Helsinki University of Technology Institute of Mathematics Reports
Espoo 2008 C19

PERSPECTIVES IN NUMERICAL ANALYSIS
TKK, MAY 27–29, 2008

Timo Eirola, Juho Könnö, Toni Lassila, Antti H. Niemi, Rolf Stenberg (eds.)

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UNIVERSITE DE TECHNOLOGIE D'HELSINKI

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Faculty of Information and Natural Sciences
Department of Mathematics and Systems Analysis

Timo Eirola, Juho Könnö, Toni Lassila, Antti H. Niemi, Rolf Stenberg (eds.): *Perspectives in Numerical Analysis 2008 – Conference material*; Helsinki University of Technology Institute of Mathematics Reports C19 (2008).

Abstract: *This report contains the program, list of participants, and abstracts for the invited presentations of the international conference Perspectives in Numerical Analysis 2008, held at the Helsinki University of Technology, May 27–29, 2008.*

AMS subject classifications: 65-06

Keywords: numerical analysis, conference abstracts

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ISBN 978-951-22-9419-0 (print)
ISBN 978-951-22-9420-6 (PDF)
ISSN 0784-6460 (print)
ISSN 1797-5875 (PDF)

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Per Lötstedt: *Simulation of stochastic reaction-diffusion processes*

Coffee

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16.30 Closing

2 List of participants

Olavi Nevanlinna, Helsinki University of Technology
Juhani Pitkäranta, Helsinki University of Technology

Organizers

Timo Eirola, Helsinki University of Technology
Rolf Stenberg, Helsinki University of Technology

Invited speakers

Ivo Babuska, University of Texas, Austin
Åke Björck, University of Linköping
Carl de Boor, University of Wisconsin, Madison
Franco Brezzi, Institute for Advanced Study, Pavia
Alain Damlamian, Université Paris XII
Leszek F. Demkowicz, University of Texas, Austin
Björn Engquist, University of Texas, Austin
Rolf Jeltsch, ETH Zurich
Claes Johnson, Royal Institute of Technology, Stockholm
R. Bruce Kellogg, University of Maryland
Martin Hanke-Bourgeois, Johannes Gutenberg Universität, Mainz
Ernst Hairer, Université de Genève
Marlis Hochbruck, Heinrich-Heine-Universität, Düsseldorf
Thomas J.R. Hughes, University of Texas, Austin
Arieh Iserles, University of Cambridge
Barbara Keyfitz, University of Houston
David Kinderlehrer, Carnegie Mellon University
Ben Leimkuhler, Edinburgh University
Christian Lubich, Universität Tübingen
Per Lötstedt, Uppsala University
Donatella Marini, University of Pavia
John E. Osborn, University of Maryland
Linda R. Petzold, University of California, Santa Barbara
Juha Pohjanpelto, Oregon State University
Rolf Rannacher, Ruprecht-Karls-Universität Heidelberg
Axel Ruhe, Royal Institute of Technology, Stockholm
Evariste Sanchez-Palencia, Université Pierre et Marie Curie, Paris
Christoph Schwab, ETH Zurich
L. Ridgway Scott, University of Chicago
Ian Sloan, University of New South Wales, Sydney
Manil Suri, University of Maryland Baltimore County
Jukka Tuomela, University of Joensuu
Jaroslav Zemánek, Polish Academy of Sciences, Warsow
Gennadi Vainikko, University of Tartu
Michael Vogelius, Rutgers, State University of New Jersey
Gerhard Wanner, Université de Genève

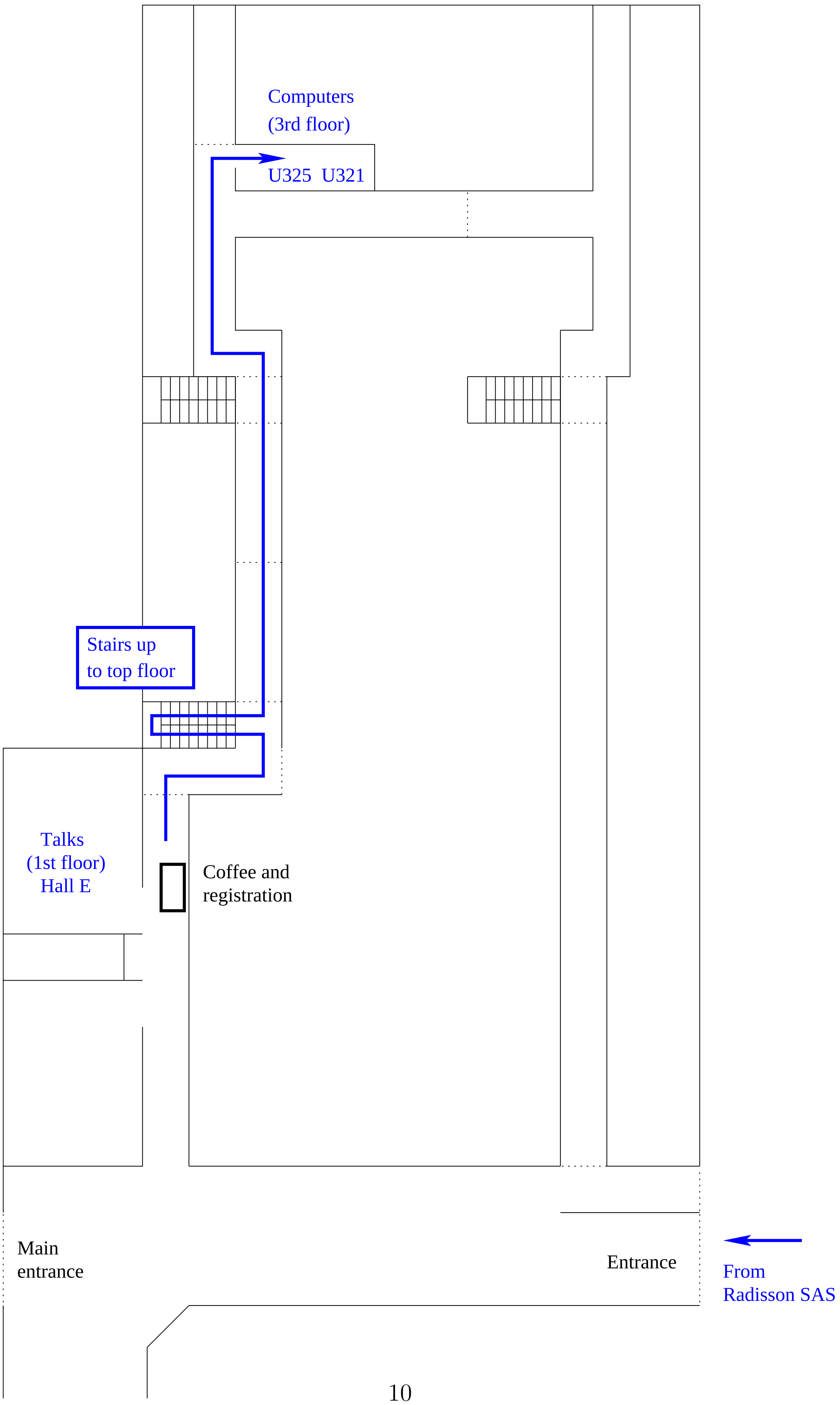
Registered attendees

Pekka Alestalo, Helsinki University of Technology
Heikki Apiola, Helsinki University of Technology
Teijo Arponen, Helsinki University of Technology
Kenrick Bingham, Helsinki University of Technology
Gustaf Gripenberg, Helsinki University of Technology
Harri Hakula, Helsinki University of Technology
Ville Havu, Helsinki University of Technology
Tapio Helin, Helsinki University of Technology
Marko Huhtanen, Helsinki University of Technology
Saara Hyvönen, Fonecta
Matti Lassas, Helsinki University of Technology
Stig-Olof Londen, Helsinki University of Technology
Mikko Lyly, CSC
Olli Mali, University of Jyväskylä
Pekka Neittaanmäki, University of Jyväskylä
Jarkko Niiranen, Helsinki University of Technology
Pertti Palo, Helsinki University of Technology
Kirsi Peltonen, Helsinki University of Technology
Hana Petzeltová, Academy of Sciences of the Czech Republic
Jan von Pfaler, Helsinki University of Technology
Santtu Ruotsalainen, Helsinki University of Technology
Esko Valkeila, Helsinki University of Technology

Organizing committee

Kurt Baarman, Helsinki University of Technology
Mikko Byckling, Helsinki University of Technology
Tuula Donskoi, Helsinki University of Technology
Mika Juntunen, Helsinki University of Technology
Marita Katavisto, Helsinki University of Technology
Juho Könnö, Helsinki University of Technology
Toni Lassila, Helsinki University of Technology
Antti H. Niemi, Helsinki University of Technology

3 Building map



4 Abstracts

Achieving Brouwer's law with geometric integrators

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ABSTRACT

In high accuracy long-time integrations of differential equations (e.g., computations for the solar system), round-off errors may dominate truncation errors. We study the influence of round-off on the conservation of first integrals such as the total energy in Hamiltonian systems. Standard implementations of numerical time integrators may show an unexpected error propagation (linear drift). For implicit Runge-Kutta methods and for an exact integration in rigid body dynamics we propose modifications of the implementation that reduces the effect of round-off. In this way, Brouwer's law can be achieved, i.e., round-off can be reduced so that it behaves like a random walk.

Thermal control of molecular dynamics

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ABSTRACT

In molecular simulation we always work with a much smaller system than would be desirable, so it is essential to provide computational devices that allow for control of the thermodynamic state corresponding to a physical environment. The emphasis in molecular dynamics applications is shifting to problems involving transient dynamics, and the flow of energy from one part of a system (one set of variables) to another. This setting places increasing demands on the techniques used to provide ergodicity and thermal regulation.

Consider a finite dimensional Hamiltonian system in $\mathbf{R}^{2N}$ with Hamiltonian $H = H(z)$, $z = (q, p)$, with q and p position and momentum vectors, respectively. By *sampling*, we mean computing the average of a function $f = f(z)$,

$$\bar{f} = \frac{1}{\Omega}\int_D f(z)\rho(z)\mathrm{d}\omega, \qquad \Omega = \int_D \rho(z)\mathrm{d}\omega,$$

with respect to a suitable measure $\rho\mathrm{d}\omega$ ($\mathrm{d}\omega$ the standard volume form in $\mathbf{R}^{2N}$), and $D \subset \mathbf{R}^{2N}$. If we consider the natural (microcanonical) measure $\rho = \delta[H - E]$ associated to Hamiltonian dynamics with energy function $H = H(z)$, then, under an ergodicity assumption, we may replace spatial averaging by the time average along a sampling trajectory (Birkhoff's Theorem). Replacing Hamiltonian dynamics by a suitable Markov process, it is possible to use temporal averages to compute canonical averages, i.e. averages with respect to the Gibbs density $\rho^{\theta}_{\mathrm{can}}(z) = e^{-H/(k_B\theta)}$. This is what is usually meant by the term "thermostat." In this talk I will describe recent and ongoing research to understand the foundations of molecular dynamics algorithms, specifically topics related to thermostatting molecular dynamics [1, 2, 3].

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Simulation of stochastic reaction-diffusion processes

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ABSTRACT

Intrinsic noise in biochemical networks can have a large impact on the macroscopic behavior of biological cells. An example is the regulation of the transcription of genes to messenger RNA (mRNA) where genes are present in one or two copies and the copy number of mRNA is small. A discrete, stochastic description of the system is necessary since the copy number is a small nonnegative integer and there is only a probability that a certain reaction will occur when two molecules meet.

Such stochastic chemical systems with diffusion are modeled with a reaction-diffusion master equation. The state of the system is the space dependent number of molecules of each participating species. The dimension of a system discretized in space is very high ('the curse of dimensionality'), making the direct computational solution of the master equation impossible. Instead, trajectories of the system are generated and mean values of the species are computed using Monte Carlo methods.

On a macroscopic level, the governing equation is a reaction-diffusion equation for the averages of the chemical species. On a mesoscopic level in our approach, the master equation for a well stirred chemical system is combined with Brownian motion in space to obtain solutions of the reaction-diffusion master equation. The space is covered by an unstructured mesh and the diffusion coefficients on the mesoscale are obtained from a finite element discretization of the Laplace operator on the macroscale. The resulting method is a flexible hybrid algorithm in that the diffusion can be handled either on the meso- or on the macroscale level. The accuracy and the efficiency of the method are illustrated in three numerical examples inspired by molecular biology.

This is a collaboration with Stefan Engblom, Lars Ferm and Andreas Hellander.

The penetration function and its application to microscale problems

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ABSTRACT

The presentation will adress the recovery of the microscale features on a unit ball $\Xi \subset \mathbb{R}^2$ from the macroscale solution U by the global-local approach. Consider the microscale equation

$$\begin{aligned} \text{div } A(x) \text{ grad } u_n = 0 \quad & \text{on} \quad \Xi, \\ u_n = g_n \quad & \text{on} \quad \partial\Xi \end{aligned}$$

Here $A(x)$ is a symmetric measurable matrix which characterizes the microstructure, $u_n \subset H^1(\Xi)$ is the weak solution of the problem and $g_n \in S_n(\Xi) \subset H^{\frac{1}{2}}(\partial\Xi)$ is the trace of the macrosolution U on $\partial\Xi$. If $g_n = g$, where g is the trace of the microsolution u on Ω, then obviously $u_n = u$.

We will consider a class Υ of the microstructures A. Further we will assume that S_n is a $2n$ dimensional space of the trigonometric polynomials of degree n on $\partial\Xi$. This is the "deal" approximation space because it is directly related to the Kolmogorov n-width theory.

We define the *penetration function*,

$$\Phi(\Upsilon, R, n) = \sup \frac{||u - u_n||_{E(\Xi_R)}}{||u||_{E(\Xi)}},$$

where g_n is the $H^{\frac{1}{2}}(\partial\Xi)$ projection of the trace g on $\partial\Xi$ of the microscale solution u on S_n, Ξ_R is the ball of radius $0 < R < 1$, $||u||_E$ is the energy norm and the supremum is taken over all $A \in \Upsilon$ and $g \in H^{\frac{1}{2}}(\partial\Xi)$. Note that for general microstructure $g \in H^{\frac{1}{2}}(\partial\Xi)$ only and is not smoother. The penetration function characterizes the best possible accuracy in the microscale feature on the ball Ξ_R which could be obtained by the global-local approach if only is known that $A \in \Upsilon$.

We prove that if Υ is the class of measurable matrices $A(x)$ with bounds $0 < \lambda_1$, and $\lambda_2 < \infty$ of the minimal and maximal eigenvalues then

$$\Phi(\Upsilon, R, n) \geq C(R) n^{-\frac{1}{2}} lg^4 n.$$

This is only a lower estimate and it is possible that $\Phi \geq C n^{-\alpha}$ with α much smaller than $\frac{1}{2}$.

We also prove the upper estimate

$$\Phi(\Upsilon, R, n) \leq C(R) n^{-\alpha},$$

where α depends only on the contrast $\kappa = \frac{\lambda_1}{\lambda_2}$ with $\alpha = \frac{\kappa}{2+\kappa}$. Nevertheless this estimate is likely very pessimistic.

To see the accuracy of the estimates we will analyze numerically the penetration function for the following class Υ_0 of matrices $A(x)$.

$$\Upsilon_0 = \{A(x) = \begin{bmatrix} a(x) & 0 \\ 0 & a(x) \end{bmatrix}, a(x) \text{ has only values } \lambda_1 \text{ or } \lambda_2\}$$

and present the numerical results. They indicate that both estimates are inaccurate. We will also show that for $a(x)$ analytic on the closed Ξ, then the penetration function Φ decreases exponentially with n.

The showed results indicate that the reconstruction of the microstructure from the macro solution is very inaccurate in contrast to the usual folklore.

Homogenization of a variational problem on a domain with oscillating boundaries with periodic unfolding

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ABSTRACT

We present a variational problem on a sequence of 2-dimensional domains with highly periodically oscillating boundaries. Using the periodic unfolding method (which will be briefly explained), the homogenized problem is obtained in the limit as the period length approaches zero. The proof is amazingly simple. Extensions in higher dimensions and with highly oscillating coefficients are also given. In this framework, a result of strong convergence is obtained which seems to be new.

Cloaking and "near" cloaking of objects

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ABSTRACT

I shall discuss some results on so-called "electromagnetic cloaking", a topic that has recently received quite a bit of "popular" attention (for example BBC, CNN and N.Y. Times each had some coverage of associated work in the "applied physics community" this past summer). Roughly speaking: a cloak is an "invisible dielectric shield" that makes a designated region in space "inaccessible" to electromagnetic inspection. I will focus on some quite elementary mathematical "mapping" techniques, that have extremely interesting implications when it comes to the construction of cloaked, or nearly cloaked regions in space. If one is willing to work with completely singular cloaks, i.e., metamaterials that have "extreme" (0 and infinite) electromagnetic properties, then "perfect" cloaking is attainable (in certain model situations). One of the focal points of our work has been to derive rigorous estimates of how nearly singular the cloak has to be in order to achieve a certain degree of invisibility.

Kepler, Newton and numerical analysis

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ABSTRACT

Numerical methods are usually constructed for solving mathematical models such as differential equations or optimization problems. In this talk is discussed the fact that numerical methods, applied inversely, also were important to ESTABLISH these models. We show in detail the discovery of the laws of planetary motion by Kepler and Newton, which stood at the beginning of modern science.

Multidimensional conservation laws: speaking of numerical methods

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ABSTRACT

Until recently, there were no analytical methods available to study systems of multidimensional conservation laws – the equations of compressible, ideal gas flow, for example. Currently, several groups have made progress by studying self-similar systems (the model of shock reflection by a wedge, for example) and solving free boundary problems for the subsonic flow (quasilinear elliptic equation) coupled to the reflected shock position. In attempting to extend this analysis beyond the simplest situation, of regular shock reflection, we have come upon the difficulty that even the local picture of a shock at a reflection point may not be known. Careful numerical simulation, first done by Allen Tesdall and John Hunter, exhibits a new phenomenon, named "Guderley Mach reflection" by the discoverers. The scenario is ripe for analysis, using the tools of free-boundary methods recently developed. It presents a fascinating example of the ability of analytical and numerical approaches to complement and stimulate each other.

Layers and corner singularities in singularly perturbed elliptic problems

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ABSTRACT

Some recent work and open problems are reviewed concerning the numerical solution of singularly perturbed elliptic boundary value problems whose solutions have boundary layers and corner singularities.

Isogeometric analysis: progress and challenges

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ABSTRACT

Geometry is the foundation of analysis yet modern methods of computational geometry have until recently had very little impact on computational mechanics. The reason may be that the Finite Element Method (FEM), as we know it today, was developed in the 1950s and 1960s, before the advent and widespread use of Computer Aided Design (CAD) programs, which occurred in the 1970s and 1980s. Many difficulties encountered with FEM emanate from its approximate, polynomial based geometry, such as, for example, mesh generation, mesh refinement, sliding contact, flows about aerodynamic shapes, buckling of thin shells, etc. It would seem that it is time to look at more powerful descriptions of geometry to provide a new basis for computational mechanics.

The purpose of this talk is to explore the new generation of computational mechanics procedures based on modern developments in computational geometry. The emphasis will be on Isogeometric Analysis in which basis functions generated from NURBS (Non-Uniform Rational B-Splines) and T-Splines are employed to construct an exact geometric model. For purposes of analysis, the basis is refined and/or its order elevated without changing the geometry or its parameterization. Analogues of finite element h- and p-refinement schemes are presented and a new, more efficient, higher-order concept, k-refinement, is described. Refinements are easily implemented and exact geometry is maintained at all levels without the necessity of subsequent communication with a CAD (Computer Aided Design) description.

In the context of structural mechanics, it is established that the basis functions are complete with respect to affine transformations, meaning that all rigid body motions and constant strain states are exactly represented. Standard patch tests are likewise satisfied. Numerical examples exhibit optimal rates of convergence for linear elasticity problems and convergence to thin elastic shell solutions. Extraordinary accuracy is noted for k-refinement in structural vibrations and wave propagation calculations. Surprising robustness is also noted in fluid mechanics problems. It is argued that Isogeometric Analysis is a viable alternative to standard, polynomial-based, finite element analysis and possesses many advantages. In particular, k-refinement seems to offer a unique combination of attributes, that is, robustness and accuracy, not possessed by classical p-methods, and is applicable to models requiring

smoother basis functions, such as, thin bending elements, and strain-gradient and phase-field theories. A new modeling paradigm for patient-specific simulation of cardiovascular fluid-structure interaction is described, and a précis of the status of current mathematical understanding is presented.

Rational Krylov algorithm for real matrix pencils with complex eigenvalues

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ABSTRACT

We compute eigenvalues of matrix pencils for which a sparse Gaussian elimination factorization of a shifted matrix is feasible.

The Rational Krylov algorithm is a generalization of the shifted and inverted Arnoldi algorithm, where several shifts are used in one run. It gives the same basis as Arnoldi, starting on a different vector from the computed Krylov space.

In the practically interesting case of a real pencil with complex eigenvalues, there is a double shift variant, where two real vectors are added in each step, and a single shift variant, where either the real or the imaginary part of the shifted pencil is used.

The main interest is model reduction for linear dynamic systems. We will report results on one simple example of a tubular reactor and one applied computation on a supersonic engine inlet.

Adaptive finite element discretization of PDE-based optimization problems

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ABSTRACT

We present a systematic approach to error control and mesh adaptation in the numerical solution of optimal control problems governed by partial differential equations. The problems considered are of the prototypical form

$$
\begin{aligned}
&J(u,q) = \tfrac{1}{2}\|u-u_d\|_V^2 + \tfrac{1}{2}\alpha\|q\|_Q^2 \to \min!\\
&-\Delta u + qu = f + q \quad \text{in} \ \ \Omega, \quad u|_{\partial\Omega} = q \ \ \text{or} \ \ \partial_n u|_{\partial\Omega} = q,
\end{aligned}
$$

which contains "distributed control", "Dirchlet" and "Neuman control", as well as "parameter estimation". By the Lagrangian formalism the optimization problem is reformulated as a saddle-point boundary value problem that is discretized by a Galerkin finite element method. The accuracy of the discretization is controlled by residual-based a posteriori error estimates. This opens the way toward systematic model reduction in the solution of the optimal control problem. The main features of this approach are illustrated by examples. Further its extension to problems with control and state constraints will be discussed. Extensions to nonstationary optimization problems are also possible.

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Automated FEM discretizations for the Stokes equation

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ABSTRACT

Current FEM software projects have made significant advances in various automated modeling techniques. We present some of the mathematical abstractions employed by these projects that allow a user to switch between finite elements, linear solvers, mesh refinement and geometry, and weak forms with very few modifications to the code. To evaluate the modularity provided by one of these abstractions, namely switching finite elements, we provide a numerical study based upon the many different discretizations of the Stokes equations.

Electric impedance tomography with only one pair of measurements

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ABSTRACT

We consider the reconstruction of an anomaly within a homogeneous body from electrostatic measurements on its boundary. Our aim is to gather as much information as possible about the anomaly using only one pair of current/voltage measurements from the entire boundary. Two different approaches will be considered. The first one adapts the convex scattering support developed by Kusiak and Sylvester to our particular problem: We reconstruct a convex domain within the body that is known to be part of the convex hull of the anomalies. In our second approach we reinvestigate a method suggested by Kwon, Seo, and Yoon, which determines a single point in order to locate the (approximate) position of the anomaly. We will compare their results with a novel approach which we call the effective dipole method. We plan to demonstrate that the effective dipole method yields a good approximation of the center of mass of the anomaly.

This is joint work with Nuutti Hyvönen and Steffi Reusswig

Blowup of incompressible Euler solutions

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ABSTRACT

We present analytical and computational evidence of blowup of initially smooth solutions of the incompressible Euler equations into non-smooth turbulent solutions, as a step towards a resolution of the Clay Mathematics Institute Navier-Stokes Millennium Problem.

The numerical analysis of fiction

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ABSTRACT

Being both a writer and mathematician, the number one question I am asked during book events is what is the connection between writing and mathematics - how one informs the other. In this talk, I expound on some similarities between the two processes. The underlying goal is mathematical outreach - putting mathematical terms in terms of the processes used in coming up with a story gives an opportunity to explain mathematical terms to non-mathematicians. In particular, I will show how the writing process can be used to motivate Fourier Series, Optimization Processes and Iterative Algorithms. It is hoped that this will be an interactive session, with comments and suggestions solicited from the audience on ways to enhance the outreach process (which hopefully is a shared goal, of high importance in today's mathematically challenged society). I will also briefly touch on previous outreach presentations that have been successful (such as a talk on infinity delivered at the 2006 International Literature Festival in Berlin).

Essentially optimal explicit Runge-Kutta methods for hyperbolic-parabolic equations

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ABSTRACT

Essentially optimal explicit Runge-Kutta methods consider more stages in order to include a particular spectrum in their stability domain and thus reduce step restrictions. This idea, so far used mostly for real line spectra, is generalized to more general spectra in form of a thin region. In this regions the eigenvalues may extend away from the real axis into the imaginary plane. We give a direct characterization of essentially optimal stability polynomials containing a maximal thin region and calculate these polynomials for various cases. Semi-discretizations of hyperbolic-parabolic equations are a relevant application which exhibit a thin region spectrum. As a model, linear scalar advection-diffusion is inverstigated. The second order stabilized Runge-Kutta methods derived from the stability polynomials are applied to advection- diffusion and compressible, viscous fluid dynamics in numerical experiments. Due to the stabilization the time step can be controlled solely from the hyperbolic CFL condition even in the presence of viscous fluxes.

Anisotropic adaptive mesh procedure for computing very thin hyperbolic shells

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ABSTRACT

We consider very thin elastic shells in the linear Koiter framework in the case when the middle surface has everywhere principal curvatures of opposite sign. The system of equations is elliptic, but the limit behaviour when the relative thickness tends to zero is hyperbolic. Internal and boundary layers appear. They have very different structure when they are along or across the zsymptotic lines of the middle surface. In order to have a good description of the layers for very small values of the relative thickness, we use an anisotrpic adaptive mesh procedure which takes automatically account of the elongated structure of the layer.

Dynamical low-rank approximation

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ABSTRACT

Dynamical low-rank approximation is a differential-equation based approach to efficiently computing low-rank approximations to time-dependent large data matrices or to solutions of large matrix differential equations. We illustrate its use in the following application areas: as an updating procedure in latent semantic indexing for information retrieval, in the compression of series of images, and in the solution of time-dependent partial differential equations, specifically on a blow-up problem of a reaction-diffusion equation in 2 and 3 spatial dimensions. In 3D and higher dimensions, space discretization yields a tensor differential equation whose solution is approximated by low-rank tensors, effectively solving a system of discretized partial differential equations in 1 spatial dimension.

The talk is based on joint work with Othmar Koch and Achim Nonnenmacher.

Space-time adaptive wavelet methods for parabolic evolution problems

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ABSTRACT

With respect to space-time tensor-product wavelet bases, parabolic initial boundary value problems are equivalently formulated as bi-infinite matrix problems. Adaptive wavelet methods are shown to yield sequences of approximate solutions which converge at the optimal rate. In case the spatial domain is of product type, the use of spatial tensor product wavelet bases is proved to overcome the so-called curse of dimensionality, i.e., the reduction of the convergence rate with increasing spatial dimension.

Joint work with Rob Stevenson, KdV Institute, Amsterdam, The Netherlands.

What is the complexity of weakly singular integral equations?

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ABSTRACT

Consider the integral equation

$$u(x) = \int_0^1 (a(x,y) \mid x-y \mid^{-\nu} + b(x,y))u(y)dy + f(x), \quad 0 \le x \le 1, \tag{1}$$

where $\nu \in (0,1)$, $f \in C^m[0,1]$, $a, b \in C^{2m}([0,1] \times [0,1])$, $m \in \mathbb{N}$, and the corresponding homogeneous equation has only the trivial solution. By a *fast* (C, C^m) *solver* of (1) we mean a solver which produces approximate solutions u_n, $n \in \mathbb{N}$, such that

- given the values of a, b and f at certain not more than $n_\star$ points depending on the solver (with $n_\star \to \infty$ as $n \to \infty$), the parameters of u_n can be determined at the cost of $\gamma_m n_\star$ arithmetical operations, and an accuracy
$$\| u - u_n \|_{C[0,1]} \le c_m n_\star^{-m} \| f \|_{C^m[0,1]} \tag{2}$$
is achieved where u is the solution of (1);

- having the parameters of u_n in hand, the value of u_n at any point $x \in [0,1]$ is available at the cost of γ'_m operations.

Here the constants c_m, γ_m, γ'_m are independent of f and n. It occurs that estimate (2) is information optimal – in the worst case, under above assumptions, a higher order of error estimate cannot be achieved allowing more arithmetical work.

In a *fast* (L^p, C^m) *solver*, $\| u - u_n \|_{L^p(0,1)} \le c_m n_\star^{-m} \| f \|_{C^m[0,1]}$ is required instead of (2). In a *quasifast* (C, C^m) *solver*, $\| u - u_n \|_{C[0,1]} \le c_m n_\star^{-m} \log n_\star \| f \|_{C^m[0,1]}$ is required instead of (2).

In the literature, fast (C, C^m) solvers have been constructed only for integral equations without singularities that for (1) corresponds to the case $a \equiv 0$. We consider (1) in general case and construct a solver which is (C, C^m) quasifast and (L^p, C^m) fast for $1 \le p < \infty$; under slightly strengthened smoothness assumptions that the mth derivatives of a and b are Hoelder continuous, this solver is also (C, C^m) fast. Hence the complexity of (1) is the same as that for integral equations with smooth kernels or close to it. Actually some boundary singularities of $a, b \in C^{2m}([0,1] \times (0,1))$ and $f \in C[0,1] \cap C^m(0,1)$ are allowed in the final formulations.

Quadrature for meshless methods

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ABSTRACT

It is well-known that creating effective quadrature schemes for Meshless Methods (MM) is an important problem (see, *e.g.,* A stabilized conforming nodal integration for Galerkin mesh free methods, J.-S. Chen, C.-T. Wu, S. Yoon, and Y. You, *Int. J. Numer. Meth. Engng.* 2001; **50**:435–466). In this talk we discuss quadrature schemes for MM of order one (MMs that reproduce linear functions). We consider the Neumann Problem and derive an estimate for the energy norm error between the exact solution and the quadrature approximate solution in terms of the mesh parameter and quantities that measure the relative errors in the stiffness matrix, in the lower order term, and in the right-hand side vector, respectively, due to the quadrature. The major hypothesis in the estimate is that the quadrature stiffness matrix has zero row sums, a hypothesis that can be easily achieved by a simple correction of the diagonal elements.

A fast directional multi-pole method for wave equations

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ABSTRACT

Boundary integral formulations of scattering problems are difficult to handle numerically due to the oscillatory nature of the kernel. The standard fast multi-pole method does not give a reduction in the computational complexity of the core matrix vector multiplication in the solution process. A new multi-level method based on directional decomposition can be proved to have near optimal order of complexity: $\mathcal{O}(N \log N)$. The number N stands here for the number of unknowns in the approximation of the boundary potential. A random sampling algorithm to further increase the efficiency will also be introduced and numerical examples will be presented.

Exponential Rosenbrock-type methods

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ABSTRACT

In this talk we present a new class of exponential integrators for the numerical integration of large-scale systems of stiff differential equations. These so-called Rosenbrock-type methods linearize the flow in each time step and make use of the matrix exponential and related functions of the numerically computed Jacobian. In contrast to standard integrators, the methods are fully explicit and do not require the numerical solution of linear systems. We analyze the convergence properties of these integrators in a semigroup framework of semilinear evolution equations in Banach spaces. In particular, we derive an abstract stability and convergence result for variable step sizes. This analysis further provides the required order conditions and thus allows to construct pairs of embedded methods. We present a third order method with two stages, and a fourth order method with three stages, respectively. The application of the required matrix functions to vectors are computed by Krylov subspace approximations. We briefly discuss these implementation issues, and we give numerical examples that demonstrate the efficiency of the new integrators.

REFERENCES

[1] M. Hochbruck, A. Ostermann, J. Schweitzer, *Exponential Rosenbrock-type methods*, Technical Report, Mathematisches Institut, Heinrich-Heine-Universität Düsseldorf. Submitted March 2008

New perspectives on microstructure evolution

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ABSTRACT

Most technologically useful materials are polycrystalline, comprised of many small grains separated by interfaces, called grain boundaries. The energetics and connectivity of this network of interfaces plays a role in many material properties and across many scales of use. Preparing arrangements of grains and boundaries, a texture, suitable for a given purpose is a central problem in materials science: it is the problem of microstructure. Texture is characterized at the mesoscale level by geometry and crystallography. A fundamental result is that this is an energy dependent material property and not some random feature of a configuration. We discuss the origins and analysis of the grain boundary character dist ibution, a basic texture measure, and survey its implications. We introduce a simplified model for interface evolution whose main objective is to understand how coarsening influences texture and discover, perhaps, some unexpected universal features. This is joint work with Shlomo Ta'asan, Katayun Barmak, Eva Eggeling, Maria Emelianenko, Dmitry Golovaty, and Yekaterina Epshteyn.

hp-adaptive finite elements for coupled acoustics/elasticity problems

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ABSTRACT

I will discuss the extension of hp-adaptive FE technology to coupled wave propagation problems. This will include a short discussion on hp data structures and necessary modifications of the original hp algorithm. I will present then three different applications of the methodology:

- Analysis of vibrations of streamers (joint work with S.Prudhomme, W. Rachowicz and W. Qiu)
- Borehole acoustics, i.e. modeling of sonic tools (joint work with Ch. Michler)
- Acoustics of the human head (joint work with M. Paszynski, P. Gatto and J. Kurtz)

All three problems share the same formulation but the underlying physics is quite different and, despite the same core technology being used, results in different challenges and research problems. The study of streamers leads to a multiscale analysis, and the borehole simulations have stimulated a rethinking of Fourier analysis. The last, most complicated of the three projects, necessitated development of new geometry reconstruction techniques and a rather complicated model of the middle ear acoustics.

Multibody dynamics: from numerical to symbolic computations and back

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ABSTRACT

The dynamic analysis of multibody systems is a very classical subject. However, in spite of the extensive litterature the problem of simulating large multibody systems remains a challenging one even in the case of holonomic systems. There are many different ways to formulate the equations of motion, each formulation with its own merits and drawbacks. Nevertheless some difficulties are related to kinematic properties of the system, i.e to the geometric properties of the configuration space, and these difficulties are likely to cause trouble whatever the method used in solving the dynamic equations.

Now it turns out that the rather recently developed tools of computational algebra can be used in the kinematic analysis of multibody systems. The key idea is that the configuration space can be represented as a zeroset of a polynomial system. Using this fact one is often able to reformulate the problem with fewer constraint singularities, or even to eliminate the singularities altogether. Hence a preliminary symbolic analysis of configuration space may actually be very important for subsequent numerical simulations.

We will recall some algebraic background and then discuss the structure of the configuration space as an algebraic variety. Then we consider some examples which show the usefulness of this kind of analysis in the (numerical) study of multibody problems.

A posteriori estimates for Discontinuous Galerkin methods

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ABSTRACT

We analyze Discontinuous Galerkin formulations for second order elliptic problems in mixed form. Using the "weighted residual" approach in an abstract framework we derive a posteriori estimates in terms of the weight operators. We then show that this unified approach applies to all the DG schemes present in the literature.

Block bidiagonal decomposition and least squares problems with multiple right-hand sides

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ABSTRACT

The bidiagonal decomposition of a matrix A plays an important role in algorithms for computing the SVD and for solving least squares and total least squares problems. In a seminal paper from 1965 Golub and Kahan gave two different methods for computing this decomposition. The first uses Householder transformations applied alternately from right and left. The second is based on a Lanczos process and forms the core of the LSQR algorithm for sparse least squares problems.

In this talk we consider block generalization of the bidiagonalization algorithms and their application to least squares and total least squares problems with multiple right hand sides. Applications to partial least squares (PLS) regression with several dependent variables will also be mentioned. The resulting methods can be interpreted as projection methods onto nested sequences of block Krylov subspaces. We describe the deflation process that needs to be applied when singular blocks occur during the decomposition. Each time a zero diagonal element occurs the block size can be reduced. This is equivalent to detecting and removing linear dependencies in the generated Krylov subspaces.

Between Ritt and Kreiss

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ABSTRACT

Let Q be a quasinilpotent operator. Some years ago, Olavi Nevanlinna suggested to study the set of complex numbers z such that the operator $I - zQ$ satisfies certain resolvent or geometric properties (like the Kreiss condition, power boundedness, etc.). We intend to report on the current research including, in particular, recent results obtained jointly with Alexander Gomilko.

Stiffness in the discrete stochastic simulation of biochemical systems

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ABSTRACT

In microscopic systems formed by living cells, the small numbers of some reactant molecules can result in dynamical behavior that is discrete and stochastic rather than continuous and deterministic. An analysis tool that respects these dynamical characteristics is the stochastic simulation algorithm (SSA). Despite recent improvements, as a procedure that simulates every reaction event, the SSA is necessarily inefficient for most realistic problems. One of the reasons for this is stiffness: the presence of both fast and slow reactions, the fastest of which are stable. We will describe the Slow-Scale Stochastic Simulation Algorithm (ssSSA), a computational framework for simulating on the scale of the slow reactions that is applicable even when fast chemical species are present in very small populations. Then we will show how the ssSSA framework can be used to determine the conditions under which Michaelis-Menten approximations in discrete stochastic simulation.

Issues in multivariate polynomial interpolation

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ABSTRACT

While univariate polynomial interpolation has been a basic tool of scientific computing for hundreds of years, multivariate polynomial interpolation is much less understood. Already the question from which polynomial space to choose an interpolant to given data has no obvious answer.

The talk presents, in some detail, one answer to this basic question, namely the "least interpolant" of Amos Ron and the speaker which, among other nice properties, is degree-reducing, then seeks some remedy for the resulting discontinuity of the interpolant as a function of the interpolation sites, then addresses the problem of a suitable representation of the interpolation error and the nature of possible limits of interpolants as some of the interpolation sites coalesce.

The last part of the talk is devoted to a more traditional setting, the complementary problem of finding correct interpolation sites for a given polynomial space, chiefly the space of polynomials of degree $\leq k$ for some k, and ends with a particular recipe for good interpolation sites in the square, the Padua points.

REFERENCES

`http://www.cs.wisc.edu/~deboor/multiint/`

High-dimensional challenges for numerical analysis

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ABSTRACT

Richard Bellmann coined the phrase "the curse of dimensionality" to describe the extraordinarily rapid increase in the difficulty of most problems as the number of variables increases. A typical problem is numerical multiple integration. It is clear that the cost of every integration formulas of product type rises exponentially with the number of dimensions. Nevertheless, problems with hundreds or even thousands of variables do arise, and are now being tackled successfully. In this talk I will touch briefly on recent advances in understanding and constructing high dimensional integration rules, but much of the focus will be on applications, in diverse fields such as mathematical finance, linear models in statistics, and flow through porous media. A general theme is that high-dimensional problems present an enduring challenge for numerical analysis.

Highly oscillatory Fredholm operators: from spectral methods to modified Fourier expansions

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ABSTRACT

In this talk we report recent advances in the calculation of spectra of complex-valued highly oscillatory Fredholm operators by the finite section method. Standard considerations based on spectral methods seem to indicate that expansions in Legendre polynomials are likely to lead to rapid convergence, hence to small matrices. However, calculation of matrix coefficients is expensive. On the other hand, modified Fourier expansions come with rapid algorithms for the calculation of coefficients. Moreover, their slower convergence is offset by the technique of hyperbolic cross. So far, all follows intuition – but numerical results seem to indicate that, surprisingly, the "slowly convergent" modified Fourier basis is actually much better! Careful asymptotic analysis reveals the truth: numerical results are right and intuition wrong!

Pseudogroups, moving frames, and exterior differential systems

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ABSTRACT

Continuous pseudogroups appear as the infinite dimensional counterparts of local Lie groups of transformations in various physical and geometrical contexts, including gauge theories, Hamiltonian mechanics and symplectic and Poisson geometry, conformal field theory, symmetry groups partial differential equations, such as the Navier–Stokes and Kadomtsev–Petviashvili equations of fluid mechanics and plasma physics, image recognizion, and geometric numerical integration.

In this talk I will report on my recent joint work with Peter Olver on extending the classical moving frames method to infinite dimensional pseudogroups. As in the finite dimensional case, moving frames can be employed to produce complete sets of differential invariants for a pseudogroup action and to effectively analyze the algebraic structure of such invariants. Moreover, I will discuss a novel reduction method based on the moving frames algorithm for exterior differential systems invariant under the action of a continuous pseudogroup and describe its applications to constructing analytic solutions to systems of partial differential equations.

Reduced symmetry elements in linear elasticity

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ABSTRACT

In continuum mechanics problems, we have to work in most cases with symmetric tensors, symmetry expressing the conservation of angular momentum.

Discretization of symmetric tensors is however difficult and a classical solution is to employ some form of reduced symmetry.

We present two ways of introducing elements with reduced symmetry. The first one is based on Stokes problems, and in the two-dimensional case allows to recover practically all interesting elements on the market. This however is (definitely) not true in three dimensions. On the other hand the second approach (based on a very nice property of several interpolation operators) works for three-dimensional problems as well, and allows, in particular, to prove the convergence of the Arnold-Falk-Winther element with simple and standard arguments, without the use of the Berstein-Gelfand-Gelfand resolution.

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ISBN 978-951-22-9419-0 (print)
ISBN 978-951-22-9420-6 (PDF)
ISSN 0784-6460 (print)
ISSN 1797-5875 (PDF)