3. Austrian Numerical Analysis Day

26.–27.4.2007

Technische Universität Wien

organized by

Institut für Analysis und Scientific Computing
Wiedner Haupstraße 8–10/E101
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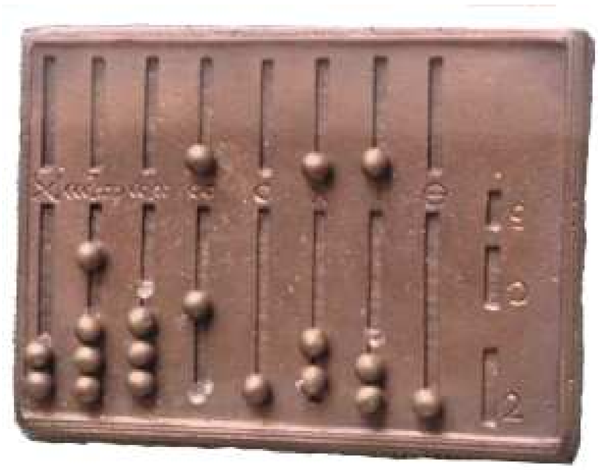

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Program

Thursday, Apr. 26, 2007

– CALIARI: prefers to give the talk on Friday, or Thursday late afternoon. –

13:00		*Opening*
13:30 – 14:00	Almedin Becirovic	*title t.b.d.*
14:00 – 14:30	Peter Balacz	Double preconditioning for Gabor frames
14:30 – 15:00	Sven Beuchler	Overlapping Additive Schwarz preconditioners for degenerated elliptic problems
15:00 – 15:30	Marco Caliari	Implementation of exponential Rosenbrock-type methods
15:30 – 16:00	Svetlana Cherednichenko	Regularization and Discretization of State Constrained Optimal Control Problems

– *coffee break* –

16:30 – 17:00	Eskil Hansen	Finite element Runge–Kutta discretizations of porous medium type equations
17:00 – 17:30	Erika Hausenblas	Numerical Approximation of Stochastic Partial Differential Equations
17:30 – 18:00	Zoltán Horvath	Numerical methods: theory and applications
18:00 – 18:30	Martin Huber	Simulation of Diffraction in periodic Media with a coupled Finite Element and Plane Wave Approach
18:30 – 19:00	Martin Kilian	Geometric Modeling in Shape Space

– *Dinner at ‘Augustinerkeller’´(Heurigenrestaurant, Wien I.)* –

Friday, Apr. 27, 2007

9:00 – 9:30	Othmar Koch	Theory and Computation of the MCTDHF Approximation for the Time-Dependent Schrödinger Equation
9:30 – 10:00	Richard Kowar	Schlierentomographie – Reconstruction of pressure fields of ultrasound transducers
10:00 – 10:30	Wolfgang Kreuzer	Numerische Probleme in der Akustik
10:30 – 11:00	Klaus Krumbiegel	Regularization of a state constrained optimal control problem with boundary control
11:00 – 11:30	Frank Lenzen	MAP estimators for Image denoising
11:30 – 12:00	Nataliya Metla	Convergence of SQP for Semilinear Elliptic Optimal Control Problems with Mixed Control-State Constraints

– *lunch break* –

13:30 – 14:00	Clemens Pechstein	FETI/BETI solvers for nonlinear magnetic field problems in unbounded domains
14:00 – 14:30	Frank Rattay	Simulationen zur Funktionellen Elektrostimulation: Effektive Elektrodenkonfigurationen zur Muskelstimulation
14:30 – 15:00	René Simon	On Schwarz-type smoothers for saddle point problems with applications to PDE-constrained optimization problems
15:00 – 15:30	Gerhard Unger	Boundary Element Methods for Eigenvalue Problems
15:30 – 16:00	Markus Windisch	Modified boundary integral equations for electromagnetic scattering problems
16:00 – 16:30	Sabine Zaglmayr	Equilibrated residual-based error estimators for Poisson and Maxwell's equations
16:30		*Closing*

Abstracts

title t.b.d.

Almedin Becirovic

abstract t.b.d.

Double preconditioning for Gabor frames

Peter Balacz

We present an application of the general idea of preconditioning in the context of Gabor frames. While most (iterative) algorithms aim at a more or less costly exact numerical calculation of the inverse Gabor frame matrix, we propose here the use of "very cheap methods" to find an approximation for it, based on (double) preconditioning. We thereby obtain very good approximations of the true dual Gabor atom at very low computational costs. Since the Gabor frame matrix commutes with certain time-frequency shifts it is natural to make use of diagonal and circulant preconditioners sharing this property.

Part of the efficiency of the proposed scheme results from the fact that all the matrices involved share a well-known block matrix structure. At least, for the smooth Gabor atoms typically used, the combination of these two preconditioners leads consistently to very good results. These claims are supported by numerical experiments in the second part of the paper. For numerical evaluations we introduce two new matrix norms, which can be calculated very efficiently by exploiting the structure of the frame.

Overlapping Additive Schwarz preconditioners for degenerated elliptic problems

Sven Beuchler

In this paper, we consider some degenerated boundary value problems on the unit square. These problems are discretized by piecewise linear finite elements on a triangular mesh of isosceles right-angled triangles. The system of linear algebraic equations is solved by a preconditioned gradient method using a domain decomposition preconditioner with overlap. We prove that the condition number of the preconditioned system is bounded by a constant which independent of the discretization parameter. Moreover, the preconditioning operation requires $\mathcal{O}(N)$ operations, where N is the number of unknowns. Several numerical experiments show the preformance of the proposed method.

This a joint work with S. Nepomnyschikh (Novosibirsk).

Implementation of exponential Rosenbrock-type methods

Marco Caliari

We present a variable step size implementation of exponential Rosenbrock-type methods. These integrators require the evaluation of exponential and related functions of the Jacobian matrix. To this aim, the Real Leja Points Method is used. We solve semilinear parabolic PDEs in one and two space dimensions and we compare our method with others from literature. We find a great potential of our method for parabolic problems with large advection in combination with moderate diffusion and mildly stiff reactions. Finally, we present an adaptive "meshfree" exponential integrator for a pure advection problem.

Regularization and Discretization of State Constrained Optimal Control Problems

Svetlana Cherednichenko

A family of elliptic optimal control problems with pointwise state and mixed constraints are considered. In particular, the main difficulties occur for cases with pure state constraints. To overcome these difficulties we use here a Lavrentiev type of regularization. We are interested in convergence rate with respect to the regularization parameter and in the error estimate for the finite element discretization of the partial differential equations with respect to the grid size. Choosing certain relation between the regularization parameter and the mesh size, we obtain convergence of order close to 1.

Finite element Runge–Kutta discretizations of porous medium type equations

Eskil Hansen

In this talk we analyze the convergence properties of a class of porous medium type equations. For spatial and time discretizations, we use standard linear finite elements and algebraically stable Runge-Kutta methods, respectively. We prove an optimal convergence result for solutions that are sufficiently smooth in time, without any assumptions on the spatial regularity. We will illustrate the convergence result with a few numerical examples.

Numerical Approximation of Stochastic Partial Differential Equations

Erika Hausenblas

First I will introduce stochastic Partial differential equations driven by Browinan motion and will give a short review about the theory. Next, I will explain the pecularities of the Brownian motion. Finally I will present some results about their approximation.

Numerical methods: theory and applications

Zoltán Horvath

In this talk we present the recent research in numerical mathematics done at the Department of Mathematics and Computational Sciences of Szechenyi Istvan University, Györ, Hungary. The wide range of the covered topics is illustrated by the following list of keywords: continuous and discrete time discrete dynamical systems (qualitative properties: invariance, monotonicity, long-time behavior, generalized maximum principle, time discretization with Runge-Kutta, Rosenbrock-type and general linear methods), numerical methods of partial differential equations (FEM, FVM and BEM for fluid flow problems and elasticity, meshless methods), optimization (global optimization) and fast Fourier transformation.

As applications of numerical methods we present our recent work with industry in automative engineering (internal and external flows, shape optimization, automated integrated CAD-based optimization), image processing (holograms) and enviromental modeling (numerical simulation of air pollution propagation in Györ).

Simulation of Diffraction in periodic Media with a coupled Finite Element and Plane Wave Approach

Martin Huber and *Joachim Schöberl*

If an electromagnetic wave incidents onto a grating it is diffracted and transmitted into certain directions. While these directions are easy to calculate and depend only on the periodicity, the computation of the corresponding intensities which depend on the shape of the grating turns out to be much more complicated.

Modeling such gratings with FEM, we have to solve Maxwell's equations on the computational domain which can be reduced to one single unit cell. In order to describe the periodic behavior of the grating, we have to formulate quasi periodic boundary conditions. A critical point is the treatment of the far-field, which is discretized by propagating plane waves and exponentialdecaying functions. The polynomial basis functions of the FEM domain have to be coupled with the plane wave basis functions. The innovation of our approach is to perform this coupling by the method of Nitsche.

By using a plane wave expansion in the far field, the simulation can be easily compared with optical experiments, where similar quantities are measured.

Geometric Modeling in Shape Space

Martin Kilian

We present a novel framework to treat shapes in the setting of Riemannian geometry. Shapes – triangular meshes or more generally straight line graphs in Euclidean space – are treated as points in a shape space. We introduce useful Riemannian metrics in this space to aid the user in design and modeling tasks, especially to explore the space of (approximately) isometric deformations of a given shape.

Much of the work relies on an efficient algorithm to compute geodesics in shape spaces; to this end, we present a multi-resolution framework to solve the boundary value problem as well as the initial value problem for geodesics. Several classical concepts like parallel transport, or the exponential map can be used in shape space to solve various geometric modeling and geometry processing tasks. Applications include shape morphing, deformation transfer, freeform deformations, intuitive shape exploration, and the computation of piecewise developable shapes such as D-forms from their unfolding.

Theory and Computation of the MCTDHF Approximation for the Time-Dependent Schrödinger Equation

Othmar Koch

We study the solution of the time-dependent Schrödinger equation for an atom or molecule with f degrees of freedom in a time-dependent electric field (typically arising from ultrashort laser pulses),

$$\mathrm{i}\,\frac{\partial\psi(x_1,\ldots,x_f,t)}{\partial t} \;=\; H(t)\psi(x_1,\ldots,x_f,t).$$

In the Hamiltonian H, the kinetic part includes a time-dependent drift term to model the influence of the electric field, and the potential part is given by the classical Coulomb potential. To reduce the computational complexity, we approximate the wave function using the multi-configuration time-dependent Hartree-Fock method. In this approach, the problem is reduced to a set of partially uncoupled, nonlinear PDEs. These are solved numerically using the method of lines.

We demonstrate the success of our solution approach by giving results computed for a one-dimensional model, where a screened Coulomb potential is used. In the case of smooth potential, it is also possible to prove the existence, uniqueness and regularity of the solution of the MCTDHF equations. Finally, we show how this model reduction technique for the time-dependent Schrödinger equation has inspired a novel, highly successful method for computing low rank approximations to time-dependent finite matrices, and give an outlook on current developments.

Schlierentomographie – Reconstruction of pressure fields of ultrasound transducers

Richard Kowar

In order to ensure safety and optimal performance of medical ultrasound transducers it is necessary to measure the acoustic pressure fields of transducers. For the estimation of such pressure fields we use light intensity data that is obtained by a Schlierensystem. Schlieren data corresponds mathematically to squared x-ray tomographic data. Acoustic pressure fields attain positive and negative values, but only the square of the line integrals are provided by the Schlieren system. Therefore the signs of the line integrals are not known, and Schlieren data cannot be reduced to data of classical X–ray CT. For the numerical estimation of pressure fields we used the loping Landweber-Kaczmarz method.

Numerische Probleme in der Akustik

Wolfgang Kreuzer

Wir wollen einen kurzen Einblick in die verschiedensten Problemstellungen geben, die im Zuge unserer Arbeit auftreten, und zwei Anwendungen speziell vorstellen. Beim ersten Problem handelt es sich um die Simulation der Ausbreitung von Vibrationen in Boeden, die als stochastische Schichten behandelt werden, da im Allgemeinen Materialparameter fuer Bodenschichten nur schwer zu bestimmen sind. Mit Hilfe von Chaospolynom-Ansatz und Karhunen-Loeve-Zerlegung ist es moeglich,das System und damit auch das daraus resultierende Gleichungssystem in einen stochastischen und einen deterministischen Teil zu trennen.

Alle rechenintensiven Routinen werden nur auf den deterministischen Teil angewandt, der relativ einfach und mit wenig Aufwand behandelt werden kann. Der aufwaendigere stochastische Teil wird mit Hilfe einer speziellen Iteration in das Gesamtsystem integriert. Eine zweites Anwendungsproblem ist die Berechnung der Verteilung des Schalldrucks am Kopf und besonders am Ohr/Pinna. Dazu wird der Kopf mit Hilfe eines 3D-Scans diskretisiert, und eine Randelemente Modell generiert. Da die Diskretisierung sehr fein sein muss, ist es notwendig das BEM-Modell mit der Fast Multipole Methode zu koppeln.

Regularization of a state constrained optimal control problem with boundary control

Klaus Krumbiegel

We consider a linear quadratic optimal control problem with pointwise state constraints and control constraints, where the control acts at the boundary. It is well known that problems with pointwise state constraints inhibit a lot of difficulties since the Lagrange multipliers are in general only Borel measures. Therefore, different regularization concepts are developed in the last years. However, a direct extension of the Lavrentiev regularization concept is not possible since the control is not defined in the domain where the state constraints are given. In order to overcome this difficulty, we regularize the state constraints by introducing a virtual control v. This control acts in the cost functional, the state equation and the regularized state constraints. The effect of regularization is influenced by different parameter functions depending on a regularization parameter $\varepsilon > 0$.

Furthermore, we derive an error estimate for the error between the optimal solution of the original problem and the regularized one. Moreover, under some assumptions on the parameter functions we obtain certain convergence rates of the regularization error. We consider several numerical examples illustrating the behaviour of the error for $\varepsilon \downarrow 0$ and for different choices of the parameter functions.

MAP estimators for Image denoising

Frank Lenzen

We present a statistical approach for image denoising based on Bayesian estimation.

We investigate three different models for noisy images u^δ, with additive Gaussian noise, with error in the pixels location and a combination of both error types.

Bayesian estimation requires a-priori information about the probability for an image u to occur, which is referred to as *prior*. We propose different priors for images based on the differences between adjacent pixels.

For each noise model we then set up the *Maximum a posteriori (MAP) estimator*, which consists in maximizing the *conditional probability* of u with given u^δ.

Finally we present some numerical results.

Convergence of SQP for Semilinear Elliptic Optimal Control Problems with Mixed Control-State Constraints

Nataliya Metla

In this talk we will consider a family of optimal control problems with pointwise control and mixed inequality constraints governed by semilinear elliptic partial differential equations (PDEs). Optimal problems involving semilinear PDEs can be efficiently solved using the sequential quadratic programming (SQP) method, which is equivalent to a generalized Newton's method. The local convergence behavior of this method relies essentially on the strong regularity of a certain generalized equation, which means Lipschitz continuous dependence of the solution of the linearized generalized equation on a perturbation parameter. In the context of PDE-constrained optimization, the linearized generalized equation represents nessesary and sufficient optimality conditions of an auxiliary linear-quadratic optimization problem.

A recent Lipschitz stability result and the convergence of the SQP method applied to such optimal control problems will be discussed. Numerical examples will be shown.

FETI/BETI solvers for nonlinear magnetic field problems in unbounded domains

Clemens Pechstein and *Ulrich Langer*

The rather popular finite element tearing and interconnecting (FETI) methods and the closely related boundary element tearing and interconnecting (BETI) methods are domain decomposition methods for solving large-scale elliptic partial differential equations (PDE). The reason of their success is firstly due to the parallel scalability, secondly the fact that the condition number of the corresponding preconditioned system grows only like $O(((1 + \log(H/h))^2)$, where H is the subdomain diameter and h denotes the discretization parameter, and finally, the robustness with respect to jumps in the coefficients of the PDE. In nonlinear magnetic field computations, one is not only confronted with large jumps of coefficients over material interfaces but often also with high variation of coefficients inside homogeneous material.

Furthermore, one likes to model the physical behaviour in a so-called exterior domain with an appropriate radiation condition. In this talk we discuss how to adapt coupled FETI/BETI methods to these needs. As model problem, we consider a nonlinear potential equation where the coefficient depends nonlinearly on the gradient of the solution. In particular, we show explicit condition number estimates for the exterior domain. Moreover, we propose and numerically analyze special preconditioners dealing with highly varying coefficients which typically arize in subdomain Newton-type Jacobi matrices.

Simulationen zur Funktionellen Elektrostimulation: Effektive Elektrodenkonfigurationen zur Muskelstimulation

Frank Rattay, Johannes Martinek, Yvonne Stickler und Karen Minassian

Funktionelle Elektrostimulation dient zur Überbrückung verloren gegangener Körperfunktionen durch gezielte Aktivierung elektrisch erregbarer Strukturen, meist von Nerven- oder Muskelfasern. Sind die unteren Extremitäten durch Rückenmarksverletzungen willentlich nicht bewegbar, so kommen drei Prinzipien zur Anwendung:

i) Stimulation von 'motorischen' Fasern des peripheren Nervensystems

ii) Direkte Stimulation von Muskelfasern bei denervierter Muskulatur (dh. die neuronale Verbindung zwischen Rückenmark und Muskelfaser fehlt verletzungsbedingt)

iii) Stimulation von Neuronengruppen, die als Mustergeneratoren im Rückenmark imstande sind rhythmische 'Laufbewegungen' auszulösen. In allen Fällen sind Form und Positionierung der Elektroden entscheidend für eine effektive Muskelaktivierung.

Zur Analyse der Wirkungsmechanismen wird ein einfaches Modell herangezogen: Infinites leitendes Medium mit punktförmigen Stromquellen. Eine lange zylindrische Struktur mit nichtlinearem Input-Output Verhalten simuliert dann die Erregung als orts- und zeitveränderliche Membranspannung einer zu untersuchenden Nerven- oder Muskelfaser. Ortsdiskretisierung der Faser liefert ein gekoppeltes Differenzialgleichungssystem, wobei in jedem Diskretisierungsintervall eine Störgröße wirkt, die den Einfluss der aktiven Elektroden repräsentiert. Die Gesamtheit dieser Störgrößen wird zur Aktivierungsfunktion f zusammengefasst und bedingt den Ort der stärksten Elektrodenwirkung auf die Zielstruktur. Im Faserendpunkt ist f proportional zu Ve' (Ortsableitung des extrazellularen Potenzials in Faserrichtung) in den anderen Bereichen zu Ve''.

Alternativ wird eine systematische Variation von Elektrodengeometrie und Signalstärken für spezielle Anwendungsfälle nach folgendem Prinzip durchgeführt. Für jede zu untersuchende Konfiguration wird zuerst mittels Finite Element Methode die Potenzialverteilung im Raum ermittelt und dann die Antwort der erregbaren Strukturen am Kompartmentmodell durch Computersimulationen ermittelt.

Für klinische Anwendungen effiziente Elektrodenkonfigurationen werden diskutiert.

(Kooperation des Institutes für Analysis und Scientific Computing der TU Wien mit dem Wilhelminenspital, Wien.)

On Schwarz-type smoothers for saddle point problems with applications to PDE-constrained optimization problems

René Simon

In this talk we consider additive (and multiplicative) Schwarz-type iteration methods for saddle point problems as smoothers in a multigrid method. Each iteration step requires the solution of several small local saddle point problems. In a previous work (by Joachim Schöberl and Walter Zulehner) the general construction of such patch smoothers for mixed problems were discussed. It was shown that, under suitable conditions, the additive Schwarz-type iteration fulfills the so-called smoothing property, an important part of a multigrid convergence proof, and the theory was applied to the Stokes problem.

Here we consider a certain class of optimization problems from optimal control. A natural property of the corresponding Karush-Kuhn-Tucker (KKT) system, a 2-by-2 block system which characterizes the solution of the optimization problems, is the positivity of the (1,1) block only on the kernel of the (2,1) block. We extend the results for the Stokes problem to PDE-contrained optimization problems and present a patch smoother, which allows a rigorous convergence analysis of the corresponding multigrid method.

Boundary Element Methods for Eigenvalue Problems

Olaf Steinbach and *Gerhard Unger*

The solution of Laplace eigenvalue problems by using boundary integral equation methods usually involves some Newton potentials which may be resolved by using a multiple reciprocity approach. Here we propose an alternative approach which is in some sense equivalent to the above. Instead of a linear eigenvalue problem for the partial differential operator we consider a nonlinear eigenvalue problem for a boundary integral operator. This nonlinear eigenvalue problem can be solved by using some approriate iterative scheme, i.e. a Newton scheme.

We will discuss the convergence and the boundary element discretization of this algorithm, and give numerical results. Moreover we will discuss alternative solution strategies and more efficient discretization techniques.

Modified boundary integral equations for electromagnetic scattering problems

Markus Windisch

For exterior electromagnetic scattering problems, the boundary integral equation method is a suitable choice for a numerical approach, because only the boundary has to be discretised, and the Silver-Müller radiation condition is incorporated. However, the unique solvability of the original problem can get lost in particular when eigenfrequencies of the scattering body appear. A first approach to overcome this problem is to use the approach of Brakhage and Werner, who introduced a combined field integral equation for the acoustic scattering problem. But this approach is considered usually in $L_2(\Gamma)$, where uniqueness results are based on Gardings inequality and Fredholm's alternative. However, the compactness of certain boundary integral operators is needed, i.e. the boundary must be assumed to be sufficiently smooth. That's why modified boundary integral equations were introduced which are formulated in the energy function spaces to ensure unique solvability also for Lipschitz polyeders.

In this talk a modified boundary integral equation will be presented that in comparison to already existing approaches neither uses a compact operator in the formulation nor uses the Hodge decomposition.

Equilibrated residual-based error estimators for Poisson and Maxwell's equations

Dietrich Braess, Joachim Schöberl and Sabine Zaglmayr

Equilibrated a-posteriori error estimators for Poisson equations rely on the following principle: Any flux σ which fulfils the equilibrium condition, $div\,\sigma = f$, can be used to obtain an upper bound for the discretization error without generic constants. We present a patch-wise construction of a flux correction $\sigma^\Delta = \sigma + \mathrm{grad}\, u_h$ that is also applicable for high-order FE-schemes and for Maxwell's equations.

The flux correction has to satisfy $div\,\sigma^\Delta = f + \Delta u_h$ in the distributional sense. The existence of a solution of the local vertex-patch problems is guaranteed by the exactness of discrete distributional de Rham sequences. The appropriate finite element spaces are a broken Raviart-Thomas space for the flux correction and an element-wise polynomial space extended by polynomials living only on the skeleton for the residual. We illustrate the advantages of our method by numerical experiments with h- and p-refinement strategies.

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