Book of Abstracts

Foundations of Computational Mathematics

Santander, 30 June – 9 July 2005

Welcome Note

The Society for the Foundations of Computational Mathematics supports fundamental research in a wide spectrum of computational mathematics and its application areas. As part of its efforts to promote research in computational mathematics, it regularly organises conferences and workshops which are a prominent meeting point for leading researchers in diverse fields that impinge on various aspects of computation. Major conferences of the Society were previously held in Park City (1995), Rio de Janeiro (1997), Oxford (1999) and Minneapolis (2002).

Similarly to previous FoCM conferences, FoCM'05 will be attended by several hundred scientists. Workshops are to be held in twenty-one fields which include: the foundations of the numerical analysis of partial differential equations, geometric integration and computational mechanics, information-based complexity, learning theory, optimization, special functions and orthogonal polynomials, approximation theory, computational algebraic geometry, computational number theory, multiresolution and adaptivity in the numerical analysis of partial differential equations, numerical linear algebra, relations with computer science: algorithmic game theory and metric embeddings, real-number complexity, computational dynamics, geometric modelling and animation, image and signal processing, stochastic computation, symbolic analysis, computational geometry and topology, mathematical control theory and applications, and random matrices.

In addition to these workshops, eighteen plenary lectures will be presented, covering a broad range of topics connected to computational mathematics.

On behalf of the Board of the Society for the Foundations of Computational Mathematics and the Local Organising Committee of the conference, we would like to use this opportunity to thank the local organisers and administrative staff of our host — the Universidad de Cantabria — for their hospitality. We would also like to express our gratitude for financial support to the International Mathematical Union, the University of Cantabria, the Departamento de Matemáticas, Estadística y Computación, the Escuela Técnica Superior de Ingenieros Industriales y Telecomunicaciones, the Vicerrectorado de Investigación de la Universidad de Cantabria, and the Programa Nacional de Acciones Complementarias (proyecto MTM2004-20180-E). We are deeply indebted to the organisers of the twenty-one workshops for their enthusiasm and tireless efforts. Above all, however, we wish to express our gratitude to all participants of this conference for being here and making this meeting such an exciting and scientifically stimulating event.

Welcome to Santander!

Luis Miguel Pardo
Chair, Local Organising Committee FoCM 2005

Endre Süli
Chair, Society for the Foundations of Computational Mathematics

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WORKSHOP 1

Foundations of numerical PDEs

ORGANISERS:

Christoph Schwab & Eitan Tadmor

MHD Equations, the div(B) Constraint, and Central Schemes

Jorge Balbas

Department of Mathematics at University of Michigan

Simulations of Magnetohydrodynamical (MHD) flows pose computational challenges that extend beyond the development of discontinuous solutions typical of non-linear hyperbolic systems. In particular, an additional constraint on the magnetic field, $\text{div}(B) = 0$, needs to be satisfied to guarantee the stability of the numerical schemes. We will discuss some of these challenges, the techniques commonly employed to overcome them, and the capability of central schemes to handle them in a rather simple manner. To this end, we present computational results that indicate a remarkable ability of certain "black box" type central schemes to address these difficulties.

Mimetic Finite Differences Methods for Diffusion Problems

Franco Brezzi

Dipartimento di Matematica at Università di Pavia

The talk will overview the basic features of Mimetic Finite Difference Methods, taking as a model problem Darcy's law for filtration in porous media. After a rather general presentation, we will concentrate on the basic ideas that allowed the extension of the method to a very wide class of geometrical situations, including polyhedra with curved faces. This last part will be based on several papers written in collaboration with K. Lipnikov and M. Shashkov from Los Alamos National Laboratory and V. Simoncini from the University of Bologna.

On Constraint Preservation in Finite Element Discretizations of Yang-Mills Equations

Snorre Christiansen

Centre of Mathematics for Applications at University of Oslo

Yang-Mills equations, in their hyperbolic form, are nonlinear wave equations generalizing those of Maxwell. They preserve a nonlinear differential constraint on the initial data, similar to electric charge. Difficulties in preserving such constraints has been perceived to be at the center of numerical instabilities observed in discretizing other evolution equations, such as Einstein's equations of general relativity. We discuss this problem, for finite element discretizations of the Yang-Mills equations, comparing with recent results obtained for the linear (Maxwell) case.

Two-sided Generalized Riemann Solvers: Advantages and Shortcomings

Rosa Donat

Department of Applied Mathematics at Universitat de València

Many modern shock capturing schemes can be classified as characteristic based schemes. These rely on a local diagonalization of the hyperbolic system that involves the Jacobian matrix of the flux function at each cell interface. It is now relatively well known that the interface state used for the computation of the Jacobian can have a significant effect on the fine features of the numerical solution [1]. A new numerical flux function is developed in [2] that takes into account the two physically relevant states at the interface, without ever constructing an artificially mixed interface state. This new flux function reduces to the well known Shu-Osher scheme [3] for scalar conservation laws, but becomes fundamentally different in the case of systems. The resulting numerical scheme can be combined with the ENO-reconstruction technology to produce state of the art HRSC schemes that have been applied in various scenarios. This talk will review recent results that derive from the use of these new schemes, with special emphasis in the advantages and shortcomings found in the simulations.

[1] R. P. Fedkiw, B. Merriman, R. Donat, S. Osher, The Penultimate Scheme for Systems of Conservation Laws: Finite Difference ENO with Marquina's Flux Splitting, Innovative methods for Numerical solutions of PDEs, Ed. M. M. Hafez, J. J. Chattot 49, 1998.
[2] R. Donat and A. Marquina, Capturing shock reflections: An improved flux formula, J. Comp. Phys., 125, 1996.
[3] C. W Shu and S. J. Osher, Efficient implementation of essentially non-oscillatory, shock-capturing schemes II. J. Comp. Phys., 83, 1989.

Central-Upwind Schemes for Balance Laws. Applications to Multifluid and Multiphase Computations

Alexander Kurganov

Mathematics Department at Tulane University

First I will briefly describe Godunov-type central-upwind schemes for hyperbolic systems of conservation and balance laws. These schemes are simple, universal and, at the same time, high-resolution methods that can be applied as a 'black-box' solver to many different problems. However, applications to balance laws typically require a special source term discretization, which should guarantee (a perfect) balance between the flux and the source terms. This will be illustrated on the example of the Saint Venant system of shallow water equations with nonflat bottom topography. Then I will focus on two more complicated applications: to compressible two-phase flows and to multi-layer shallow water equations, for which a treatment of nonconservative products seems to be the most challenging part in designing a reliable numerical method.

Some Questions in Computational Chemistry

Claude Le Bris

CERMICS at École Nationale des Ponts et Chaussées

We will make an overview of various techniques used in computational chemistry for the calculations of electronic structure. Such calculations require the solution of some nonlinear eigenvalue problems. In particular, advanced techniques for large systems will be addressed.

High-resolution Finite Volume Methods and Approximate Riemann Solvers for Hyperbolic Systems

Randall LeVeque

Department of Applied Mathematics at University of Washington

High-resolution finite volume methods for hyperbolic systems of PDEs are often based on Godunov's method, with the addition of second-order correction terms that are limited in some manner to avoid nonphysical oscillations and sharpen the resolution of steep gradients or discontinuities such as shock waves. This is often coupled with upwinding based on a characteristic decomposition or the solution of the Riemann problem between the neighboring states. A variety of slope limiting or flux limiting methods have been proposed and successfully used. The wave-propagation method is a general formulation of such methods that limits the waves resulting from the Riemann solution and uses the resulting waves to define the high-resolution correction terms. This approach has allowed the development of general-purpose software that applies to a wide range of hyperbolic problems, including problems that are not in conservation form and to quasi-steady balance laws where the flux gradient is nearly balanced by a source term. In practice approximate Riemann solvers are often used, ranging from very simple approximations such as the HLL solver to more sophisticated and expensive solvers that better mimic important aspects of the exact solution. Several of these can be unified by interpreting them in the framework of "relaxation Riemann solvers" that are related to relaxation schemes for hyperbolic systems.

Mesh Adaptivity and Artificial Diffusion in Hyperbolic Problems

Charalambos Makridakis

Department of Applied Mathematics at University of Crete

We consider finite element, finite difference schemes and adaptive strategies for the approximation of nonlinear hyperbolic systems of conservation laws. It is known that finite elements are not a very popular choice for computing singular solutions of hyperbolic problems. When applied directly to the system they will result computational solutions with oscillatory character close to shocks and/or not convergent approximations. This well known phenomenon is of course related to the fact that direct finite element discretizations behave like dispersion approximations. Similar behavior is observed in the study of related dispersive difference schemes approximating conservation laws.

To overcome this difficulty in using standard schemes, several modifications have been proposed in the literature by adding artificial viscosity and / or extra stabilization terms in the schemes. The higher order versions of these methods are complicated and with poor theoretical backup. Recently many of these schemes have been tested with various mesh adaptation methods. Our motivation was to consider schemes designed to be used in conjunction with appropriate mesh refinement. We will show that mesh refinement strategies can change our view on the application of many of the known schemes. This is because the mesh distribution influences not only the accuracy of the scheme but also its stability behavior.

In this talk we (1) consider new finite element schemes for HCL designed to be used with mesh adaptivity. (2) discuss adaptive strategies for shock computations based on estimator functionals or a posteriori error control. (3) conclude to new and rather unexpected observations for the behavior of Entropy Conservative difference schemes. Classical dispersive-type finite element and finite difference schemes are also considered. We then try to explain why many of these schemes when used in conjunction with appropriate adaptive strategies yield computational solutions with surprisingly stable behavior.

We conclude that the qualitative effect of mesh adaptivity is the responsible mechanism and not the 'resolution' of boundary layers/shocks. These conclusions are also applicable to convection - diffusion problems where similar numerical problems occur.

Boundary Concentrated FEM

Jens Melenk

Mathematics at University of Reading

It is well-known for elliptic problems with smooth coefficients that the solution is smooth in the interior of the domain; low regularity is only possible near the boundary. The hp-version of the finite element method (hp-FEM) with variable order polynomial degree distribution allows us to exploit this observation to get optimal (in the sense of n-widths) approximation methods by using meshes where the element size grows proportionally to the element's distance to the boundary and the approximation order is suitably linked to the element size. In this way most degrees of freedom are concentrated near the boundary, and whence comes the name of this variant of the hp-FEM.

A focus of this talk, will be (near) optimal solution techniques for the arising linear system. The first approach we discuss is based on multilevel techniques for this variant of the hp-FEM. The second approach considered is based on the concept of H-matrices, recently introduced by W. Hackbusch.

The boundary concentrated FEM is variant of the hp-FEM; many of the implementation issues discussed for it apply in fact to the hp-FEM in general.

Finite Element Methods for Moving Surfaces and Applications to Stressed Epitaxial Films, Shape Optimization, and Image Processing

Ricardo Nochetto

Mathematics and IPST at University of Maryland

Using shape differential calculus, which expresses variations of bulk and surface energy with respect to domain changes, and Euler implicit time discretization, we formulate gradient flows for these energies which yield geometric laws for the motion of domain boundaries (curves or surfaces). We next present a semi-implicit variational formulation which requires no explicit parametrization of the surface, and is sufficiently flexible to accommodate several scalar products for the computation of normal velocity, depending on the application. This leads to linear systems of lower order elliptic PDE to solve at each time step, in both the surface and bulk. We develop adaptive finite element methods (AFEM), and propose a Schur complement approach to solve the resulting linear SPD systems.

We first apply this idea to surface diffusion, namely to the geometric motion of a surface with normal velocity proportional to the surface Laplacian of mean curvature, and couple it with elasticity in the bulk; this is a simple model for stressed epitaxial films. We present several numerical experiments for surface diffusion including pinch-off in finite time and topological changes. We also present preliminary computations for the coupled system exhibiting formation of dislocations. We next discuss applications to shape optimization and image processing, that is to the minimization of functionals subject to differential constraints, and present preliminary simulations. We discuss time and space adaptivity to handle the multiscale nature of these problems, as well as mesh generation, mesh distortion and mesh smoothing.

This work is joint with E. Baensch, G. Dogan, P. Morin, and M. Verani.

Bregman Iteration and the Dual of BV in Inverse Problems in Imaging and elsewhere

Stanley Osher

Department of Mathematics at University of California, Los Angeles

We shall review some new results obtained with: M. Burger, S. Kindermann, D. Goldfarb, O. Scherzer, W. Yin and J.J. Xu in image processing and general inverse problems. State-of-the-art image restoration methods result from easy to explain nonlinear optimization and functional analysis considerations.

Recent Advances in Computational Ferromagnetism

Andreas Prohl

Seminar für Angewandte Mathematik at ETH Zürich

Micromagnetics is a continuum variational theory describing magnetization pattern in ferromagnetic media. Its multiscale nature due to different inherent spatio-temporal physical and geometric scales, together with nonlocal phenomena and a nonconvex side-constraint leads to a rich behavior and pattern formation. This variety of effects is also the reason for severe problems in constructing reliable numerical methods, which are reviewed in this talk.

High Order Finite Volume Schemes for Balance Laws with Stiff Source

Giovanni Russo

Dipartimento di Matematica ed Informatica at Università di Catania

Finite difference methods are usually preferred over their finite volume counterparts for the development of high order schemes for the numerical solution of hyperbolic systems of balance laws with a stiff source. The unstaggered version of such schemes is usually developed by a method-of-line approach: the derivative of the flux is discretized in a conservative way, using some high order nonlinear reconstruction on the flux, to prevent spurious oscillations, and the system of PDE's is reduced to a large system of ODE's, which contains a non stiff part (the flux term) and a stiff part (the relaxation). At this point, the system of ODE's can be solved by some Implicit-Explicit (IMEX) scheme, in which the source term is treated implicitly, while the flux term is treated explicitly. The advantage of finite difference is that the source term does not couple the cells, and therefore the implicit step can be efficiently solved, treating each cell separately. The same procedure cannot be applied with a finite volume scheme, since the cell average of the source is not equal to the source evaluated at the cell average, and the source term couples the cells. In our finite volume methods, a different approach to time discretization, called Central Runge Kutta (CRK), treats the numerical solution (cell average) with a conservative scheme for the flux, while the stage values at the edge of each cell (pointwise) are treated by a non conservative scheme, in which the source term is decoupled from the other cells, and therefore implicit schemes can be effectively used for the source. During the talk the development of finite difference on staggered grids will be also discussed, and high order finite volume methods for stiff balance laws will be illustrated both in the staggered and unstaggered version.

Moving Mesh Methods for Computational Fluid Dynamics

Tao Tang

Department of Mathematics at Hong Kong Baptist University

This talk will describe some recent developments on moving mesh methods. In particular, we review their applications to computational fluid dynamics. The following website contains some materials related to this talk:
`http://www.math.hkbu.edu.hk/~ttang/MMmovie`

Locking-free Finite Element Methods Based on the Hu-Washizu Formulation for Linear and Geometrically Nonlinear Elasticity

Barbara Wohlmuth

Institut für Angewandte Analysis und Numerische Simulation at Universität Stuttgart

It is well-known that the low-order elements based on four-noded quadrilaterals or eight-noded hexahedra have two drawbacks in finite element computation. The first one is the locking effect in nearly incompressible case; in other words, they do not converge uniformly with respect to the Lamé parameter λ. The second one is that these standard elements lead to poor accuracy in bending-dominated problems when coarse meshes are used. In the first part of the talk, we examine the classical Hu-Washizu mixed formulation for plane and three dimensional problems in linear elasticity with the emphasis on behavior in the incompressible limit. The classical continuous problem is embedded in a family of Hu-Washizu problems parameterized by a scalar α for which $\alpha = \lambda/\mu$ corresponds to the classical formulation, with λ and μ being the Lamé parameters. We discuss the uniform well-posedness in the incompressible limit of the continuous problem for $\alpha = -1$. Finite element approximations are based on the choice of piecewise bilinear or trilinear approximations for the displacements on quadrilateral or hexahedral meshes. Conditions for uniform convergence are made explicit. These conditions are shown to be met by particular choices of bases for stresses and strains that include well-known bases as well as newly constructed ones. Though a discrete version of the spherical part of the stress exhibits checkerboard modes, we establish a λ-independent optimal a priori error estimates for the displacement and for the postprocessed stress. Furthermore, starting from a suitable three-field formulation we introduce a two-field mixed formulation for geometrically nonlinear elasticity with Saint-Venant Kirchhoff law. In the second part, we demonstrate the performance of our approach through different numerical examples.