Mathematisches Forschungsinstitut Oberwolfach

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Schnelle Löser für Partielle Differentialgleichungen

June 1st – June 7th, 2003

The Oberwolfach conference gave the highly qualified basis for a variety in ongoing work and future research of fast solvers for partial differential equations. The meeting was organized by Randolph E. Bank (La Jolla, U.S.A.), Wolfgang Hackbusch (Leipzig), and Gabriel Wittum (Heidelberg).
In its focus were research in fastest numerical methods, algebraic multigrid methods, domain decompositions, convergence analysis for adaptive finite element methods, parallelization algorithms and applications. The variety of schemes and topics under the roof of fast solvers was remarkable.

Recent developments and ideas were presented and discussed in the fields of multigrid algorithms for special problems like variational inequalities or option pricing model as well as in the generalized framework of algebraic methods (cf. the contributions of D. Braess, R. D. Falgout). The topic of domain decomposition solvers and methods was covered by presented investigations in newly developed parallel adaptive meshing paradigms and hierarchical methods e.g. for diffusion problems on fractures (cf. the contribution R. E. Bank, R. Kornhuber, O. B. Widlund).
New understandings in adaptive discretization methods and Mortar elements were provided (cf. the presentation M. Dryja, B. Wohlmuth) and new proofs in the field of convergence theory, especially for smoothing and grid adaptivity, and adaptive finite element methods were widely discussed (cf. the contributions of K. Johannsen, A. Reusken, R. Stevenson, C. Wieners, J. Xu, W. Zulehner).
New trends in the growing field of wavelets and wavelet applications and in the field of sparse grids were also marked during the conference (cf. the contributions of W. Dahmen, A. Kunoth, H. Yserentant). Special attention was also on improved parallelization for reservoir simulation and fastest computation of coefficients (cf. the contribution I. Garrido, N. Neuss). Furthermore, some presentations demonstrated the great impact and the importance of numerical mathematics in practical applications especially in medical science and finance (cf. the presentation of P. Deuflhard, G. Haase, C. Reisinger).

The fruitful discussions in small groups were as important as the discussions with the very competent audience during or immediately after the presentations. The conference showed that fast solvers for partial differential equations are still an important and interesting research field with a large variety of different aspects.

Abstracts

A Domain Decomposition Solver for a Parallel Adaptive Meshing Paradigm

Randolph E. Bank (La Jolla, U.S.A)
(joint work with S. Lu)

We describe a domain decomposition algorithm for use in the parallel adaptive meshing paradigm of Bank and Holst. Our algorithm has low communication, makes extensive use of existing sequential solvers, and exploits in several important ways data generated as part of the adaptive meshing paradigm. Numerical examples illustrate the effectiveness of the procedure.

A Cascadic Multigrid Method for Variational Inequalities

Dietrich Braess (Bochum, Germany)

Obstacle problems, contact problems, and Signorini's problem are variational problems with unilateral constraints. Therefore, Schur complement methods are not the appropriate tools. When classical multigrid algorithms are used, there is also a difficulty. The variational problem on the level l is performed with a cone K_{h_l} that is not the intersection of the given cone with the linear finite element space.
We overcome this difficulty by making use of a cascadic multigrid algorithm. In this way we avoid the transfer from the fine to coarse grids. A cg-version is also considered in connection with relaxation and the smoothing procedure. Numerical results show the good performance of the algorithm.

Multigrid Algorithms for C^0 Interior Penalty Methods

Susanne C. Brenner (Columbia, U.S.A)

In this talk we discuss C^0 interior penalty methods for the model problem $\Delta^2 u - \beta \Delta u = f$ ($\beta \geq 0$). The convergence of multigrid algorithms (V, F, W and variable V-cycle) is analyzed.

Adaptive Multiscale Application of Operators

Wolfgang Dahmen (Aachen, Germany)
(joint work with A. Cohen and R. DeVore)

This talk is concerned with the adaptive application of (linear and nonlinear) operators in wavelet coordinates. There are two principal steps, namely first the reliable prediction of significant wavelet coefficients of the result of such applications from those of the input, and second the accurate and efficient computation of the significant output coefficients. Some of the main conceptual ingredients of such schemes are discussed. Moreover, we indicate how this leads to adaptive solution schemes for variational problems that can be shown to have asymptotically optimal complexity.

The Smile of the Mathematicians

Peter Deuflhard (Berlin, Germany)
(joint work with F. Zeilhofer and R. Sader)

The talk presented details of a joint project in the field of computer assisted oral and facial surgery. The task of the mathematician is (a) to help in the planning of the operation, (b) to predict the post-operative facial appearance of the individual patient and, which gave the title of the talk, also of the facial expressions – assuming the operation has been performed successfully as planned. Task (a) includes the construction of a 3D virtual patient from medical images of the real patient, which involves mathematical segmentation, 3D grid generation, and grid coarsening. On this basis, different scenarios of an operation, prescribed in detail by the surgeons, can be analyzed. Task (b) involves the numerical solution of partial differential equations: facial appearance means the solution of the Lame-Navier equation (linear and geometrically nonlinear elasticity model), smile requires additionally a detailed patient specific muscle model (from 2 up to 32 muscles). Documented predictions based on the still rather simple model turn out to agree with the actual post-operative appearance to a surprising extent (0.5 mm discrepancies only). The smile based on only two muscles seems to be realistic as well.

Neumann-Neumann method for mortar finite element discretization of elliptic problems

Maksymilian Dryja (Warsaw, Poland)

A discretization of PDEs on nonmatching triangulation is a modern approach for solving difficult differential problems, for example, with singular solutions. In the first part of talk a finite element discretization of elliptic problems with discontinuous coefficients will be discussed. For that the so-called mortar technique will be used (different triangulation in different subregions of original region where the differential problem is imposed). In the second part of talk a parallel algorithm for solving the resulting discrete problem will be designed and analyzed. It is based on a domain decomposition method and is called the Neumann-Neumann algorithm. It is proved that the method is almost optimal and very well suited for parallel computations.

On Generalizing the AMG Framework

Robert D. Falgout (Livermore, U.S.A)

In recent years, much work has been done to increase the robustness of Algebraic Multigrid (AMG) methods. The classical AMG method of Ruge and Stüben used heuristics based on properties of M-matrices. Although this algorithm works remarkably well for a wide variety of problems [3], the M-matrix assumption still limits its applicability. To address this, a new class of algorithms was developed based on multigrid theory: AMGe [1], element-free AMGe[4], and spectral AMGe [2]. All of these algorithms assume a basic framework in their construction. Namely, they assume that relaxation is a simple pointwise method, then they build the coarse-grid correction step to eliminate the so-called *algebraically smooth* error left over by the relaxation process. In the AMGe methods above, this is done with the help of a *measure* (or weak-approximation property) that defines the approximation property that interpolation must satisfy in order to achieve uniform convergence assuming a pointwise relaxation. In this talk, we introduce a new measure for constructing algebraic multigrid methods. The purpose of this new measure is to generalize the AMG framework to include problems such as Maxwell's Equations, which has a particularly large null-space when discretized using the common Nédélec finite elements. In the old framework, it is necessary to take all $O(N)$ of these null-space components to the coarse grid, which results in a non-optimal method. This problem can be overcome by using something other than pointwise relaxation to damp a subspace of these near-null-space components on the fine grid. Examples include overlapping block relaxation or the so-called Hiptmair smoother (Brandt's distributive relaxation). The measure proposed here takes into account the smoothing process and changes the AMGe heuristic in a subtle but important way. The hope is that this new measure will allow us to develop AMG methods that can handle difficult problems such as Maxwell's equations or Helmholtz.

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Reservoir Simulation: Time Parallelization

Izaskun Garrido (Bergen, Norway)

We present two implicit molar mass formulations with analytical computation of the Jacobian. Besides, based on the classical Alternating Schwarz method, we also derive new time-parallel algorithms, which act as a predictor corrector improving both speed and accuracy with respect to the sequential solvers. These new algorithms reduce significantly the numerical effort for the computation of the molar masses, and we illustrate their performance with several numerical examples on our complex reservoir simulator, Athene.

Existence and Computation of a Low Kronecker-Rank Approximant to the Solution of a Tensor System with Tensor Right-Hand Side

Lars Grasedyck (Leipzig, Germany)

In the talk we construct an approximation to the solution x of a linear system of equations $Ax = b$ of tensor product structure as it typically arises for finite element and finite difference discretizations of partial differential operators on tensor grids. For a right-hand side b of tensor product structure we can prove that the solution x can be approximated by a sum of $\mathcal{O}(\log(\varepsilon)^2)$ tensor product vectors where ε is the relative approximation error. The talk closes with numerical examples for systems of size 1024^{256}.

Algebraic Multigrid in a Medical Source Identification Problem

Gundolf Haase (Linz, Austria)
(joint work with S. Reitzinger)

Solving huge systems of equations requires an optimal solver, i.e., the memory requirements and the time for solving should be proportional to the number of unknowns. Recent research has enhanced multigrid methods and algebraic multigrid methods (AMG) which are now fulfilling these requirements for many problem classes, i.e., 3D Maxwell equations. Although AMG possesses the above optimal properties a commercial user could be dissatisfied of the computational performance in comparison to highly optimized standard solvers. A lot of performance can be gained by designing data structures with respect to state-of-the-art computer architectures, parallelization and redesign of numerical algorithms.
The parallelization needs some modifications in the coarsening process such that the inter grid transfer operators fulfil a certain condition on the pattern of the interpolation/restriction. This guarantees that the parallel AMG is only a simple modification of the sequential AMG. The presented parallelization strategy for AMG results in very good speedups.
Discretized differential equations have to be solved several thousand times inside the solution process of an inverse problem. We got for this special application of AMG a significant gain in CPU time (factor 4 and more) due to additional acceleration of our code PEBBLES by simultaneous handling of several data sets, cache aware programming and by merging of multigrid subroutines. Together with a parallelization, the solution time of the original code was accelerated from 8 days to 5 hours on a 12 processor parallel computer.

SOR_a - A SOR-type smoother for strongly non-symmetric positive-definite matrices

Klaus Johannsen (Heidelberg, Germany)

Discrete systems arising from elliptic PDE's can be solved efficiently using multigrid methods. In many cases of practical importance the resulting linear equations are symmetric or weakly non-symmetric and standard multigrid components can be applied successfully. Nevertheless, strongly non-symmetric discrete problems may arise in practically relevant situations and standard multigrid components fail. We present a SOR-type smoother for strongly non-symmetric problems. In case where local mode analysis can be applied, we show the smoothing property in the Euklidian norm for a large class of positive definite matrices. The method can be extended to general positive-definite systems. Considering Finite-Element discretizations of the convection-diffusion equation numerical experiments confirm the theoretical results. In case of symmetric problems SOR_a reduces to the standard Gauss-Seidel.

Direct Schur Complement Method Based on Hierarchical Matrix Formats

Boris N. Khoromskij (Leipzig, Germany)
(joint work with W. Hackbusch and R. Kriemann)

A class of hierarchical matrices ($\mathcal{H}$-matrices) allows the data-sparse approximation to integral and more general nonlocal operators (say, the elliptic Green function and Poincaré-Steklov operators) with almost linear complexity. We consider the $\mathcal{H}$-matrix-based approximation to the Schur complement on the interface [2] corresponding to the finite element discretisation of an elliptic operator $\mathcal{L}$ in $\mathbb{R}^2$. As with the standard Schur complement domain decomposition methods, we split the elliptic inverse $\mathcal{L}^{-1}$ as a sum of local inverses associated with subdomains (this can be implemented in parallel), and the corresponding Poincaré-Steklov operator on the interface. We focus on the data-sparse approximation to the Poincaré-Steklov operator and its inverse emphasizing the following three cases: (i) Piecewise constant coefficients; (ii) Piecewise smooth coefficients; (iii) Rather general L_∞-coefficients.

In cases (i) and (ii), using the hierarchical formats based on weakened admissibility criteria (cf. [1]), we elaborate the *approximate Schur complement inverse* in an explicit form that is proved to have a linear-logarithmic cost $O(N_\Gamma \log^q N_\Gamma)$, where N_Γ is the number of degrees of freedom on the interface. We also derive the asymptotically optimal error estimate in the case of piecewise linear finite elements. In case (iii), our method manifests a linear-logarithmic complexity in the discrete problem size N_Ω.

Numerical examples confirm the almost linear cost of our direct Schur complement method. In particular, for the discrete Laplacian on 255×255 and 511×511 grids with 6×6 decomposition, we have $N_\Gamma = 2525$ and $N_\Gamma = 5085$, respectively. The elapsed CPU times to compute the explicit Schur complement inverses on the interface with the relative error $1.1e-03$ are $29.0sec$ and $74.0sec$, correspondingly (SUN 6800).

References

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Hierarchical Decomposition of Domains with Fractures

Ralf Kornhuber (Berlin, Germany)
(joint work with S. Gebauer and H. Yserentant)

We consider a diffusion problem with strongly varying diffusion coefficients. More precisely, the diffusion k_0 in a subdomain consisting of a network of fractures is much larger than it is in the remaining porous matrix. The network of fractures consists of long thin rectangles with width ε. Such kind of problems occur not only in hydrology (where the above notions come from) but also has other applications in engineering sciences or medicine. The main difficulty in constructing fast solvers is that the permeability k_0 may become arbitrary large while the width $\varepsilon > 0$ may become arbitrary small.

In order to reduce the degrees of freedom, we use an anisotropic quadrilateral partition of the network of fractures while the porous matrix is partitioned in the usual way by isotropic triangles. For the resulting discrete problem we present an hierarchical domain decomposition algorithm with appropriate multigrid solvers for the subproblems. It turns out that under reasonable assumptions on the mesh parameters our algorithm converges robustly for arbitrary large permeability k_0 and vanishing width ε. These theoretical findings are illustrated by numerical computations.

(Adaptive) Wavelet Methods for Control Problems with PDE Constraints

Angela Kunoth (Bonn, Germany)
(joint work with C. Burstedde and W. Dahmen)

For the fast numerical solution of a control problem governed by a stationary PDE with distributed or Neumann boundary control, an adaptive algorithm is proposed based on wavelets. A quadratic cost functional involving different norms of the state and the control is to be minimized subject to constraints in weak form. Placing the problem into the framework of (biorthogonal) wavelets allows to formulate the functional and the constraints equivalently in terms of sequence norms of wavelet expansion coefficients and constraints in form of an automorphism. The resulting first order necessary conditions are then derived as a (still infinite) weakly coupled system of equations. We investigate numerically the choice of different equivalent norms in the cost functional. It will be seen that including Gramian matrices positively influence the quality of the solution.
Once this system is obtained, the machinery developed by Cohen, Dahmen and DeVore can be employed for the design of an adaptive method which can be interpreted as an inexact gradient method. In each iteration step the primal and the dual system needs to be solved up to a prescribed accuracy. In particular, we show that the adaptive algorithm is asymptotically optimal, that is, the convergence rate achieved for computing the solution up to the target tolerance is asymptotically the same as given by the wavelet-best N -term approximation of the solution, and the total computational work is proportional to the number of unknowns.

An Algebraic Convergence Theory for Primal and Dual Substructuring Methods by Constraints

Jan Mandel (Denver, U.S.A)
(joint work with C. R. Dohrmann, S. and R. Tezaur)

We formulate the FETI-DP and BDDC substructuring methods in a common framework as methods based on general inter-substructure constraints, and provide a simplified convergence theory. The basic blocks of the implementations are common to both methods. Algebraic condition number bounds are provided in terms of the matrices of the problem and the method, and the bounds for BDDC are reduced to those for FETI-DP. The algebraic bounds imply the usual polylogarithmic bounds for finite elements, independent of coefficient jumps between substructures. Computational experiments confirm that the methods perform similarly and show that in fact their spectra of the preconditioned operator are same.

Fast computation of effective coefficients

Nicolas Neuss (Heidelberg, Germany)

In natural and engineering sciences people are often interested in determining effective parameters. In this talk we consider the calculation of such parameters in the case of media with periodic micro structure. The essential part of such calculations is the numerical solution of a cell problem which is defined either on the unit cube or on a semi-infinite boundary cell. The solution to this cell problem is smooth such that a fast numerical approximation requires the use of high-order finite elements. Additionally, the so-called blending technique has to be used for approximating smooth boundaries and interfaces.
Multigrid is used for solving the arising linear systems. A special ingredient is the smoothing with a vertex-centred block Gauss-Seidel smoother which is shown to be robust with respect to the discretization order p.
Using this method we can compute effective constants very fast and with high precision. For this purpose, we used the the PDE tool box "Femlisp" which is written completely in the AI language Common Lisp. Essential advantages compared with traditional languages like C, C++ or Fortran are the interactive development environment, automatic memory management, dynamic typing, compilation at runtime, and dynamic object-oriented programming.

Multigrid Methods for Option Pricing Problems on Sparse Grids

Christoph Reisinger (Heidelberg, Germany)

The distribution of a diffusion process is given by the solution of a parabolic equation. If the process is bounded, reversion conditions hold and the corresponding PDE degenerates at the boundary. This raises questions about the regularity of the solution and challenges the numerical method to find it.
A very relevant and widely studied example of such a multi-dimensional state space consists of financial assets, frequently depending on several parameters that are not directly observable on the market and stochastic themselves. The price of an option on a claim depending on such risky assets can then be seen as its expectation under a risk neutral measure.
The governing equations are often high-dimensional, but very diffusive such that they have smooth solutions, which can be well represented on sparse grids. We will focus on the solution of the linear systems that constitute the sparse grid combination technique. In addition to the specific anisotropic behaviour at the boundary we have to cope with strongly stretched grids then. We test the robustness of multi-dimensional plane smoothers with respect to linear complexity of the algorithm. This is essential if we want to take advantage of the inherent parallelism of the combination technique, since we need to have a good a priori estimate of the solution time when we distribute the grids to the processors.
Most traded options, moreover, allow early exercise. This poses an optimal stopping time problem, which translates into a linear complementarity problem in the PDE context. We infer the above strategies to this type of variational inequalities and obtain comparable results as in the linear case.

Convergence analysis of multigrid for convection diffusion equations

Arnold Reusken (Aachen, Germany)

In this talk we present a convergence analysis of a multigrid solver for a system of linear algebraic equations resulting from the discretization of a convection-diffusion model problem using the streamline diffusion finite element method. The multigrid method is based on canonical inter-grid transfer operators, a "direct discretization" approach for the coarse-grid operators and a smoother of line-Jacobi type. A robust (diffusion and h-independent) bound for the contraction number of the two-grid method and the multigrid W-cycle are proved for a special class of convection-diffusion problems, namely with Neumann conditions on the outflow boundary, Dirichlet conditions on the rest of the boundary and a flow direction that is constant and aligned with grid-lines. Our convergence analysis is based on modified smoothing and approximation properties. The arithmetic complexity of one multigrid iteration is optimal up to a logarithmic term.

Lattice equations

Stefan Sauter (Zürich, Switzerland)

Lattice equations have many applications in structural mechanics especially for lightweight constructions. In our talk, we present the stability analysis of the equations of elasticity on embedded graphs. We will prove sufficient and necessary conditions for stability.
In the second part of the talk we will present the "Recovery Method" for solving the lattice equations. The idea is to transform by a local energy matching principle the lattice equations to a partial differential equation along with a standard finite element discretisation. We prove the equivalence of the resulting energies.

An optimal adaptiv finite element method

Rob Stevenson (Utrecht, Netherland)

We present an adaptive finite element method for solving second order elliptic equations which is (quasi-)optimal in the following sense: If the solution is such that for some $s > 0$, the errors in energy norm of the best continuous piecewise linear approximations subordinate to any partition with N triangles are $O(N^{-s})$, then given an $\epsilon > 0$, the adaptive method produces an approximation with an error less than ϵ subordinate to a partition with $O(\epsilon^{-1/s})$ triangles, taking only $O(\epsilon^{-1/s})$ operations. Our method is based on ideas from [Binev, Dahmen and DeVore '02], who added a coarsening routine to the method from [Morin, Nochetto and Siebert '00]. Differences are that we employ non-conforming partitions, our coarsening routine is based on a transformation to a wavelet basis, all our results are valid uniformly in the size of possible jumps of the diffusion coefficients, and that we allow more general right-hand sides. All tolerances in our adaptive method depend on a posteriori estimate of the current error instead an a priori one, which can be expected to give quantitative advantages.

Comparison of deflation and coarse grid correction

Pieter Wesseling (Delft, Netherland)
(joint work with R. Nabben and C. Vuik)

Let $Ax = b$ ($A \in R^n$, SPD) be a linear system arising from discretization of a partial differential equation. Let the columns of an n-by-r matrix Z span a r-dimensional subspace. Suitable subspaces may arise from coarse grid correction in domain decomposition, or be chosen on physical grounds; how to do this in problems with large jumps in coefficients is discussed in Vuik et al., Ap. Num. Math. 41:219, 2002. Whatever Z may be, in order to accelerate convergence of iterative methods one may use Z for coarse grid correction or for deflation. Define $E = Z'AZ$, $P_d = I - AZE^{-1}Z'$, $P_c = I + ZE^{-1}Z'$. P_d and P_c are the deflation and the coarse grid preconditioner, respectively; the latter is of additive Schwarz type. Of course, in addition further preconditioners may be applied in both cases. It is shown theoretically that P_d is a better preconditioner than P_c. Numerical experiments confirm this.

Dual-Primal FETI Algorithms for Linear Elasticity

Olof B. Widlund (New York, U.S.A)
(joint work with A. Klawonn)

The FETI algorithms form one of three families of domain decomposition methods that have been implemented and severely tested on the very largest existing parallel computer systems; the other two are the Balancing Neumann- Neumann methods and the Overlapping Schwarz methods with at least two levels.
The analysis of the FETI methods has posed a very real challenge but by now a coherent theory has emerged. Algorithmically and theoretically, the main research emphasis is now on the Dual-Primal FETI methods. Previous theoretical work on scalar elliptic problems, such as those arising in heat conduction in highly heterogeneous materials, has recently been extended to linear compressible elastic materials with the goal of obtaining convergence rates of the iteration which are independent of even large changes in the Lame parameters across the interface between the subdomains. At the same time, it is important to keep the cost related to the coarse global problem of the preconditioner, which is required to ensure scalability, small. There are also interesting problems of numerical linear algebra related to these algorithms.
The authors acknowledge the importance of a series of conversations with Charbel Farhat, Michel Lesoinne, and Kendall Pierson for the development of the results.

Local multigrid analysis

Christian Wieners (Erlangen, Germany)

In the context of the multilevel analysis by Bramble-Pasciak-Xu local multigrid methods can be analyzed. This requires a fully nested and conforming setting, which is not satisfied in many applications. Therefore, we are interested in a local multigrid analysis based on the classical splitting in approximation property and smoothing property.
Motivated by numerical experiments, we observe for a two-level method with local smoothing in a non-Galerkin setting an improvement by multiple smoothing (in the regular case $O(1/m)$) up to some saturation for the convergence rate given by a multiplicative overlapping Schwarz method with exact solving on the global coarse mesh and local fine mesh.

An appropriate convergence analysis is presented which leads in the nested case to the estimate of the spectral radius of the two-level method

$$\rho((id - R_j Q_j A_j)^m (id - I_j^*)) \leq \sqrt{1 - 1/C_P^2} + \frac{C_{B,\beta}^2 C_R^\beta}{m^\beta}$$

depending on the number of smoothing step m and the regularity parameter β. Furthermore, C_P estimates the overlapping Schwarz method, $C_{B,\beta}$ and C_R are estimates corresponding to approximation property and smoothing property, respectively.

A γ-cycle multigrid method for Mortar finite elements

Barbara Wohlmuth (Stuttgart, Germany)

Mortar methods, based on dual Lagrange multipliers, provide a flexible tool for the numerical approximation of partial differential equations. The associated finite element spaces are, in general, nonconforming and non-nested. Optimal multigrid results have previously been established for $\mathcal{W}$-cycle and the variable $\mathcal{V}$-cycle multigrid methods.
In this talk, we introduce a new multigrid method based on a nested sequence of modified mortar spaces for which we can establish level independent $\mathcal{V}$-cycle convergence. To obtain nested mortar spaces, we apply a product form of certain corrections at the interfaces. Numerical results demonstrate the efficiency of the resulting multigrid solver.

Multilevel techniques for grid adaptation

Jinchao Xu (Penn State, U.S.A)

Some recent studies are reported in this talk on using multilevel techniques in grid adaptation. Results presented include gradient and Hessian recovery schemes by using averaging and smoothing (as in multigrid), interpolation error estimates for both isotropic and anisotropic grids and multilevel techniques for global grid moving and local grid refining/moving. Some applications will also be given.

A theoretical justification of sparse grids methods for the solution of the electronic Schrödinger equation

Harry Yserentant (Tübingen, Germany)

The electronic Schrödinger equation describes the motion of electrons under Coulomb interaction forces in the field of clamped nuclei and forms the basis of quantum chemistry. The talk was concerned with the regularity properties of the corresponding wavefunctions that are compatible with the Pauli principle. It was shown that these solutions possess certain square integrable mixed weak derivatives of order up to $N+1$ with N the number of electrons. The result mathematically substantiates approximation methods that are based on the idea of sparse grids or hyperbolic cross spaces. It lets expect that such schemes represent a promising alternative to current methods for the solution of the electronic Schrödinger equation like Hartree-Fock methods or density functional theory and that it could even become possible to reduce the computational complexity of an N–electron problem to that of a one-electron or a two-electron problem.

On kernel–preserving Schwarz-type smoothers for saddle point problems

Walter Zulehner (Linz, Austria)
(joint work with Joachim Schöberl)

Iterative methods which keep some problem–dependent subspace invariant have been proven to be appropriate smoothers for multigrid methods. The Braess–Sarazin smoother for saddle point problems belongs to this class, where the invariant subspace is the kernel of the operator describing the constraints. Performing one step of this iterative method, however, requires the accurate solution of some global linear system for the dual variables. Another iterative method with invariant subspace has been proposed by Joachim Schöberl for parameter dependent elliptic problems and the limiting saddle point problem. If this smoother is accompanied with some specific (kernel–preserving) prolongation robust multigrid convergence results were shown by Schöberl. The smoother as well as the prolongation can be realized by solving a number of local problems.
In this talk it will be shown that multigrid convergence can also be achieved for standard prolongation and local kernel–preserving smoothers for saddle point problems.

Edited by Jens Eberhard

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