# Technische Universität Graz



# Workshop 2nd Austrian Numerical Analysis Day

Graz, 27.-28.4.2006

O. Steinbach (ed.)



Berichte aus dem Institut für Numerische Mathematik

Book of Abstracts 2006/2

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# Berichte aus dem Institut für Numerische Mathematik

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# Programm

Donnerstag, 27.4.2006			
14.00 - 14.30	J. M. Melenk (Wien)		
	On Adaptivity in hp–FEM		
14.30 - 15.00	M. Thalhammer (Innsbruck)		
	Exponential Splitting for Parabolic Problems		
15.00 - 15.30	S. Beuchler (Linz)		
	Sparse Shape Functions for Triangular FEM		
15.30 - 16.00	S. Engleder (Graz)		
	Modified Boundary Integral Formulations for the		
	Helmholtz Equation		
16.00 - 16.30	Kaffee		
16.30 - 17.00	B. Vexler (Linz)		
	Adaptive Space–Times Finite Element Methods for		
	Parabolic Optimization Problems		
17.00 - 17.30	K. Krumbiegel (Linz)		
	Linear–Quadratic Optimal Control Problems:		
	Error Estimates and Numerical Treatment		
17.30 - 18.00	A. Rösch (Linz)		
	Numerical Analysis for Optimal Control Problems		
	in Nonconvex Domains		
18.00 - 18.30	B. Carpentieri (Graz)		
	Adaptively Preconditioned Krylov Methods for Solving		
	General Linear Systems		
19.00	Gemeinsames Abendessen		

Freitag, 28.4.2006				
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	Numerical Problems in Gabor Analysis			
9.00 - 9.30	G. Of (Graz)			
	Fast Boundary Element Methods and Applications			
9.30 - 10.00	C. Pechstein (Linz)			
	Finite and Boundary Element Tearing and Interconnecting Solvers			
	for Nonlinear Potential Problems in Bounded and Unbounded			
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10.30 - 11.00	J. Kraus (Linz)			
	Multilevel Preconditioning of 2D Rannacher–Turek			
	Finite Element Problems			
11.00 - 11.30	C. Pöschl (Innsbruck)			
	Duality and Higher Order TV–Regularization			
11.30 - 12.30	Mittag			
12.30 - 13.00	D. Praetorius (Wien)			
	Numerical Analysis for the Landau-Lifshitz Minimization Problem			
	in Micromagnetics			
13.00 - 13.30	S. Zaglmayr (Linz)			
	High Order Nédélec Elements for Electromagnetic			
	Field Computation			
13.30 - 14.00	A. Sinwel (Linz)			
	Tangential–Displacement and Normal–Normal–Stress			
	Continuous Mixed Finite Elements for Elasticity			
14.00 - 14.30	A. Ostermann (Innsbruck)			
	Exponential Rosenbrock–Type Methods			

#### Sparse shape functions for triangular FEM

S. Beuchler

#### Universität Linz

In this talk, the second order boundary value problem  $-\nabla \cdot (\mathcal{A}(x, y)\nabla u) = f$  is discretized by the Finite Element Method using piecewise polynomial functions of degree p on a triangular mesh. On the reference element, we define integrated Jacobi polynomials as interior ansatz functions. If  $\mathcal{A}$  is a constant function on each triangle and each triangle has straight edges, we prove that the element stiffness matrix has not more than  $\frac{25}{2}p^2$  nonzero matrix entries.

Two applications of this result are given.

Numerical examples show the advantages of the proposed basis. This talk is joint work with Joachim Schöberl (Aachen).

## Adaptively preconditioned Krylov methods for solving general linear systems

B. Carpentieri Karl–Franzens Universität Graz

The solution of linear systems of equations is a crucial component of the simulation in many engineering and scientific applications. Direct solution methods based on variants of Gaussian elimination are often the method of choice because they are fairly robust and predictable in terms of accuracy and cost. When direct methods become too demanding for the memory of the coefficient matrix of the linear system is only accessible via matrix-vector products, iterative solution strategies can be a reliable alternative. Iterative methods can be also combined with direct method to design robust hybrid solvers. It is now well understood that iterative methods, although they can solve the bottleneck of memory, have to be used in combination with efficient preconditioners to be cost effective on realistic applications. In this talk, we present a class of adaptive preconditioners for both symmetric and unsymmetric Krylov methods. The proposed class of algorithms can be used as stand-alone preconditioners for solving the linear system, or as a refinement technique constructed on top of an existing *first-level* preconditioner to enhance its robustness on tough problems. Experiments are reported on sparse linear systems extracted from the harwell–Boeing matrix collections and dense linear systems arising from realistic electromagnetic applications to assess the effectiveness and to analyse the cost of the proposed method.

## Modified Boundary Integral Formulations for the Helmholtz Equation

<u>S. Engleder</u>, O. Steinbach Technische Universität Graz

Although the exterior boundary value problems for the Helmholtz equation with either Dirichlet or Neumann boundary conditions are unique solvable, related boundary integral equations may not be solvable, or the solutions are not unique. In particular, the boundary integral operators are not injective when the wave number  $k^2$  is an eigenvalue of the interior Dirichlet or Neumann eigenvalue problem, respectively. Considering linear combinations of different boundary integral formulations this results in combined boundary integral equations, which are unique solvable for all wave numbers. The most known formulations are those of Brakhage–Werner and Burton–Miller. However, since the combined boundary integral equation involves boundary integral operators of both first and second kind, the analytical framework offers different settings. The classical combined boundary integral equations are considered in  $L_2(\Gamma)$ , where the uniqueness results are based on Gårdings inequality and Fredholm's alternative. To ensure the compactness of certain boundary integral operators, sufficient smoothness of the surface  $\Gamma$  is required. Recently, different regularized formulations are discussed, which ensure the unique solvability even for Lipschitz surfaces  $\Gamma$ .

Here we will describe a modified regularized boundary integral formulation for the Helmholtz equation with either Dirichlet or Neumann boundary conditions. Moreover, we analyse the associated boundary element approximation and we give first numerical results.

# References

 S. Engleder, O. Steinbach: Modified boundary integral formulations for the Helmholtz equation. Bericht 2006/1, Berichte aus dem Institut f
ür Numerische Mathematik, TU Graz, 2006.

#### Numerical Problems in Gabor Analysis

H. G. Feichtinger Universität Wien

Gabor analysis is an important branch within time-frequency analysis, based on the use of the so-called short time Fourier transform (STFT) or sliding window Fourier transform of a function ("signal") f. One may think of some audio signal which is locally decomposed into harmonics, very much like a musical score. It was the idea of D.Gabor (who received the Nobel Prize for this pioneering work on the foundations of holography) to decompose an arbitrary signal into a double series where the building blocks are time-frequency shifted versions of a Gaussian. The reason to take a Gaussian is due to the fact that it is the minimizer in the Heisenberg uncertainty relation. Interpreting this accoustically, one can generate arbitrary noises and melodies by playing sufficiently fast (and with arbitrarily many fingers) on a piano which is tuned sufficiently fine. It turned out that the original approach is only realizable by redundant systems. However, one can enforce uniqueness by choosing coefficients of minimial  $\ell^2$ -norm. Moreover, one can show that the canonical Gabor coefficients of a function can be computed efficiently as sample values of an STFT by using the so called dual Gabor window.

Gabor multipliers are operators which can be realized by pointwise multiplication of the Gabor coefficients (before synthesis). For instance this may be used to denoise an accoustic signal or to separate certain (time-frequency) parts of a signal. Since "good" Gabor systems are never orthonormal bases, Gabor multipliers behave completely different (e.g. with respect to composition or inversion) than Fourier multipliers. The talk will shortly summarize basics on Gabor analysis including several numerical and algorithmic aspects such as best approximation of matrices with Gabor multipliers, methods to compute dual Gabor frames etc. . If time permits we will point out the relevance of such algorithms for current projects at the Numerical Harmonic Analysis Group (NuHAG) under supervision of the speaker, in particular EUCETIFA (Marie Curie Excellence Grant 2005-2009) and MOHAWI (2005-2008). Details can be found on the NuHAG homepage http://www.univie.ac.at/nuhag-php/home/index.php

# Multilevel preconditioning of 2D Rannacher–Turek finite element problems

I. Georgiev<sup>1</sup>, <u>J. Kraus</u><sup>2</sup>, S. Margenov<sup>1</sup> <sup>1</sup>Bulgarian Academy of Sciences, Sofia <sup>2</sup>Johann Radon Institut (RICAM), Linz

Preconditioners based on various multilevel extensions of two-level finite element methods (FEM) lead to iterative methods which often have an optimal order computational complexity with respect to the number of degrees of freedom of the system. Such methods were first presented in [1, 2], and are based on (recursive) two-level splittings of the finite element space. The key role in the derivation of optimal convergence rate estimates plays the constant  $\gamma$  in the so-called Cauchy– Bunyakowski–Schwarz (CBS) inequality, associated with the angle between the two subspaces of the splitting. More precisely, the value of the upper bound for  $\gamma \in (0, 1)$ is a part of the construction of various multilevel extensions of the related two-level methods.

In the present talk we concentrate on algebraic two-level and multilevel preconditioners for second-order elliptic boundary-value problems discretized using Rannacher-Turek non-conforming rotated bilinear finite elements on quadrilaterals. An important point to make is that in this case the finite element spaces corresponding to two successive levels of mesh refinement are not nested (in general). To handle this, a proper two-level basis is required in order to fit the general framework for the construction of two-level preconditioners for conforming finite elements and to generalize the methods to the multilevel case. The proposed variants of hierarchical two-level basis are first introduced in a rather general setting. Then, the involved parameters are studied and optimized. As will be shown, the obtained bounds give rise to optimal order algebraic multilevel iteration (AMLI) methods.

# References

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# Linear–quadratic optimal control problems error estimates and numerical treatment

<u>K. Krumbiegel</u>, A. Rösch Johann Radon Institut (RICAM), Linz

We consider a linear-quadratic optimal control problem governed by an elliptic partial differential equation with pointwise control constraints. Such problems are often treated by multilevel iterative methods. We present an error estimation technique for the iterates with respect to the solution. These error estimates can be used as stopping criteria for the iterative methods. The presented theory is illustrated by numerical examples. Here, we used the primal-dual active set strategy and a CG-algorithm as iterative methods.

### On adaptivity in *hp*–FEM

T. Eibner<sup>1</sup>, <u>J. M. Melenk<sup>2</sup></u> <sup>1</sup>TU Chemnitz, <sup>2</sup>TU Wien

In the hp-version of the finite element method convergence can be achieved by refining the mesh refinement or increasing the approximation order or a combination of both. In fact, suitable combinations of both techniques can lead, for a large problem classes, to very fast convergence.

Many adaptive algorithms are based on two ingredients: an error estimator and a marking strategy. The error estimator discussed in the talk is of residual type. This estimator is shown to be reliable for elliptic problems in 2 and 3 dimensions; for 2D problems, the efficiency estimate is slightly suboptimal (optimal in the mesh parameters but suboptimal by essentially one factor p, where p is maximal approximation order). Numerical experiments for the pure p-version FEM show that this reliability-efficiency gap is not an artifact of the proof. The numerical experiments with the p-version FEM applied to problems with an isolated singularity also show that the appearance of the reliability-efficiency gap of the estimator depends significantly on whether the singularity is located at a mesh point or not.

In the hp-version of the finite element method (hp-FEM), convergence can be achieved either through mesh refinement or by increasing the approximation order. We presented an hp-adaptive algorithm where the decision whether to perform h-refinement or p-enrichment is based on locally testing for analyticity. Analyticity is detected by estimating the decay rate of the coefficients of the elementwise expansion of the hp-FEM solution in orthogonal polynomials: elements where the coefficients decay rapidly are candidates for p-enrichment whereas those with slow increase are candidates for h-refinement.

#### Fast Boundary Element Methods and Applications

<u>G. Of</u>, O. Steinbach Technische Universität Graz

Fast boundary element methods are applied for engineering and industrial real life problems with homogeneous partial differential equations in complicated structures. Examples are the computation of capacity curves of micromechanical sensors, the simulation of spray painting processes and the elastic deformation of mechanical transformation tools and of a foam. For the discretization of the symmetric boundary integral formulation a Galerkin boundary element method is used, where all boundary integral operators can be reduced to the single and douple layer potential of the Laplace equation. From this we obtain a fast boundary element method by using the fast multipole method. A main feature of this method is a fast realization of the Dirichlet to Neumann map by the so-called Steklov-Poincare operator. Finally we discuss the preconditioned iterative solution process of the resulting linear systems.

#### Exponential Rosenbrock-type methods

# A. Ostermann Universität Innsbruck

Exponential integrators have been developed for the numerical solution of semilinear evolution equations  $\partial_t u = Au + g(u)$ . In contrast to implicit Runge–Kutta methods, they make explicit use of the decomposition of the vector field into a linear part Au and a (possibly) nonlinear remainder g(u). This decomposition is usually kept constant along the integration.

In my talk, which is based on joint work with Marlis Hochbruck and Julia Schweitzer (Düsseldorf), I will present a new class of exponential integrators that update the above decomposition in each step by linearising the vector field along the numerical solution (whence the name Rosenbrock-type methods). This strategy has two advantages. On the one hand, it simplifies the actual construction of high-order methods, on the other hand it leads to methods with much smaller error constants. I will discuss in detail the implementation of an exponential integrator of order four with variable step size selection based on a local error control. This new method is explicit, and its performance compares very well with that of implicit Runge–Kutta methods (for instance RADAU5).

# References

- M. Hochbruck, A. Ostermann: Explicit exponential Runge-Kutta methods for semilinear parabolic problems. SIAM J. Numer. Anal. 43, 1069-1090 (2005)
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# Finite and boundary element tearing and interconnecting solvers for nonlinear potential problems in bounded and unbounded domains

U. Langer, <u>C. Pechstein</u> Johannes Kepler Universität Linz

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. As a model problem, we consider the potential equation  $-\nabla \cdot [\nu(|\nabla u|)\nabla u] = f$  with a nonlinear coefficient  $\nu$ .

Domain decomposition (DD) methods like the rather popular finite element tearing and interconnecting (FETI) methods, dual-primal FETI (FETI-DP) methods and balanced domain decomposition by constraints (BDDC) techniques offer preconditioners which are robust with respect to jumps in the coefficients across subdomain interfaces. Furthermore, the boundary element method (BEM) allows a rather comfortable treatment of unbounded domains and air gaps, whereas source terms and nonlinearities can be modelled with finite elements. In order to benefit from the advantages of both methods, BEM and FEM are coupled within a DD framework, the coupled finite and boundary element tearing and interconnecting (FETI/BETI) methods. Applying Newton's method, the spectrum of the Jacobi matrices in the nonlinear subdomains may show high variation. A special FETI preconditioner is proposed to overcome these problems.

Finally, we discuss our first numerical results obtained from the solution of a twodimensional magnetostatic problem.

## References

- U. Langer, C. Pechstein: Coupled Finite and Boundary Element Tearing and Interconnecting Methods Applied to Nonlinear Potential Problems. SFB Report 2006-01. Johannes Kepler University Linz. http://www.sfb013.uni-linz.ac.at
- [2] U. Langer, C. Pechstein: Coupled Finite and Boundary Element Tearing and Interconnecting Solvers for Nonlinear Potential Problems. Submitted to ZAMM.
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#### Duality and higher order TV-regularization

C. Pöschl Universität Innsbruck

This talk is concerned with variational scale space methods for analysis of data  $u^{\delta}$ . In particular we investigate the families of regularization methods

$$\mathcal{F}(u) := \mathcal{S}(u) + \alpha \|D^k u\| \quad (k = 1, 2, \ldots), (\alpha > 0),$$

where

- (1)  $||D^k u||$  denotes the total variation of the (k-1)-th derivative of u and
- (2)  $\mathcal{S}(u)$  is a similarity measure. Typical examples are  $\mathcal{S}(u) = \frac{1}{p} \int_{\Omega} |u u^{\delta}|^p$

Y. Meyer charakterized minimizers of the ROF-functional, where  $S(u) = \frac{1}{2} \int_{\Omega} (u - u^{\delta})^2$  and k = 1, in terms of the *G*-norm. This research has significant impact on the research in image analysis.

Moreover, exploiting the Fenchel duality concept we exemplarily derive solutions for minimizers of the ROF-functional for denoising one-dimensional data (repeating the results of Strong & Chan and Y. Meyer), the  $L^1 - BV(\Omega)$  regularization (repeating the results of Chan & Esedoglu), and also for novel metrical regularization techniques as well as regularization techniques with higher order penalization.

# Numerical Analysis for the Landau–Lifshitz Minimization Problem in Micromagnetics

#### D. Praetorius

TU Wien

The Landau-Lifshitz minimization problem in micromagnetics is to find a minimizer  $\mathbf{m}: \Omega \to \mathbb{R}^d E(\mathbf{m}) = \int_{\Omega} \phi(\mathbf{m}) dx - \int_{\Omega} \mathbf{f} \cdot \mathbf{m} dx + \frac{1}{2} \int_{\mathbb{R}^d} |\nabla u|^2 dx + \alpha \int_{\Omega} |\nabla \mathbf{m}|^2 dx$  under the side constraint  $|\mathbf{m}| = 1$ . Here,  $\Omega \subset \mathbb{R}^d$  is the spatial domain of the magnet,  $\phi$  is the anisotropy density of the material,  $\mathbf{f}$  is an applied exterior field, and u is the magnetic potential which solves the magnetostatic (Maxwell) equation in the entire space  $\mathbb{R}^d$ . For large-soft bodies, the exchange parameter  $\alpha \geq 0$  vanishes. Then, there are no classical solutions of the minimization problem, and one has to consider appropriate relaxations. One possible relaxation introduced by DESIMONE is to consider a convexified problem.

In our talk, we provide a discretization of the convexified problem, where the side constraint is replaced by a penalization strategy. Numerical aspects addressed in the presentation include a priori and a posteriori error control with a reliabilityefficiency gap and adaptive mesh-design.

### Numerical analysis for optimal control problems in nonconvex domains

A. Rösch Johann Radon Institut (RICAM), Linz

Optimal control problems have to be discretized for numerical computations. Consequently, many papers on error estimates and approximation properties of discretized optimal control problems are published in the last years. Discretization approaches with higher approximation order benefit strongly from the regularity of the optimal solution. Therefore, such approaches have to be adapt to nonconvex domains. We generalize here results of the superconvergence approach by Meyer and Rösch [1]. The corner singularities are treated by a-priori mesh grading such that we are able to prove results of the same quality as in the case of regular solutions. Numerical experiments are presented at the end of the talk. This is a joint work with Thomas Apel and Gunter Winkler from Munich.

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## Tangential–Displacement and Normal–Normal–Stress Continuous Mixed Finite Elements for Elasticity

J. Schöberl, <u>A. Sinwel</u>

Johann Radon Institut (RICAM), Linz

We introduce finite elements to approximate the Hellinger–Reissner formulation of elasticity. For the displacements, we use vector–valued, tangential continuous Nedelec elements, whereas we use symmetric, tensor–valued, normal–normal continuous elements for the stresses. These elements are suitable for nearly incompressible materials, where the Poisson ratio tends to 1/2. Also they do not suffer from shear locking when anisotropic elements are used.

We present the analysis of these elements. We see that the discrete system satisfies a stability condition without need for further stabilization. We discuss the implementation of the new elements, and give numerical results.

## Exponential splitting for parabolic problems

M. Thalhammer Universität Innsbruck

Recent advances in numerical linear algebra enable the efficient calculation of the matrix exponential and related functions, also for matrices of large dimension. As a consequence, exponential integration methods are presently attracting a lot of research interest. In particular, they show a favourable behaviour in the time integration of hyperbolic and parabolic initial-boundary value problems and therefore provide an alternative to established schemes.

In this talk, I will consider an exponential splitting method for parabolic problems and study its error behaviour. For the theoretical investigation of the time integration method, it is useful to employ the abstract framework of analytic semigroups, which will be reviewed in brief.

# Adaptive space-time finite element methods for parabolic optimization problems

B. Vexler

Johann Radon Institut (RICAM), Linz

In this talk we discuss a posteriori error estimates for space-time finite element discretization of parabolic optimization problems. The provided error estimates assess the discretization error with respect to a given quantity of interest and separate the influence of different parts of the discretization (time, space, and control discretization). This allows to set up an efficient adaptive algorithm which successively improves the accuracy of the computed solution by construction of locally refined meshes for time and space discretizations.

#### High Order Nédélec Elements for Electromagnetic Field Computation

# <u>S. Zaglmayr</u>, J. Schöberl Johann Radon Institut (RICAM), Linz

Electromagnetic problems are formulated in the function space H(curl), which naturally contains the continuity of tangential components across sub-domains. This calls for the construction of finite elements with tangential continuity. The goal of the presented work is the efficient computation of Maxwell boundary value problems using high-order H(curl)-conforming finite elements.

In the first part, we introduce a systematic strategy for the realization of arbitrary order hierarchical (edge-,face-, and cell-based) shape functions for common element geometries. Our new approach bases on using gradients of higher-order  $H^1$ -conforming shape functions explicitely in the construction of the Nédélec shape functions. In fact this implies a local exact sequence property for each edge, face, cell, which allows arbitrary and variable polynomial degree on each edge, face, and cell.

In the second part, we focus on efficient Additive Schwarz preconditioning for  $A(u, v) = \nu(curlu, curlv) + \epsilon(u, v)$ , which occur in time-stepping methods for Maxwell's equations and in the regularized formulation of the magnetostatic boundary value problem. We show that the local complete sequence property provides robustness with respect to the parameters  $\nu, \epsilon$  even for cheap ASM-block preconditioning. We illustrate the dependency of the condition number on the polynomial degree in 3d for several block variants of ASM by numerical experiments.

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# Erschienene Preprints ab Nummer 2005/1

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