriori error estimators give precise information about the location of the error and can be used to adapt the grid such that the global error is less than a given tolerance. Nevertheless, for conservation laws, people use grid indicators like the discrete gradients of the discrete solution to adapt the grid. But in this way, you will get no real information about the distribution of the error. Only the location of steep gradients of the numerical solution will be indicated.

Rigorous results about of posteriori error estimates for conservation laws in multi dimensions were not available up to now. Tadmor has proved an a posteriori error estimate for nonlinear conservation laws in 1–D. Süli has considered linear hyperbolic systems, Johnson convection dominated diffusion problems, and Cockburn special error estimates for nonlinear conservation laws in multi dimensions.

In this lecture, we present some new results about a posteriori error estimates for nonlinear scalar conservation laws in the L^1–norm. It turns out that the grid in the whole cone of dependence has to be adapted in order to satisfy the prescribed tolerance in a given domain in the (x,t)–plane. In particular, this error estimate takes care of the transported parts of the error. The theoretical results are confirmed by numerical experiments.

Furthermore, we present some numerical examples concerning higher order discretizations, the comparison between results obtained on hexahedrons and tetrahedrons, local grid adaption, and the parallelization for complex flow problems in multi dimensions.

Ulrich Langer

On the Use of (Parallel) Global Extraction Methods

In the engineering literature, the so-called Global Extraction Element-by-Element (GE-EBE) Methods have been successfully used for solving real-life mechanical problems, especially, in 3D, although the EBE preconditioners C haven't any asymptotical preconditioning effects on the stiffness matrix K at all, i.e. the spectral condition number $\kappa(C^{-1}K)$ behaves like $O(h^{-2})$, say, for elasticity problems. However, the method has quite good scaling properties. From a theoretical point of view, the GE-EBE preconditioner is nothing else than an additive Schwarz preconditioner generated by an overlapping splitting of the finite element space into subspaces spanned by the element ansatz functions. The author proposes to use the GE-EBE methods and their patch counterpart (GE-PBP) either as smoothers, especially, in their multiplicative version, or as preconditioners in their multilevel additive version. In the multilevel version, such preconditioners are asymptotically optimal. The GE-PBP smoother is especially suited for the use in algebraic multigrid methods based on graph coarsening strategies. The numerical results presented confirm the good smoothing properties of GE-PBP smoothers as well as the preconditioning properties of multilevel additive GE-PBP preconditioners. Finally, the author discusses prallalization aspects.

Matthias Meinke

Numerical Flow Simulation

Results of recent flow simulations carried out at the computing center of the RWTH Aachen and the High-Performance Computing Center Stuttgart will be reported. The flow simulations comprise steady, compressible two- and three-dimensional, aerodynamic non-reacting and reacting flows, incompressible turbulent flows in plane and round jets, unsteady, compressible three-dimensional flow in a cylinder of a piston engine, and unsteady, three-dimensional, incompressible swirling flow in a divergent pipe including breakdown. The simulations of the aerodynamic flows were carried out simultaneously with experimental investigations of the supersonic and hypersonic flow around a model of the first stage of a space transportation system, its shape resembling that of a thick delta wing with a round leading edge. The comparison of both sets of results demonstrates the accuracy of the numerical simulation, which were obtained with solutions of the parabolized and complete Navier-Stokes equations. The jet flows were predicted with the method of large-eddy simulation, recently extended to the descrption of round jets. The simulation of the flow in a piston engine was restricted to the computation of the time-dependent, three-dimensional velocity, pressure, density und temperature variation during the intake and compression stroke for an engine with two inlet valves. The results, obtained with a finite-volume solution of the Navier-Stokes equations exhibit the formation of two vortex rings, also observed in experiments, their merging and deformation during the intake and compression stroke. Complete agreement with the experimental data of Sarpkaya was obtained for the simulation of vortex breakdown of swirling flow in a pipe. All results are obtained with explicit or implicit integration on block-structured curvilinear grids. The number of grid points varied from 300.000 in the computation of the turbulent jet flow to approximately 2 millions in the simulations of the flow in the piston engine. All algorithms are vectorized and parallelized. Characteristic computing times and memory requirements are reported for the different applications.

Helmut Neunzert

Domain Decomposition for Fluid Mechanical Problems Based on Kinetic Models

Most fluidmechanical equations are asymptotic limits of kinetic models.
This has 2 consequences:

1. In problems with domains in which the macroscopic equation is valid and others in which the kinetic equation has to be solved, three questions may be posed:

   a) The Where-questions: Where is the macroscopic equation valid? Tiwari (97) has developed and investigated several criteria - the best one based on Grad's 13-moment expansion.

   b) The How-question: How should one match the solution of say Euler and Boltzmann? Marshak conditions were investigated by Arnold & Giving (96), half space problems for the transition were considered by A. Klar (95-97)

   c) The Which-question: Which codes fit optimally together?

2. One may use the kinetic origin of the macroscopic questions for designing better codes for these equations. Examples are "kinetic schemes" and lattice Boltzmann. Coupling particle schemes based on kinetic schemes for Euler with "PARBOSS" particle schemes for Boltzmann gives an extemely efficient hybrid code for reentry problems in space flight (Tiwari 97).

Erwin Stein

Concepts and Structures of the Adaptive 2D-3D Finite-Element Program PARAFEP in C++ for MIMD-Parallel Computers with Solution–, Dimension- and Model-Adaptivity

We consider thin-walled elastoplastic structural problems with disturbed layers which can give rise to dimension- and model-adaptivity of simplified, e.g. 2D-differential operators.

A hierarchy of classes for parametriced finite elements is given in $C++$. Lanczos algorithms with hierarchical preconditioning are used where global matrix-vector products are realized efficiently. Hierarchical mesh refinements with 3D-8-node elements and transitions to 2D-elements need new strategies for repartitioning element graphs for parallel processing.

Quasioptimal load balancing for iterative solving is achieved by combined data distribution w.r.t. elements and degrees of freedom.

Adaptive refinement of node-regular hexaeder elements is given in a complete form, using intermediate configurations where tri-eder elements with 1/32 of volume appear inwards.

Locally computed upper bound Neumann-error estimators are presented for solution-, dimension- and model-adaptivity for model expansions.

3D- and 2D-3D-structural problems were solved on a 16-processor Pentium-system (with 2 Gigabyte storage) with parallel cards in each processor, connected in a 2D-torus ring. Execution times for 3D-problems with $0,9 \cdot 10^6$ unknowns, $b = 0,5 \cdot 10^4$, are $t_{cpu} = 4min$, and for 2D-problems with $u = 1,35 \cdot 10^6$ unknowns the execution time is $t_{cpu} = 6,5min$.

Jörg Steinbach

Fixed-Domain Fomulations for a Degenerate Free Boundary Problem with Applications in Injection/Compression Moulding

An evolutionary variational inequality approach to a degenerate moving free boundary problem is discussed. The main features of this variational inequality formulation of obstacle type are an elliptic differential operator, a memory term, time-dependent convex (constraint) sets and different types of boundary conditions.

The study of such inequality problems is motivated by their applications, e.g. a temperature-dependent Hele-Shaw flow, the electro-chemical machining process or a quasi-stationary Stefan type problem with zero-specific heat.

The evolutionary inequality problem as a fixed domain formulation is the result of the application of a generalized Baiocchi-type transformation to the free boundary problem.

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Both finite element and finite volume approximations are analysed in a variational framework for the numerical solution of the evulationary inequality problem in two and three space dimensions.

Finally, an overview is given on the mathematical modelling of injection and compression moulding by means of a generalized Hele-Shaw flow which includes thermal and possible non-Newtonian effects. The presented simulation results for these applications are concerned with the study of the influence of geometrical and opterating conditions as well as with a comparison to a different mathematical model, the distance model as a geometrical approach for injection moulding.

Andre Thess

Computational Magnetohydrodynamics

Magenetohydrodynamics (MHD) is the study of the movement of electrically conducting fluids under the influence of electromagnetic fields. MHD phenomena arise in areas as diverse as steelmaking, aluminium production, cystal growth, fusion technology, turbulence research, and the dynamics of Earth's magnetic field. The present lecture will provide an overview of some basic MHD phenomena which, in spite of their apparent simplicity, present new challenges to computational fluid dynamics. Emphasis will be placed on phenomena at high kinetic and low magnetic Reynolds number, as relevant to engineering applications.

Lutz Tobiska

Order of Convergence of Drag and Lift Coefficients in Incompressible Flow Problems

A method for computing the drag and lift coefficients of bodies in a channel by nonconforming finite element approximations of the incompressible Navier-Stokes-equations is proposed. For the new formulas a priori error estimates are given which cover both the standard nonconforming finite element method and also stabilized discretizations of upwind type to handle the case of higher Reynolds numbers. For the two-dimensional DFG-benchmark problem of a laminar flow around a cylinder numerical results of the drag and lift coefficient are presented. Both the theoretical and numerical investigations show that the new method gives more precise values compared with calculating the drag and lift coefficients directly from the corresponding surface integrals.

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Ulrich Trottenberg

Anordnung industrieller Anwendungen: Parallelität, Adaptivität, Kopplungsalgorithmen

Der Vortrag diskutiert an Hand konkreter Projekte (EUROPORT; POPINDA, CISPAR) aktuelle Trends des Wissenschaftlichen Rechnens. Dabei wird der spezielle Aspekt der industriellen Softwareentwicklung in den Vordergrund gestellt.

Durch EUROPORT ist eine Vielzahl industrieller Programme zur Simulation und Untersuchung von Einzelphänomenen (Strömungslöser, Strukturcodes und viele andere) erfolglreich parallelisiert worden.

Um außer der Parallelität auch Skalierbarkeit und Adaptivität zu garantieren, muß tiefer in die Programmstrukturen und die Algorithmik eingegriffen werden: Im POPINDA-Projekt ist der FLOWER-Code entstanden, ein 3D-Navier-Stokes-Löser für volle Flugzeugkonfigurationen auf blockstrukturierten Gittern. Der FLOWER-Code ist das Produktionsprogramm der Airbus-Entwicklung. Die zugrundeliegende 3D-Kommunikationsbibliothek garantiert skalierbare Parallelität und Adaptivität.

Noch einen Schritt weiter, auch über die EUROPORT-Ergebnisse hinaus, geht die Anforderung der Industrie, für die gekoppelte Simulation verschiedener physikalischer Effekte (Strömungs-Struktur-Wechselwirkung usw.) bessere Design- und Simulationstools zur Verfügung zu haben. Diese Kopplungsproblematik steht in EU-Projekt CISPAR im Vordergrund. Die algorithmische und softwaretechnische Lösung dieser Problematik wird durch die Kopplungsbibliothek COCOLIB gewährleistet.

Pieter Wesseling

Hyperbolic Conservation Laws and Staggered Grids

With the aim of developing a unified computing method that works well both for compressible and incompressible flow, the classical staggered scheme of Harlow and Welch (MAC scheme, 1965) is extended to the compressible case. The limit $M \downarrow O$ (M=Mach number) is made regular by appropriate scaling of the pressure. Convergence of the scheme to correct physical solutions is verified by comparison with exact solutions of Riemann problems. Both the Euler equations of gas dynamics, and the p-system with arbitrary equations of state are considered. Contrary to most methods designed for the Euler equations, the staggered scheme generalizes commediately to the p-system. This is also true for the Osher-Solomon scheme, but the scheme requires much more computing time. As an example of the p-system, cavitating flow is modeled by postulating a fictitious medium with an equation of state that switches between the equations of state of water and vapour. This equation of state is nonconvex with two turning points. The Riemann solution has an interesting structure that is captured correctly both by the Osher-Solomon and the staggered scheme.

Ragnar Winther

Preconditioners for Systems of Differential Equations

The purpose of this talk is to present a unified approach to preconditioned iterative methods for discretizations of systems of differential equations. We will explain how the mapping properties of the systems lead naturally to preconditioners which are composed of preconditioners for simpler positive definite subproblems. Theoretical and computational results will be presented for various models, for example Stokes problem, mixed formulation of a second order elliptic equation and the Reissner-Mindlin plate model. We will also present some related results on domain embedding preconditioners for problems with essential boundary conditions.

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