Mathematisches Forschungsinstitut Oberwolfach

Report No. 24/2005

Schnelle Löser für partielle Differentialgleichungen

Organised by
Randolph E. Bank (La Jolla)
Wolfgang Hackbusch(Leipzig)
Gabriel Wittum (Heidelberg)

May 22nd – May 28th, 2005

Abstract. The workshop *Schnelle Löser für partielle Differentialgleichungen*, organised by Randolph E. Bank (La Jolla), Wolfgang Hackbusch(Leipzig), Gabriel Wittum (Heidelberg) was held May 22nd - May 28th, 2005. This meeting was well attended by 47 participants with broad geographic representation from 9 countries and 3 continents. This workshop was a nice blend of researchers with various backgrounds.

Mathematics Subject Classification (2000): 65N55, 65M55, 65M60, 65N30, 65N50, 65F10, 65F50, 65H10, 65K10.

Introduction by the Organisers

The conference was organized by Randolph E. Bank, UCSD, La Jolla, Wolfgang Hackbusch, MPI Leipzig, and Gabriel Wittum, University of Heidelberg. This was the fourth one in a series of conferences on fast solvers held at Oberwolfach since 1999. The idea of these workshops is to bring together experts from the different thriving areas of solvers and offer a platform for scientific exchange and progress. The field of solvers for the algebraic systems arising from the discretization of partial differential equations has developed to a major area of numerical mathematics and scientific computing. Solvers are an essential part of simulation codes for problems from science and technology, in many cases determining the complexity of the whole simulation. By virtue of that, the choice of the solver can decide on the realiability of a simulation and if it can be done at all. Thus, solvers are a substantial mathematical component of most simulation tools and a major contribution of mathematics to quite a lot of applied disciplines. This has increased

the interest in mathematics of colleagues from the applied sciencies over the last decade substantially.
Major areas of solvers represented at the workshop are: Multigrid methods, H-matrices, domain decomposition methods, and conjugate gradient methods. Often these methods are combined, e.g. multigrid is mostly used as a preconditioner nowadays. Besides that, several talks were given on other aspects of solving partial differential equations, such as discretization schemes and the algebraic properties of the resulting stiffness matrices, overall solution strategies, and application areas where solving plays a crucial rôle. A total of 27 presentations gave a nice overview over the current research, open problems and new developments. Intense discussions provided the opportunity to go into details of novel algorithms and approaches.
In multigrid methods, a lot of research is going in the direction of developing robust methods for special applications. This is a challenging topic requiring mathematical expertise as well as understanding of the model and the application process itself. Another major topic is Algebraic Multigrid. AMG methods are already wide spread in several applied communities. However, a lot of open problems remains and the final algorithm is not yet in sight. Several talks also were related to performance issues of multigrid on certain computer architectures such as super scalar or parallel computers. Multigrid research is thriving more than ever.
A whole bunch of talks were about domain decomposition methods. These methods are of particular interest for multiphysics problems and parallelization issues. Several new developments have been reported and discussed, giving interesting future perspectives. Often techiques from domain decomposition analysis can be used to analyze other methods e.g. multigrid. A novel technique useful together with domain decomposition and multigrid, but can also stand on its own, are hierarchical matrices (H-matrices). Here, several talks have shown the impressive level of development these methods already have since their introduction in 1998. Further talks have discussed solver techniques for application problems e.g. low Mach-number flow or electromagnetics. as well as other problem areas like optimization. Moreover, talks about novel techniques like meshless methods and several other solver techniques have been given.
In total, the workshop was very successful in bringing together international-level experts from different areas and disciplines. Meanwhile, the Oberwolfach workshop on *Schnelle Löser für partielle Differentialgleichungen* is established as major event in the solver community and a mainstay for novel developments.

Workshop: Schnelle Löser für partielle Differentialgleichungen

Table of Contents

Abstracts

Analysis of a finite PML approximation to a Maxwell's scattering problem

J.H. Bramble
(joint work with J.E. Pasciak)

We consider the frequency domain Maxwell scattering problem

$$
\begin{aligned}
&-\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\boldsymbol{E}+k^2\boldsymbol{E}=\mathbf{0} \text{ in } \Omega^c,\\
&\boldsymbol{n}\times\boldsymbol{E}=\boldsymbol{n}\times\boldsymbol{g} \text{ on } \partial\Omega,\\
&\lim_{\rho\to\infty}\rho((\boldsymbol{\nabla}\times\boldsymbol{E})\times\hat{\boldsymbol{x}}-ik\boldsymbol{E})=\mathbf{0}.
\end{aligned}
\tag{1}
$$

Here Ω is a bounded domain in $\mathbb{R}^3$, $\rho=|\boldsymbol{x}|$, and $\hat{\boldsymbol{x}}=\boldsymbol{x}/\rho$. In this talk, we will consider approximations to (1) using a truncated domain perfectly matched layer (PML).

Recently, there has been intensive computational and theoretical research toward understanding the properties of PML approximations. The research into the computational aspects of these methods is the subject of many papers in the engineering literature and we shall not attempt to discuss them here. The original PML method was suggested by Bérenger in [2] and [1]. The observation that a PML method could be considered as a complex change of variable was made by Chew and Weedon [4]. Using this technique, Collino and Monk [5] derived PML equations based on rectangular and polar coordinates. There, they also showed the existence and uniqueness of solutions of the truncated acoustic PML except for a countable number of wave numbers. The formulation of PML equations for (1) in spherical coordinates can be found in [8]. Lassas and Sommersalo [6] proved the existence and uniqueness of the PML acoustic approximation on a truncated domain where the outer boundary was circular. In a later paper [7], they extended these results to smooth convex domains in $\mathbb{R}^n$.

To date, there has been relatively little analysis of the truncated electromagnetic PML equations. In this talk we describe a new analytical approach the study of the electromagnetic PML equation.

Following [6], we use a transitional layer based on spherical geometry which results in a constant coefficient problem outside the transition. As discussed in [4, 5], the PML problem can be viewed as a complex coordinate transformation. Given σ_0, r_1, and r_2, with Ω contained in the ball of radius r_1 and $r_1 < r_2$, we start with a function $\widetilde{\sigma}\in C^2(\mathbb{R}^+)$ satisfying

$$
\begin{aligned}
&\widetilde{\sigma}(\rho)=0 \quad \text{for } 0\le\rho\le r_1,\\
&\widetilde{\sigma}(\rho)=\sigma_0 \quad \text{for } \rho\ge r_2,\\
&\widetilde{\sigma}(\rho) \text{ increasing for } \rho\in(r_1,r_2).
\end{aligned}
$$

Following [8], we define

$$\tilde{\rho} = \rho(1 + i\widetilde{\sigma}) \equiv \rho\widetilde{d}$$

The PML solution is developed as follows. Away from the scatterer, the solution of (1) can be expanded in a series of Hankel functions, i.e.,

$$\boldsymbol{E} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \boldsymbol{a}_{n,m} h_n^1(k\rho) Y_n^m(\theta, \phi), \quad \text{for } \rho \geq r_1.$$

Here $h_n^1(r)$ are spherical Bessel functions of the third kind (Hankel functions) and Y_n^m are spherical harmonics (see, e.g., [8] for details). The (infinite domain) PML solution is defined by

$$\widetilde{\boldsymbol{E}} = \begin{cases} \boldsymbol{E}(\boldsymbol{x}) \quad \text{for } |\boldsymbol{x}| \leq r_1, \\ \displaystyle\sum_{n=1}^{\infty} \sum_{m=-n}^{n} \boldsymbol{a}_{n,m} h_n^1(k\tilde{\rho}) Y_n^m(\theta, \phi), \\ \qquad \text{for } \rho = |\boldsymbol{x}| \geq r_1. \end{cases}$$

By construction $\widetilde{\boldsymbol{E}}$ and $\boldsymbol{E}$ coincide on Ω_1. Furthermore, the complex shift in the argument of h_n^1 above guarantees exponential decay of $\widetilde{\boldsymbol{E}}$.

It turns out that $\widetilde{\boldsymbol{E}}$ satisfies Maxwell's equations using the spherical coordinates $(\tilde{\rho}, \theta, \phi)$ [8]. More precisely,

$$\begin{aligned} -\widetilde{\boldsymbol{\nabla}} \times \widetilde{\boldsymbol{\nabla}} \times \widetilde{\boldsymbol{E}} + k^2 \widetilde{\boldsymbol{E}} &= \boldsymbol{0} \text{ in } \Omega^c, \\ \boldsymbol{n} \times \widetilde{\boldsymbol{E}} &= \boldsymbol{n} \times \boldsymbol{g} \text{ on } \partial\Omega, \\ \widetilde{\boldsymbol{E}} &\text{ bounded at } \infty. \end{aligned} \tag{2}$$

For $\widetilde{\boldsymbol{E}}$ expanded in spherical coordinates,

$$\widetilde{\boldsymbol{E}} = \widetilde{\boldsymbol{E}}_\rho \boldsymbol{e}_\rho + \widetilde{\boldsymbol{E}}_\theta \boldsymbol{e}_\theta + \widetilde{\boldsymbol{E}}_\phi \boldsymbol{e}_\phi,$$

we have

$$\begin{aligned} \widetilde{\boldsymbol{\nabla}} \times \widetilde{\boldsymbol{E}} = {} & \frac{1}{\tilde{\rho} \sin\theta} \left(\frac{\partial}{\partial\theta} (\sin\theta\, \widetilde{\boldsymbol{E}}_\phi) - \frac{\partial \widetilde{\boldsymbol{E}}_\theta}{\partial\phi} \right) \boldsymbol{e}_\rho \\ & + \frac{1}{\tilde{\rho}} \left(\frac{1}{\sin\theta} \frac{\partial \widetilde{\boldsymbol{E}}_\rho}{\partial\phi} - \frac{\partial}{\partial\tilde{\rho}} (\tilde{\rho} \widetilde{\boldsymbol{E}}_\phi) \right) \boldsymbol{e}_\theta \\ & + \frac{1}{\tilde{\rho}} \left(\frac{\partial(\tilde{\rho} \widetilde{\boldsymbol{E}}_\theta)}{\partial\tilde{\rho}} - \frac{\partial \widetilde{\boldsymbol{E}}_\rho}{\partial\theta} \right) \boldsymbol{e}_\phi. \end{aligned}$$

Since the solution of (2) coincides with that of (1) on Ω_1 while rapidly decaying as ρ tends to infinity, it is natural to truncate to a finite computational domain Ω_∞ and impose a convenient boundary condition on the outer boundary of Ω_∞ (which we denote by Γ_∞). The truncated domain need only have a minimally smooth outer boundary (e.g., Lipschitz continuous).

We consider the truncated PML problem involving a vector function $\widetilde{\boldsymbol{E_t}}$ defined on Ω_∞ and satisfying

$$
\begin{aligned}
-\widetilde{\boldsymbol{\nabla}} \times \widetilde{\boldsymbol{\nabla}} \times \widetilde{\boldsymbol{E_t}} + k^2 \widetilde{\boldsymbol{E_t}} &= \mathbf{0} \text{ in } \Omega_\infty, \\
\boldsymbol{n} \times \widetilde{\boldsymbol{E_t}} &= \boldsymbol{n} \times \boldsymbol{g} \text{ on } \partial\Omega, \\
\boldsymbol{n} \times \widetilde{\boldsymbol{E_t}} &= \mathbf{0} \text{ on } \Gamma_\infty.
\end{aligned} \tag{3}
$$

The existence and uniqueness of solutions to the truncated PML problem (3) will be shown provided that the truncated domain is sufficiently large, e.g., contains a sphere of radius R_t. Specifically, we keep the PML transition layer fixed while increasing the size computational domain.

To show uniqueness we consider a weak problem which is related to (3), specifically, we consider $\boldsymbol{\Theta} \in \boldsymbol{H}_0(\mathbf{curl})(\Omega_\infty)$ satisfying

$$
\begin{aligned}
-(\boldsymbol{\mu}^{-1} \boldsymbol{\nabla} \times \boldsymbol{\Theta}, \boldsymbol{\nabla} \times \boldsymbol{\Psi})_{\Omega^c} \\
+ k^2 (\boldsymbol{\mu}\boldsymbol{\Theta}, \boldsymbol{\Psi}) = 0
\end{aligned} \tag{4}
$$

for all $\boldsymbol{\Psi} \in \boldsymbol{H}_0(\mathbf{curl})(\Omega_\infty)$. We prove the following theorem.

Theorem 0.1. *For R_t sufficiently large, the only solution $\boldsymbol{\Theta} \in \boldsymbol{H}_0(\mathbf{curl})(\Omega_\infty)$ satisfying (4) is $\boldsymbol{\Theta} = \mathbf{0}$.*

The existence of solutions is not a simple matter even when uniqueness has been verified. To show the existence of solutions of (3), we consider a related div-curl formulation. This involves setting up a variational formulation for a pair of vectors $(\boldsymbol{e}, \boldsymbol{h})$ satisfying two connected div-curl systems. This is a weak formulation where $\boldsymbol{e}$ and $\boldsymbol{h}$ are sought in $\boldsymbol{L}^2(\Omega_\infty)$ and are tested against functions in various vector and scalar subspaces of $H^1(\Omega_\infty)$ similar to the approach of [3]. This approach allows us to prove the following two theorems:

Theorem 0.2. *Let $\boldsymbol{g}$ admit an $\boldsymbol{H}(\mathbf{curl}; \Omega_\infty)$-extension $\widehat{\boldsymbol{g}}$ supported in Ω_1 (the ball of radius r_1 minus Ω). Then for R_t sufficiently large, the truncated PML problem (3) has a unique solution $\widetilde{\boldsymbol{E_t}}$.*

Theorem 0.3. *Let $\widetilde{\boldsymbol{E}}$ be the solution of (2) and $\widetilde{\boldsymbol{E_t}}$ be the solution of (3). For R_t sufficiently large,*

$$
\|\widetilde{\boldsymbol{E_t}} - \widetilde{\boldsymbol{E}}\|_{\boldsymbol{L}^2(\Omega_3)} \leq C e^{-2\sigma_0 k R_t} \|\widehat{\boldsymbol{g}}\|_{\boldsymbol{H}(\mathbf{curl};\Omega_1)}.
$$

Here Ω_3 is a ball of radius r_3 minus Ω for any fixed r_3 (Ω_3 can include the transition region, i.e., $r_3 > r_2$).

References

[1] J.-P. Berenger. A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, 114(2):185–200, 1994.

[2] J.-P. Berenger. Three-dimensional perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, 127(2):363–379, 1996.

[3] J. H. Bramble, T. V. Kolev, and J. E. Pasciak. A least-squares method for the time-harmonic Maxwell equations. 2003. preprint.

[4] W. Chew and W. Weedon. A 3d perfectly matched medium for modified Maxwell's equations with streched coordinates. *Microwave Opt. Techno. Lett.*, 13(7):599–604, 1994.
[5] F. Collino and P. Monk. The perfectly matched layer in curvilinear coordinates. *SIAM J. Sci. Comp.*, 19(6):2061–2090, 1998.
[6] M. Lassas and E. Somersalo. On the existence and convergence of the solution of PML equations. *Computing*, 60(3):229–241, 1998.
[7] M. Lassas and E. Somersalo. Analysis of the PML equations in general convex geometry. *Proc. Roy. Soc. Edinburgh Sect. A*, 131(5):1183–1207, 2001.
[8] P. Monk. *Finite Element Methods for Maxwell's Equations*. Numerical Mathematics and Scientific Computation. Oxford University Press, Oxford, UK, 2003.

Optimality of a standard adaptive finite element method

Rob Stevenson

Adaptive finite element methods for solving elliptic boundary value problems have the potential to produce a sequence of approximations to the solution that converges with a rate that is optimal in view of the polynomial order that is applied, also in the, common, situation that finite element approximations with respect to uniformly refined partitions exhibit a reduced rate due to a lacking (Sobolev) regularity of the solution. The basic idea of an adaptive finite element method is, given some finite element approximation, to create a refined partition by subdividing those elements where local error estimators indicate that the error is large, and then, on this refined partition, to compute the next approximation, after which the process can be repeated. Although, because of their success in practice, during the last 25 years the use of these adaptive methods became more and more widely spread, apart from results in the one-dimensional case by Babuška and Vogelius ([1]), their convergence was not shown before the work by Dörfler ([6]), that was later extended by Morin, Nochetto and Siebert ([7]).

Although these results meant a break through in the theoretical understanding of adaptive methods, they do not tell anything about the rate of convergence, and so, in particular, they do not show that adaptive methods are more effective than, or even competitive with non-adaptive ones in the situation that the solution has a lacking regularity.

Recently, in [2], Binev, Dahmen and DeVore developed an adaptive finite element method which they showed to be of optimal computational complexity. Whenever for some $s > 0$, the solution is in the approximation class $\mathcal{A}^s$, meaning that there exists a sequence of partitions of the domain into n elements such that the best finite element approximation with respect to this partition has an error in energy norm of order n^{-s}, then the adaptive method produces a sequence of approximations that converge with the same rate, where, moreover, the cost of computing such an approximation is of the order of the number of elements in the underlying partition. A combination of the (near) characterization of $\mathcal{A}^s$ in terms of Besov spaces from [3], and Besov regularity theorems from [5, 4], indicate that under very mild conditions the value of s is indeed only restricted by the polynomial order. An additional condition was required on the right-hand side, the discussion of which we postpone to the end of this abstract.

The key to obtain the optimal computational complexity result was the addition of a so-called coarsening or derefinement routine to the method from [7], that has to be applied after each fixed number of iterations, as well as, in view of the cost, to replace the exact Galerkin solvers by inexact ones. Thanks to the linear convergence of the method from [7], and the fact that after this coarsening, the underlying partition can be shown to have, up to some constant factor, the smallest possible cardinality in relation to the current error, optimal computational complexity could be shown.

The result of [2] is of great theoretical importance, but the adaptive method seems not very practical. The implementation of the coarsening procedure is not trivial, whereas, moreover, numerical results indicate that coarsening is not needed for obtaining an optimal method. In this talk, we will present a proof of this fact (see [8]). We construct an adaptive finite element method, that, except that we solve the Galerkin systems inexactly, is very similar to the one from [7], and show that it has optimal computational complexity.

As in [2, 7], we restrict ourselves to the model case of the Poisson equation in two space dimensions, linear finite elements, and partitions that are created by newest vertex bisection. Our results, however, rely on three ingredients only, two dealing with residual based a posteriori error estimators, and one dealing with bounding the number of bisections needed to find the smallest conforming refinement of a partition. The two results on a posteriori error estimators extend to more general second order elliptic differential operators, to more space dimensions, and to higher order finite elements. It can be expected that also the result about newest vertex bisection extends to more space dimensions, which, however, has to be investigated.

To solve a boundary value problem on a computer, it is indispensable to be able to approximate the right-hand side by some finite representation within a given tolerance. As (implicitly) in [7, 2], we use piecewise constant approximations, but, in particular for higher order elements, by a modification of the adaptive refinement routine, piecewise polynomial approximations of higher order can be applied as well. Our aforementioned result concerning optimal computational complexity is valid only under the additional assumption that if the solution $u \in \mathcal{A}^s$, then for any n we know how to approximate the right-hand side f by a piecewise constant function with respect to a partition of n elements such that the error in the dual norm is of order n^{-s}. For $s \in (0, \frac{1}{2}]$, which is the relevant range for piecewise linear elements, we conjecture that if $u \in \mathcal{A}^s$, then such approximations for the corresponding right-hand side exist, which, however, is something different than knowing how to construct them. For $f \in L_2(\Omega)$, however, the additional assumption is always satisfied, where for constructing the approximations of the right-hand side we may even rely on uniform refinements.

The adaptive methods from [7, 2] apply only to $f \in L_2(\Omega)$. Our additional assumption on the right-hand side is weaker than that of [2], but for $f \in H^{-1}(\Omega)$ not in $L_2(\Omega)$, it has to be verified for the right-hand side at hand.

References

[1] I. Babuška, and M. Vogelius. Feedback and adaptive finite element solution of one-dimensional boundary value problems. *Numer. Math.*, 44(1), 1984.

[2] P. Binev, W. Dahmen, and R. DeVore. Adaptive finite element methods with convergence rates. *Numer. Math.*, 97(2):219 – 268, 2004.

[3] P. Binev, W. Dahmen, R. DeVore, and P. Petruchev. Approximation classes for adaptive methods. *Serdica Math. J.*, 28:391–416, 2002.

[4] S. Dahlke. Besov regularity for elliptic boundary value problems in polygonal domains. *Appl. Math. Lett.*, 12(6):31–36, 1999.

[5] S. Dahlke and R. DeVore. Besov regularity for elliptic boundary value problems. *Comm. Partial Differential Equations*, 22(1 & 2):1–16, 1997.

[6] W. Dörfler. A convergent adaptive algorithm for Poisson's equation. *SIAM J. Numer. Anal.*, 33:1106–1124, 1996.

[7] P. Morin, R. Nochetto, and K. Siebert. Data oscillation and convergence of adaptive FEM. *SIAM J. Numer. Anal.*, 38(2):466–488, 2000.

[8] R.P. Stevenson. Optimality of a standard adaptive finite element method. Preprint No. 1329, Department of Mathematics, Utrecht University, May 2005. Submitted.

Algebraic Multigrid in an Application

Gundolf Haase

(joint work with Michael Kuhn, Stefan Reitzinger, Carsten Wolters)

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., solving the potential problem occurring in an inverse source reconstruction problem from medicine.

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 according to the pattern condition formulated in [2] such that the inter grid transfer operators fulfill 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 [1]. Together with a parallelization, the solution time of the original reconstruction problem was accelerated from 8 days to 5 hours on a 12 processor parallel computer [3].

Using the lead field basis approach to calculate the influence matrix for MEG [4] accelerates the inverse problem solving dramatically with the costs of storing a large matrix for the lead field basis. The rows of this matrix can be stored in parallel in the same way as parallel vectors in the parallelization of AMG [2]. This allows a parallelization of the inverse problem solver by routines from a toolbox.

References

[1] G. Haase and S. Reitzinger, *Cache Issues of Algebraic Multigrid Methods for Linear Systems with Multiple Right-Hand Sides*, SIAM SISC(2005), accepted for publication.

[2] G. Haase and M. Kuhn and S. Reitzinger, *Parallel AMG on Distributed Memory Computers*, SIAM SISC **24**(2) (2002), 410–427.

[3] A. Anwander and M. Kuhn and S. Reitzinger and C. Wolters *A parallel algebraic multigrid solver for finite element based source localization in the human brain* Comp. Vis. Sci., **5**(3) (2002), 165–177.

[4] C. Wolters and L. Grasedyck and W. Hackbusch, *Efficient Computation of Lead Field Bases and Influence Matrix for the FEM-based EEG and MEG Inverse Problem* Inverse Problems, **20**(4) (2004), 1099–1116.

Adjoint methods are particle methods: Implications for Eulerian-Lagrangian modeling of multiphase multicomponent transport

Thomas F. Russell

(joint work with Bjørn-Ove Heimsund, Helge K. Dahle, Magne S. Espedal)

Advection-dominated problems are notoriously difficult to solve numerically because of trade-offs between numerical diffusion and non-physical oscillations. With standard Eulerian methods, these trade-offs can often be avoided only by using impractically fine grids and small time steps. The Eulerian-Lagrangian localized adjoint method (ELLAM) [CRHE] is an efficient method originally developed for linear advection-diffusion equations. By treating advection in a Lagrangian manner via operator splitting, it has no CFL restrictions on the time step and it reduces the non-symmetry of the advection-diffusion operator. This enables accurate computations with coarser grids and larger time steps than Eulerian methods typically permit. ELLAM can be viewed as an extension of the modified method of characteristics (MMOC) [DR] that is fully mass-conservative and handles all types of boundary conditions rigorously. See [RC] and the references therein for more information.

ELLAM is often used for simulating flows in porous media, and in many types of reservoir flows strong non-linear flux functions are found, a prominent example being the Buckley-Leverett equation for two-phase immiscible flow. Problems with non-linear fluxes are computationally demanding, and efficient methods are necessary for handling large-scale cases. Work on extending ELLAM to the Buckley-Leverett equation [DER] has used particular splittings of the flux function [EE] in order to handle nonlinear features. It has not been clear how to extend ELLAM

to nonlinear systems of advection-dominated PDEs, such as those that describe multiphase multicomponent transport.

In this talk [RHDE] we make a key observation that shows the way toward extensions of adjoint-based Eulerian-Lagrangian methods, including ELLAM, to complex nonlinear systems. MMOC and related schemes introduce their Lagrangian discretization by a direct approximation of the advective part of the primal differential operator, where a common physical interpretation is in terms of propagation of waves. ELLAM works in a dual framework and demands that space-time test functions satisfy an adjoint equation that incorporates the Lagrangian velocity. *The key insight is that this adjoint operator has a natural physical interpretation in terms of propagation of particles or masses, and that this velocity is a particle velocity.*

The primal system exhibits the usual difficulties of nonlinear hyperbolic conservation laws: crossing of characteristic curves, formation of shocks, questions of well-posedness. The dual system is different: unlike primal waves that can break, dual masses do not disappear, and trailing particles do not overtake leading ones. Mathematically, this is reflected in the fact that the adjoint equation is linear, with its complexities embedded in the nonlinear dependence of its coefficients on the solution of the primal problem. Its space-time characteristics cannot cross, though their directions can change discontinuously when a primal-dependent coefficient experiences a jump, causing a discontinuous change in particle velocity.

The dual adjoint formulation is generalizable to complex transport systems, because such systems can always be viewed as propagating mass particles. In multiphase flows, these particles propagate in phases; each phase will have an adjoint equation and associated test function, and the overall formulation will superpose the phases. *The dual space is the natural framework for a particle-based formulation that always makes sense physically;* this will enable ELLAM to be extended to complex flows, whereas the applicability of MMOC-like schemes has been restricted.

This talk presents the adjoint formulation, closely related to the original linear ELLAM schemes. The approach does not involve any splitting of nonlinear flux functions. It is developed in detail for a scalar multidimensional equation, including the relationship between the primal and dual formulations. These concepts are illustrated in some examples, focusing on the interaction between the primal waves and the particle motion. Next, an algorithm for the solution of general hyperbolic 1D equations is outlined, and results are presented for the Burgers and the Buckley-Leverett equations, as well as solutions of a 2D Buckley-Leverett equation using the 1D algorithm on streamlines. Finally, the formulation for compositional petroleum reservoir simulation is outlined, involving multiphase multicomponent flow and transport.

References

[CRHE] M. A. Celia, T. F. Russell, I. Herrera, and R. E. Ewing. An Eulerian–Lagrangian localized adjoint method for the advection–diffusion equation. *Advances in Water Resources*, 13:187–206, 1990.

[DER] H. K. Dahle, R. E. Ewing, and T. F. Russell. Eulerian–Lagrangian localized adjoint methods for a nonlinear advection–diffusion equation. *Computer Methods in Applied Mechanics and Engineering*, 122:223–250, 1995.

[DR] J. Douglas, Jr., and T. F. Russell. Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures. *SIAM J. Numer. Anal.*, 19:871–885, 1982.

[EE] M. S. Espedal and R. E. Ewing. Characteristic Petrov-Galerkin subdomain methods for two-phase immiscible flow. *Comp. Meth. in Appl. Mech. and Eng.*, 64:113–135, 1987.

[RC] T. F. Russell and M. A. Celia. An overview of research on Eulerian–Lagrangian localized adjoint methods (ELLAM). *Advances in Water Resources*, 25(8–12):1215–1231, 2002.

[RHDE] T. F. Russell, B. O. Heimsund, H. K. Dahle, and M. S. Espedal. Adjoint methods are particle methods. Preprint, 2005.

A Cache oblivious adaptive parallel Multilevel Implementation of the Finite Element Method using Space filling Curves

Christoph Zenger

(joint work with Michael Bader)

Implementations of the adaptive Finite Element Method usually use vectors, tree or haching to access data. In all cases during the process of the computation the data are accessed in a nonlocal highly irregular way. As a consequence the jumps in the address space produce cache misses slowing down the execution of the program considerably. This problem gets more and more severe for modern computer architectures because processer speed grows much faster then the speed with which data are read from memory. In this paper we describe an implementation of an adaptive finite element scheme which is based on a fixed number of stacks. The data needed in the course of the computation are always read from top of one of the stacks and are later pushed to another stack for later use. The grid is based on a space tree and allows local refinement restricted by some mild conditions assuring compatibility. As a further advantage the memory overhead for the description of the geometry of the underlying domain and for the the refinement structure is very small (only a few bits per degree of freedom). Not all space filling curves are suitable for this approach. An implementation based on the Peano curve is published in [GMPZ1, GMPZ2] for two and three dimensions. In this talk we discuss an implementation based on the Sierpinski curve in two dimensions which uses only four stacks. The three dimensional analogue is under construction.

References

[GMPZ1] F. Günther, M. Mehl, M. Pögl, and C. Zenger, A cache-aware algorithm for PDEs on hierarchical data structures based on space-filling curves. SIAM Journal on Scientific Computing, in review.

[GMPZ2] F. Günther, M. Mehl, M. Pögl, Ch. Zenger, A cache-aware algorithm for PDEs on hierarchical data structures. Conference Proceedings PARA '04, Kopenhagen, June 2004, LNCS, Springer, submitted.

Heterogeneous Domain Decomposition Methods for Coupled Darcy/Stokes Flow Problems

Ronald H.W. Hoppe
(joint work with Paulo Porta, Yuri Vassilevski)

In this contribution, we consider heterogeneous domain decomposition methods for coupled surface/subsurface flow problems

$$-\boldsymbol{\nabla}\cdot\mathbf{T}(\mathbf{u}_1,p_1) = \mathbf{f}_1 \quad \text{in } \Omega_1 \,, \tag{1a}$$

$$\boldsymbol{\nabla}\cdot\mathbf{u}_1 = 0 \quad \text{in } \Omega_1 \,, \tag{1b}$$

$$\mathbf{u}_1 = \mathbf{u}_1^D \quad \text{on } \Gamma_1^D \,, \tag{1c}$$

$$\mathbf{n}_1\cdot\mathbf{T}(\mathbf{u}_1,p_1) = \mathbf{h}_1 \quad \text{on } \Gamma_1^N \,, \tag{1d}$$

$$\boldsymbol{\nabla}\cdot\mathbf{q} = \mathbf{f}_2 \quad \text{in } \Omega_2 \,, \tag{2a}$$

$$\varphi = \varphi^D \quad \text{on } \Gamma_2^D \,, \tag{2b}$$

$$\mathbf{n}_2\cdot\mathbf{q} = \mathbf{h}_2 \quad \text{on } \Gamma_2^N \,. \tag{2c}$$

Here, the equations (1a)-(1d) describe the stationary Stokes flow in the subdomain Ω_1 in terms of the velocity $\mathbf{u}_1$ and the pressure p_1 with $\mathbf{T}(\mathbf{u}_1,p_1)$ being the stress tensor. The equations (2a)-(2c) stand for the Darcy flow in the subdomain Ω_2 with $\mathbf{q}$ denoting the specific discharge vector that is related to the piezometric head φ and the velocity vector $\mathbf{u}_2$ by Darcy's law $\varepsilon\mathbf{u}_2 = \mathbf{q} = -\mathbf{K}\,\boldsymbol{\nabla}\varphi$, where ε is the porosity and $\mathbf{K}$ refers to the hydraulic conductivity tensor.

We first address the issue of mathematical modeling of coupled Darcy and Stokes flow problems with emphasis on the transmission conditions at the interface Γ between the two domains governed by the surface and the subsurface flows, respectively:

$$\mathbf{n}_1\cdot\mathbf{u}_1 + \mathbf{n}_2\cdot\mathbf{u}_2 = 0 \,, \tag{3a}$$

$$\Big(\mathbf{n}_1\cdot\mathbf{T}(u_1,p_1)\Big)\cdot\mathbf{n}_1 = g\varphi \,, \tag{3b}$$

$$\Big(\mathbf{n}_1\cdot\mathbf{T}(\mathbf{u}_1,p_1)\Big)\cdot\boldsymbol{\tau}_i = \frac{\alpha}{2\,\sqrt{(\boldsymbol{\tau}_i\cdot\boldsymbol{\kappa})\cdot\boldsymbol{\tau}_i}}\,(u_1-u_2)\cdot\boldsymbol{\tau}_i \,,\ 1\le i\le 2 \,. \tag{3c}$$

Equation (3a) states the continuity of the fluxes, whereas (3b),(3c) represent the continuity of the normal and tangential components of the normal stresses where g in (3b) stands for the gravitation acceleration modulus. In particular, (3c) is known as the Beavers-Joseph-Saffman condition [3] where $\boldsymbol{\kappa}$ is the symmetric permeability tensor and the nonnegative constant α is the slip coefficient.

We consider three solution techniques based on the variational formulation of the coupled problem and finite element discretizations with respect to simplicial triangulations of the computational domain:

The first one, which has been originally suggested by Discacciati and Quarteroni [1, 2], is an iterative substructuring approach involving a Neumann-Dirichlet type

iteration that requires $\alpha = 0$ in the Beavers-Joseph-Saffman transmission condition so that (3c) can be treated as an additional boundary condition. In particular, the ND-iteration requires the successive solution of a Neumann problem for the Darcy equation on Ω_2 and a Dirichlet problem for the Stokes system on Ω_1. In terms of associated Steklov-Poincaré operators S_1 and S_2, it can be interpreted and analyzed as a preconditioned Richardson iteration

$$\lambda^{k+1} \;=\; \lambda^k \;+\; \theta\; S_1^{-1}\Big(\eta \;-\; (S_1 + S_2)\;\lambda^k\Big)\;,\; k \geq 0\;. \tag{4}$$

Here, $\lambda^k \in \hat{H}_{00}^{1/2}(\Gamma)$, which is the subspace of functions in $H_{00}^{1/2}(\Gamma)$ with vanishing integral mean, and $0 < \theta < 1$ is an under-relaxation parameter. However, a detailed analysis shows that the applicability of the ND-iteration is limited to porous media with high conductivity, whereas it is not competitive for other types of porous media.

Therefore, in such cases we suggest a direct method which is based on the recovery of the discrete Neumann-Dirichlet iteration operator. Since the direct method in its original form is computationally costly, we focus on its practical realization by using some sort of aggregated finite element spaces by aggregation of basis functions associated with the nodal points of the triangulation of the interface.

Finally, it is possible to reduce the problem to one stated on the interface between the surface and the subsurface regime. This can be done either by relying on the continuity of the fluxes or on the continuity of the normal stresses. The first approach requires some compatibility condition which again severely limits its practical applicability. Such a compatibility condition, however, is not required for the second approach which also allows the interpretation as a preconditioned Richardson iteration, but with a somewhat reversed role of the Poincaré-Steklov operators

$$\phi_\Gamma^{k+1} \;=\; \phi_\Gamma^k + \theta\; S_2^{-1}\Big(f_2 - (S_2 + M_\lambda Q_\Gamma C^{-1} Q_\Gamma^T M_\phi)\;\phi_\Gamma^k\Big)\;,\; k \geq 0\;. \tag{5}$$

Here, C^{-1} stands for the solution of a Stokes problem on Ω_1. The FE discretized Stokes and Darcy problems are numerically solved by GMRES and PCG, respectively, whereas GMRES is also used for the interface equation to be solved in the realization of (5).

Numerical results for a benchmark problem illustrate the performance of the different approaches. As a somewhat realistic scenario, we study the simulation of the confluence of the rivers Wertach and Lech close to the city of Augsburg.

References

[1] M. Discacciati and A. Quarteroni; *Analysis of a domain decomposition method for the coupling of Stokes and Darcy equations.* Proc. Europ. Conf. on Numer. Math. and Advanced Applications, ENUMATH 2001 (F. Brezzi et al., eds.), pp. 3-20, Springer, Milano, 2003

[2] M. Discacciati and A. Quarteroni, *Convergence analysis of a subdomain iterative method for the finite element approximation of Stokes and Darcy equations.* Comp. Visual. Sci., 6, 2004

[3] W. Jäger and A. Mikelic, *On the interface boundary condition of Beavers, Joseph, and Saffman.* SIAM J. Appl. Math. 60, 1111–1127, 2000

Analysis of a Domain Decomposition Algorithm

Randolph E. Bank

In [4, 5], we introduced a general approach to parallel adaptive meshing for systems of elliptic partial differential equations. This approach was motivated by the desire to keep communications costs low, and to allow sequential adaptive software (such as the software package PLTMG [1] used in this work) to be employed without extensive recoding.

The original paradigm has three main components:

> **Step I: Load Balancing.** We solve a small problem on a coarse mesh, and use a posteriori error estimates to partition the mesh. Each subregion has approximately the same error, although subregions may vary considerably in terms of numbers of elements or gridpoints.
>
> **Step II: Adaptive Meshing.** Each processor is provided the complete coarse mesh and instructed to sequentially solve the *entire* problem, with the stipulation that its adaptive refinement should be limited largely to its own partition. The target number of elements and grid points for each problem is the same. At the end of this step, the mesh is regularized such that the global mesh described in Step III is conforming.
>
> **Step III: Global Solve.** The final global mesh consists of the union of the refined partitions provided by each processor. A final solution is computed using domain decomposition.

With this paradigm, the load balancing problem is reduced to the numerical solution of a small elliptic problem on a single processor, using a sequential adaptive solver such as PLTMG, without requiring any modifications to the sequential solver. The bulk of the calculation in the adaptive meshing step also takes place independently on each processor and can also be performed with a sequential solver with no modifications necessary for communication.

In [2], we considered a variant of the above approach in which the load balancing occurs on a much finer mesh. The motivation was to address some possible problems arising from the use of a coarse grid in computing the load balance. This variant also has three main components.

> **Step I: Load Balancing.** On a single processor we adaptively create a *fine* mesh of size N_p, and use a posteriori error estimates to partition the mesh such that each subregion has approximately equal error, similar to Step I of the original paradigm.
>
> **Step II: Adaptive Meshing.** Each processor is provided the complete adaptive mesh and instructed to sequentially solve the *entire* problem. However, in this case each processor should adaptively *coarsen* regions corresponding to other processors, and adaptively refine its own subregion. The size of the problem on each processor remains N_p, but this adaptive rezoning strategy concentrates the degrees of freedom in the processor's subregion. At the end of this step, the mesh is regularized such that the global mesh is conforming.

Step III: Global Solve. This step is the same as in the original paradigm.

Using the variant, the initial mesh can be of any size. Indeed, our choice of N_p is mainly for convenience and to simplify notation; any combination of coarsening and refinement could be allowed in Step II. Allowing the mesh in Step I to be finer increases the cost of both the solution and the load balance in Step I, but it allows flexibility in overcoming potential deficiencies of a very coarse mesh in the original paradigm. See [4, 5, 6] for numerical examples of the original paradigm and [2, 3] for examples comparing the original and variant paradigms.

Although both the original paradigm and the variant use the same domain decomposition solver in Step III, the variant algorithm produced some unforeseen consequences. In particular, in the PLTMG package, in Step II of the paradigm, edges lying on the interface system can be refined as necessary. Vertices added during refinement steps can be deleted during coarsening steps, but the original vertices defining the interface system must remain in the mesh during Steps II and III of either paradigm. This restriction insures that the subdomains remain geometrically conforming across all processors, and also plays an important role in the mesh regularization algorithm applied at the end of Step II.

This point is of little consequence for the original paradigm because it is based mainly on refinement. However, it is quite significant for the variant. Indeed, for the variant, coarsening is limited to the *interiors* of subdomains corresponding to other processors, while the parts of the interface system lying in the coarse parts of the domain remain largely unchanged. Thus in the domain decomposition solver the local problem has an unusual structure, in that it is highly refined on its own subdomain and its part of the interface system, it is very coarse in the interior of other subregions, and it has the original level of refinement on the coarse parts of the interface system.

Interestingly, and perhaps obvious with hindsight, this unusual structure significantly improved the already very good convergence rate of the domain decomposition solver. In particular, for many problems, the observed rate of convergence appears to be independent of both the global problem size N and the number of processors p, while the solver applied to meshes generated using the original paradigm (thus with less refined interface systems in the coarse region) had convergence rates that were independent of N but (empirically) exhibited a logarithmic dependence on p.

The purpose of this work is to analyze the domain decomposition solver in the environment provided by the variant paradigm. For an idealized version of the algorithm we are indeed able to show that the rate of convergence is independent of both N and p. Our analysis here is interesting for several reasons. First, the overall iteration does not have a symmetric error propagator, even in the case where the underlying continuous problem and its conforming finite element discretization are self-adjoint and positive definite. Thus we do not take an approach based on estimating generalized condition numbers, but rather make direct norm estimates for the error reduction. Second, while the approximate solution of the global

problem belongs to a usual, globally conforming, finite element space, (in our case, continuous piecewise linear finite elements on a shape regular triangulation) the domain decomposition iteration itself is based on a saddle point formulation for nonconforming finite element spaces. The Lagrange multipliers, which are used to impose continuity at vertices along the interface, have the flavor of Dirac delta functions when viewed in the finite element context. An additional complication in the analysis arises from the fact that these Lagrange multipliers are not actually computed or updated as part of the iteration.

References

[1] R. E. Bank, *PLTMG: A software package for solving elliptic partial differential equations, users' guide 9.0*, tech. report, Department of Mathematics, University of California at San Diego, 2004.

[2] R. E. Bank, *Some variants of the Bank-Holst parallel adaptive meshing paradigm*, Computing and Visualization in Science, (accepted).

[3] R. E. Bank, *A domain decomposition for a parallel adaptive meshing algorithm*, in Sixteenth International Symposium on Domain Decomposition Methods for Partial Differential Equations, Lecture Notes in Computational Science and Engineering, Springer-Verlag, to appear.

[4] R. E. Bank and M. J. Holst, *A new paradigm for parallel adaptive meshing algorithms*, SIAM J. on Scientific Computing, 22 (2000), pp. 1411–1443.

[5] R. E. Bank and M. J. Holst, *A new paradigm for parallel adaptive meshing algorithms*, SIAM Review, 45 (2003), pp. 292–323.

[6] R. E. Bank and S. Lu, *A domain decomposition solver for a parallel adaptive meshing paradigm*, SIAM J. on Scientific Computing, 26 (2004), pp. 105–127 (electronic).

Inexact Data–Sparse Boundary Element Tearing and Interconnecting

Ulrich Langer

(joint work with Günther Of, Olaf Steinbach and Walter Zulehner)

In [LSa] we have recently introduced the Boundary Element Tearing and Interconnecting (BETI) methods as boundary element counterparts of the well–established Finite Element Tearing and Interconnecting (FETI) methods which were proposed by Farhat and Roux in 1991. We refer the reader to the monograph [TW] by Toselli and Widlund for more information and references to FETI and FETI–DP methods. The coupled BETI/FETI methods were introduced in [LSb]. It is widely recognized that Boundary Element Methods (BEM) have some advantages over the Finite Element Methods (FEM) in the treatment of unbounded regions. But we can also benefit from the BEM in some other situations like in the case of large air subdomains without sources in electromagnetics or in the case of moving parts or interfaces in magnetomechanics. The coupling of BEM and FEM within a domain decomposition framework seems to be very attractive. The symmetric FEM–BEM coupling technique was originally proposed by Costabel (1987). The symmetric coupling technique was then used by Hsiao and Wendland (1991) to construct a (primal) boundary element (BE) substructuring method. Similar to

the finite element substructuring method they eliminate the interior subdomain unknowns, which are the fluxes (tractions) in the BEM, and arrive at the symmetric and positive definite boundary element Schur complement system that can be solved by a direct or an iterative method. For large–scale problems, a preconditioned conjugate gradient method should be used for efficiency reasons. However, in every iteration step, the interior boundary element subdomain unknowns must be eliminated, i.e. a discrete single layer potential must be inverted to compute the solution of a Dirichlet boundary value problem in every subdomain. To avoid the expensive elimination of these interior boundary element unknowns, an inexact boundary element substructuring method was introduced in [La] which requires the solution of a saddle point problem. The saddle point problem was solved by the preconditioned conjugate gradient method proposed by Bramble and Pasciak (1988) for solving systems of algebraic equations with symmetric, but indefinite system matrices. The availability of good preconditioners is very essential for the efficiency of the solver. In the inexact BE substructuring case preconditioners for the local (subdomain) discrete single layer potential operators and for the global (skeleton) boundary element Schur complement are needed. The latter should also provide the global information exchange. Carstensen, Kuhn and Langer proposed such preconditioners and gave a rigorous analysis of the solver in the case of dense matrices [CKL]. Inexact finite element substructuring solvers were proposed and investigated by Boergers (1989), Haase, Langer and Meyer (1990) and others. The first inexact FETI solver was introduced and analyzed by Klawonn and Widlund (2000). Let us mention that inexact versions are usually more efficient than Schur complement techniques, especially in the case of sufficiently large local subproblems. This is typical for really large scale problems. On PC clusters, also mid–size problems can benefit from inexact solution techniques.

In this talk we introduce inexact BETI methods which lead to three–fold saddle point problems in the first instance. However, applying an appropriate projection, we can reduce the three–fold saddle point problem to a two–fold saddle point problem. Following the approach given in [Zu], we present preconditioned Krylov subspace solution methods for two–fold saddle point problems and give sharp convergence rate estimates. The standard boundary element discretization of boundary integral operators with nonlocal kernel functions would lead to fully populated matrices. This is totally unacceptable for 3D boundary value problems. Indeed, already the matrix–by–vector multiplication costs $\mathcal{O}(N_h^2)$ arithmetical operations in the case of dense matrices. Here N_h denotes the number of boundary unknowns which is of the order $\mathcal{O}(h^{-(d-1)})$, where h denotes the usual mesh size parameter and d is the spatial dimension ($d = 2$, or $d = 3$). The same complexity is required for the storage demand. Data–sparse approximations of the system matrix, such as multipole techniques, panel clustering methods, $\mathcal{H}$–matrix approaches, and Adaptive Cross Approximation methods, can reduce the complexity to almost $\mathcal{O}(N_h)$, up to polylogarithmic perturbations, for both the arithmetical expenses and the memory demand. Here we use the Fast Multipole Method in order to approximate

the single layer potential, the double layer potential and the hypersingular boundary integral operators which appear in the symmetric boundary integral domain decomposition formulation. Our preconditioned Krylov subspace solvers for two–fold saddle point problems require appropriately scaled preconditioners for the local (subdomain) discrete single layer potential operators, for the local boundary element Schur complements and for the BETI matrix in their data–sparse (fast multipole) representations. We propose data–sparse preconditioners which result in an almost optimal solver requiring $\mathcal{O}((H/h)^{(d-1)}(1+\log(H/h))^q \log \varepsilon^{-1})$ arithmetical operations in a parallel regime and $\mathcal{O}((H/h)^{(d-1)}(1+\log(H/h))^2)$ storage units per processor, where $q = 3$ and $\varepsilon \in (0,1)$ is the relative accuracy of the iteration error in a suitable norm. H and h denote the usual scalings of the subdomains and the boundary elements, respectively. Other local data–sparse preconditioners are proposed in [LOSZa] and [LOSZb] which result in the same arithmetical complexity estimate as given above, but with $q = 5$ and $q = 4$, respectively. Moreover, our solvers are insensitive to large jumps in the coefficients of the potential equation that is considered as model problem throughout the paper. These results can be generalized to linear elasticity boundary value problems in bounded and unbounded regions. The full version of this paper can be found in [LOSZa].

This work has been supported by the Austrian Science Fund 'Fonds zur Förderung der wissenschaftlichen Forschung (FWF)' under the grants P14953 and SFB F013 'Numerical and Symbolic Scientific Computing', and by the German Research Foundation 'Deutsche Forschungsgemeinschaft (DFG)' under the grant SFB 404 'Multifield Problems in Continuum Mechanics'.

References

[CKL] C. Carstensen, M. Kuhn, U. Langer, Fast parallel solvers for symmetric boundary element domain decomposition equations. Numer. Math., 79, 1998, 321–347.

[La] U. Langer, Parallel iterative solution of symmetric coupled FE/BE–equations via domain decomposition. Contemp. Math. 157, 1994, 335–344.

[LOSZa] U. Langer, G. Of, O. Steinbach, W. Zulehner, Inexact data–sparse boundary element tearing and interconnecting methods, RICAM–Report 2005-07, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, 2005.

[LOSZb] U. Langer, G. Of, O. Steinbach, W. Zulehner, Inexact fast multipole boundary element tearing and interconnecting methods. In: Proceedings of the 16th International Conference on Domain Decomposition, Lecture Notes in Computational Sciences and Engineering, Springer, Heidelberg, 2005 (to appear).

[LSa] U. Langer, O. Steinbach, Boundary element tearing and interconnecting methods, Computing, 71 (3), 2003, 205–228.

[LSb] U. Langer, O. Steinbach, Coupled boundary and finite element tearing and interconnecting methods. In: Proceedings of the 15th International Conference on Domain Decomposition (R. Kornhuber, R. Hoppe, J. Periaux, O. Pironneau, O. Widlund, J. Xu eds.), Lecture Notes in Computational Sciences and Engineering, vol. 40, Springer, Heidelberg, pp. 83–97, 2004.

[TW] A. Toselli, O. Widlund, Domain Decomposition Methods – Algorithms and Theory. Springer Series in Computational Mathematics, vol. 34, Springer, New York, 2004.

[Zu] W. Zulehner, Uzawa–type methods for block–structured indefinite linear systems, SFB–Report 2005-05, SFB F013, Johannes Kepler University Linz, Austria, 2005.

Sharpening the Predictive Properties of Compatible Relaxation

Robert D. Falgout
(joint work with J. Brannick, T. Manteuffel, S. McCormick, P. Vassilevski, L. Zikatanov)

The notion of *compatible relaxation* (CR) was introduced by Brandt in [1] as a modified relaxation scheme that keeps the coarse-level variables invariant. Brandt stated that the convergence rate of CR is a general measure for the quality of the set of coarse variables. A supporting theory for these ideas was presented in [2], from which we developed a CR-based algebraic coarsening algorithm for use in algebraic multigrid (AMG) methods. In [3], a new sharp convergence theory was developed for AMG. The form of this new theory bears a striking resemblance to its predecessor and suggests the possibility of improving the CR measure. We use the relationship between these two theories below to motivate a new approach for CR, one that has the potential of being a sharper measure of coarse grid quality and a better predictor of AMG convergence.

We will use the notation in [2, 3]. Consider solving the linear system

$$A\mathbf{u} = \mathbf{f}, \tag{1}$$

where A is a real symmetric positive definite (SPD) matrix, with $\mathbf{u}, \mathbf{f} \in \Re^n$. Define the smoother error propagator by

$$I - M^{-1}A, \tag{2}$$

and assume that the smoother is convergent (in energy norm) so that $(M+M^T-A)$ is SPD. Denote the symmetrized smoother operator by

$$\widetilde{M} = M(M^T + M - A)^{-1}M^T, \tag{3}$$

i.e., $\widetilde{M}$ is the "M" in (2) for the symmetric smoother $(I - M^{-T}A)(I - M^{-1}A)$.

Let $P : \Re^{n_c} \to \Re^n$ be the *interpolation* (or *prolongation*) operator, where $\Re^{n_c}$ is a lower-dimensional (*coarse*) vector space, and let $R : \Re^n \to \Re^{n_c}$ be some restriction operator (it is not the restriction operator used in the actual multigrid method) such that $RP = I_c$, the identity on $\Re^{n_c}$. We can think of R as defining the *coarse-grid variables*, i.e., $\mathbf{u}_c = R\mathbf{u}$. Note that PR is a projection onto range(P). For any SPD matrix X and any full-rank matrix B, we denote the X-orthogonal projection onto range(B) by

$$\pi_X(B) = B(B^T X B)^{-1} B^T X. \tag{4}$$

When $B = P$, we will drop the parentheses so that $\pi_X := \pi_X(P)$.

Consider now the two-grid multigrid operator,

$$E_{TG} = (I - M^{-1}A)(I - \pi_A). \tag{5}$$

The next two theorems summarize the main convergence results in [2, 3].

THEOREM *(from* [2]*)*

$$\|E_{TG}\|_A^2 \leq 1 - \frac{1}{K};\ K = \sup_{\mathbf{e}} \frac{\|(I - PR)\mathbf{e}\|_{\widetilde{M}}^2}{\|\mathbf{e}\|_A^2}. \tag{6}$$

THEOREM *(from* [3]*)*

$$\|E_{TG}\|_A^2 = 1 - \frac{1}{K_\sharp};\ K_\sharp = \sup_{\mathbf{e}} \frac{\left\|(I - \pi_{\widetilde{M}})\mathbf{e}\right\|_{\widetilde{M}}^2}{\|\mathbf{e}\|_A^2}. \tag{7}$$

From the two theorems, we note that the only difference between the quantities K and $K_\sharp$ is the form of the projection. More specifically, we see that $K = K_\sharp$ (i.e., the two "measures" are the same) if

$$R = (P^T \widetilde{M} P)^{-1} P^T \widetilde{M}. \tag{8}$$

Since compatible relaxation in [2] was based entirely on the form of R, this suggests the possibility of defining more predictive CR methods by simply using a "better" R. From equation (8), we see that the "best" R is rather complicated and impractical. However, we can find a simpler form for R by noting that the multigrid operator in (5) is invariant to post-scaling of interpolation. In particular, we can equivalently use the interpolation operator $\bar{P} = P(RP)^{-1}$ in the theory, since $R\bar{P} = I_c$, as required. Now, if we compare the numerator for K in (6) to the numerator for $K_\sharp$ in (7), it is clear that the optimal R is given by

$$R = P^T \widetilde{M}, \tag{9}$$

which is much simpler than in (8). It also makes more intuitive sense that the coarse-grid variables are best defined as the transpose of interpolation (times the smoother).

Note that the "best" R is a function of P, something that is not allowed in [2]. Furthermore, we want to use CR to help build P, so we cannot use P in the CR algorithm. However, equation (9) does provide guidance for choosing an R that might provide better prediction of two-grid multigrid rates. Assuming we have a means of finding such an R, let us consider an example of how we might use it in a CR method.

Assume that P has the classical form

$$P = \begin{bmatrix} W_p \\ I \end{bmatrix}. \tag{10}$$

Now, define the coarse-grid variables to be some kind of averaging of the form

$$R = \begin{bmatrix} W^T & I \end{bmatrix}. \tag{11}$$

Then, we can define S such that $RS = 0$ by

$$S = \begin{bmatrix} I \\ -W^T \end{bmatrix}. \tag{12}$$

From here, we can define the primary version of CR

$$I - (S^T M S)^{-1}(S^T A S). \tag{13}$$

This may or may not be easily computable, depending on M, etc. What we would really like to use (at least it is always easily computable) is the habituated form of CR given by

$$S^T(I - M^{-1}A)S. \tag{14}$$

The problem here is that the theory in [2] requires that S be normalized such that $S^T S = I_f$. This again is not easily computable or practical. However, we can avoid this problem by using a modified form of habituated CR as we now describe.

Consider the following related forms of habituated CR:

$$\pi(S)(I - M^{-1}A) = (I - \pi(R^T))(I - M^{-1}A). \tag{15}$$

The idea is to define the CR method as in (15) where we approximate the action of $(S^T S)^{-1}$ and $(RR^T)^{-1}$ with operators C_s and C_r, respectively. In particular, we are interested in the case where these operators result by applying a simple iterative method to the appropriate set of equations (e.g., $(S^T S)\mathbf{u}_s = \mathbf{f}_s$) with zero initial guess. That is, consider the following two habituated CR methods (the second method is the one proposed by Livne [4] and Brandt):

$$SC_s S^T(I - M^{-1}A); \tag{16}$$

$$(I - R^T C_r R)(I - M^{-1}A). \tag{17}$$

In [2], we show that the convergence rate of the habituated CR method in (14) can be used to estimate the quality of the coarse grid and to predict the convergence rate of the 2-grid method. We can prove a similar result for the two new CR methods in (16) and (17).

As a simple example of the potential of these new CR methods to give sharp prediction of two-grid multigrid rates, consider a 9-pt finite element discretization of a 2D Laplacian problem on a square. Define $R = P^T$ = full weighting. Using symmetric cycles for AMG and the CR methods, we get

$$\begin{aligned} \left\|(I - M^{-T}A)(I - \pi_A)(I - M^{-1}A)\right\|_A &= 0.1711 \\ \left\|(I - M^{-T}A)(I - \pi(R^T))(I - M^{-1}A)\right\|_A &= 0.1713. \end{aligned}$$

If we run the method in (17) using Gauss-Seidel to produce C_r, we get

$$\begin{aligned} \left\|(I - M^{-T}A)(I - R^T C_r R)(I - M^{-1}A)\right\| &= 0.186 \text{ (1 GS)} \\ &= 0.173 \text{ (3 GS)}. \end{aligned}$$

By comparison, the primary CR method in (13) with the usual $R = [0,\ I]$ gives a prediction for (18) of 0.5.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

References

[1] A. Brandt, *General highly accurate algebraic coarsening*, Electronic Transactions on Numerical Analysis, 10 (2000), pp. 1–20.
[2] R. D. Falgout and P. S. Vassilevski, *On Generalizing the AMG Framework*, SIAM J. Numer. Anal., 42 (2004), pp. 1669–1693.
[3] R. D. Falgout, P. S. Vassilevski, and L. T. Zikatanov, *On Two-Grid Convergence Estimates*, Numer. Linear Algebra Appl., to appear.
[4] O. E. Livne, *Coarsening by Compatible Relaxation*, Numer. Linear Algebra Appl., 11 (2004), pp. 205–227.

A Symmetric Smoother for NIPG

Klaus Johannsen

Discontinuous Galerkin (DG) methods, traditionally used for the solution of hyperbolic equations [Co, JP], have recently gained much attention in application to elliptic problems. Whereas multigrid solution schemes are well-understood in case of conforming Galerkin discretizations, its analysis for DG methods began only recently. In the case of the symmetric penalized SIPG method [GRW, Wh] standard multigrid theory has been applied successfully [GK]. In the case of non-symmetric DG, the behavior of basic iterative methods have been investigated in [HR, HHRa, HHRb] by means of Fourier analysis and numerical experiments in [BR]. An rigorous treatment of the non-symmetric variants is not know to the author.

In this contribution we investigate the smoothing property of a variant of the symmetric Gauss-Seidel applied to the non-symmetric NIPG method. We consider arbitrary unstructured, quasi-uniform meshes and polynomial degrees of any order. Let A denote the NIPG discretization of the Laplacian operator. We split A into the symmetric and the anti-symmetric part

$$A_s = 1/2(A + A^T), \qquad A_a = 1/2(A - A^T).$$

The key of the argumentation is an estimate of the antisymmetric part A_a with respect to A_s

$$-\xi A_s \leq iA_a \leq \xi A_s,$$

for a $\xi > 0$ depending on the penalty parameter only. The estimate could be shown using standard arguments from functional analysis. Using this estimate, the classical smoothing property could be shown to hold in the Euclidian norm for the smoother defined by

$$S = \mathbb{I} - W^{-1}A,$$
$$W := \text{symmetric Gauss-Seidel approximation of } A_s.$$

A standard argumentation leads to h-independent multigrid convergence for the $W(\nu,\nu)$-cycle multigrid iteration, provided the number of smoothing steps ν is large enough. For details, see [Ha]. A dependence of the smoothing property on the penalty parameter of the NIPG discretization is made explicite.

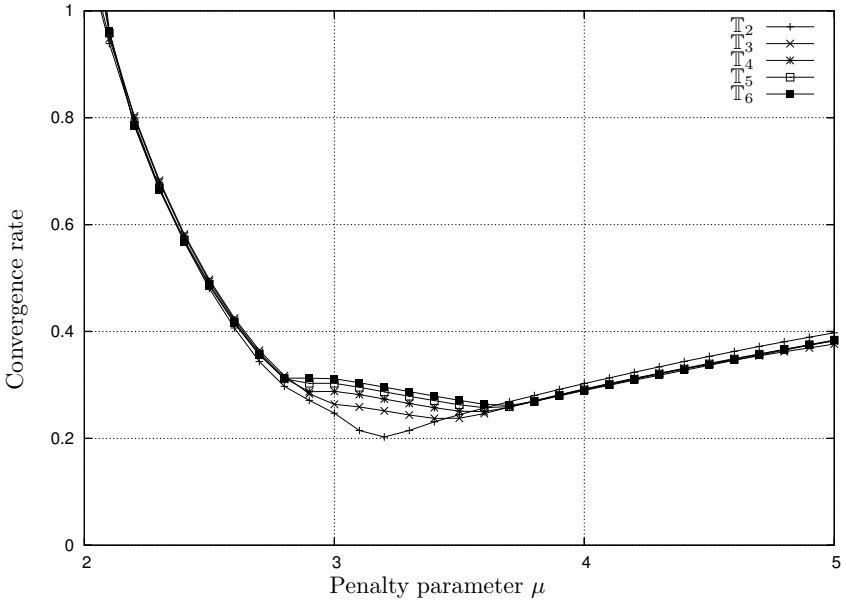

FIGURE 1. Convergence of the $V(1,1)$-cycle multigrid applied to a model problem using the basis P_2 in dependence on the penalty parameter μ. The graphs correspond to different grid levels.

Numerical experiments confirm the theoretical findings. As an illustration, we show the convergence rates of the $V(1,1)$-cycle multigrid applied to a P_2-discretization of a two-dimensional model problem for varying penalty parameter μ on different levels of the multigrid hierarchy in the figure below. As can be seen clearly, the multigrid convergence does not depend on the mesh size. On the other hand, a strong dependence on the penalty parameter μ can be observed. A too a small penalty parameters leads to the divergence of the scheme, which is in accordance with the theory.

REFERENCES

[BR] P. Bastian, V. Reichenberger, Multigrid for higher order discontinuous Galerkin finite elements applied to groundwater flow, Technical Report 2000-37, SFB 359, Heidelberg University, 2000.

[Co] B. Cockburn, Discontinuous Galerkin methods for convection dominated problems, In: High-Order Methods for Computational Physics, T. Barth, H. Deconink (eds), Springer-Verlag, New York, 9:69-224, 1999.

[GK] J. Gopalakrishnan, G. Kanschat, A Multilevel Discontinuous Galerkin Method, Numer. Math., 3:527-550, 2003.

[GRW] V. Girault, B. Riviere, M.F. Wheeler, Improved energy estimates for inerior penalty, constraint and discontinuous Galerkin methods for elliptic problems. Part I. Computational Geosciences, 3:337-360,1999.

[Ha] W. Hackbusch, Multi-Grid Methods and Applications, Springer-Verlag, Berlin, Heidelberg, 1985.

[HR] P.W. Hemker, M.H. van Raalte, Fourier two-level analysis for higher dimensional discontinuous Galerkin, Technical Report MAS-R0227, ISSN 1386-3703, CWI, Amsterdam, 2002.

[HHRa] P.W. Hemker, W. Hoffmann, M.H. van Raalte, Fourier two-level analysis for higher dimensional discontinuous Galerkin, Technical Report MAS-R0217, ISSN 1386-3703, CWI, Amsterdam, 2002.

[HHRb] P.W. Hemker, W. Hoffmann, M.H. van Raalte, Two-level Fourier analysis of a multigrid approach for discontinuous Galerkin discretisation, Technical Report MAS-R0206, ISSN 1386-3703, CWI, Amsterdam, 2002.

[JP] C. Johnson, J. Pitkäranta, An analysis of the discontinuous Galerkin method for a scalar hyperbolic equation, Mathematics of Computation, 46:1-26,1986.

[Wh] M.F. Wheeler, An elliptic collocation-finite element method with interior penalties, SIAM J Numer. Anal., 15:152-161, 1978.

Hierarchical Matrices based on Domain Decomposition

Lars Grasedyck

(joint work with Ronald Kriemann and Sabine Le Borne)

Most direct methods for sparse linear systems perform an LU factorisation of the original matrix after some reordering of the indices in order to reduce fill-ins. One such popular reordering method is the so-called *nested dissection* which exploits the concept of separation. The idea of nested dissection has been introduced more than 30 years ago [Ge] and since then attracted considerable attention (see, e.g., [BT, HR] and the references therein). The main idea is to separate a (matrix) graph into three parts, two of which have no coupling between each other. The third one, referred to as an interior boundary or separator, contains couplings with (possibly both of) the other two parts. The nodes of the separator are numbered last. This process is then repeated recursively in each subgraph. An illustration of the resulting sparsity pattern is shown in Figure 1 for the first two decomposition steps. In domain decomposition terminology, we recursively subdivide our domain

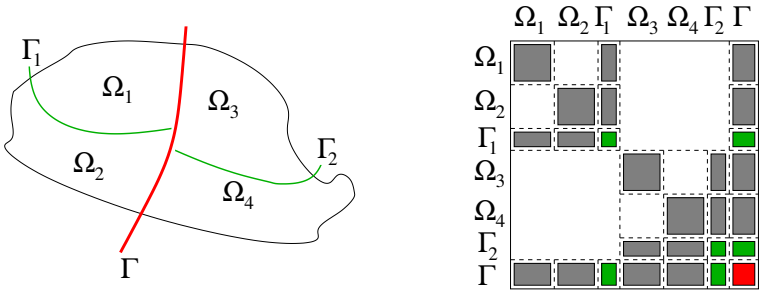

Figure 1. Nested dissection and resulting matrix sparsity structure

into two disjoint subdomains and an interior boundary.

A favourable property of such an ordering is that a subsequent LU factorisation maintains a major part of this sparsity structure, i.e., there occurs no fill-in in the large, off-diagonal zero matrix blocks. In fact, in the case of regular two-dimensional grids, the computational complexity amounts to $\mathcal{O}(N^{1.5})$ for a matrix $A \in \mathbb{R}^{N\times N}$. In order to obtain a (nearly) optimal complexity, we propose to approximate all nonzero, off-diagonal blocks in $\mathcal{H}$-matrix representation and compute them using $\mathcal{H}$-matrix arithmetic. The (small) blocks along the diagonal and the corresponding LU factorisations will be stored as full matrices.

We apply the new domain decomposition based $\mathcal{H}$-LU factorisation [Li, GL] to a volume-conduction model of the head [Wo], see Figure 2, where the system has to be solved for many right-hand sides. It turns out that our new solver is up to 5 times faster than the optimised algebraic multigrid method PEBBLES [HKR]. Both approaches use the leadfield-bases acceleration from [WGH]. At the last Oberwolfach workshop "Schnelle Löser für partielle Differentialgleichungen" in 2003, the time to setup the influence matrix was reduced from 8 days down to 5 hours by use of a parallel machine and optimisation for multiple right-hand sides. By use of the leadfield-bases acceleration and the hierarchical matrix technique we could reduce this to 15 minutes on a single processor machine. In the second

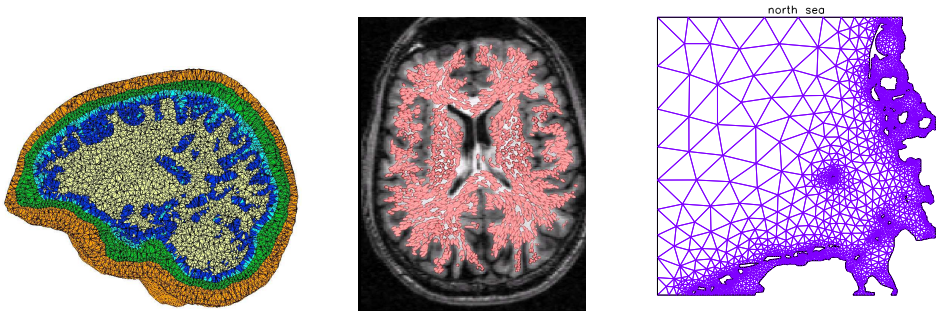

FIGURE 2. Left: 5 layer head geometry; Right: North sea mesh

part of the talk we present a black-box clustering algorithm that uses only the sparse stiffness matrix as input. The cluster tree as well as the blocking of the matrix, based on a black-box admissibility criterion, are constructed using nested dissection applied to the matrix graph. We compare the new black-box solver to the standard algebraic multigrid solver PLTMG for some examples, see Figure 2, provided by PLTMG [Ba].

REFERENCES

[Ge] A. George. Nested dissection of a regular finite element mesh. *SIAM J. Numer. Anal.*, 10:345–363, 1973.

[Ba] R. E. Bank. PLTMG: A software package for solving elliptic partial differential equations, users guide 9.0.. Technical report, University of California, San Diego, 2004.

[BT] I. Brainman and S. Toledo. Nested-dissection orderings for sparse LU with partial pivoting. *SIAM J. Mat. Anal. Appl.*, 23:998–1012, 2002.

[Gr] L. Grasedyck. *Theorie und Anwendungen Hierarchischer Matrizen*. Doctoral thesis, Universität Kiel, 2001.

[GH] L. Grasedyck and W. Hackbusch. Construction and arithmetics of $\mathcal{H}$-matrices. *Computing*, 70:295–334, 2003.

[GL] L. Grasedyck and S. LeBorne. H-matrix preconditioners in convection-dominated problems. *SIAM J. Mat. Anal.* accepted.

[HKR] G. Haase, M. Kuhn, and S. Reitzinger. Parallel AMG on distributed memory computers. *SIAM J. Sci.Comp.*, 24(2):410–427, 2002.

[HKK] W. Hackbusch, B. Khoromskij, and R. Kriemann. Hierarchical matrices based on a weak admissibility criterion. *Computing*, 73:207–243, 2004.

[Ha] W. Hackbusch. Direct domain decomposition using the hierarchical matrix technique. In O. Widlund I. Herrera, D. Keyes and R. Yates, editors, *Domain Decomposition Methods in Science and Engineering*, pages 39–50. UNAM, 2003.

[HKb] W. Hackbusch and B. Khoromskij. A sparse matrix arithmetic based on $\mathcal{H}$-matrices. Part II: Application to multi-dimensional problems. *Computing*, 64:21–47, 2000.

[HR] B. Hendrickson and E. Rothberg. Improving the run time and quality of nested dissection ordering. *SIAM J. Sci. Comp.*, 20:468–489, 1998.

[Le] S. LeBorne. Hierarchical matrices for convection-dominated problems. In J. Périaux O. Pironneau O. Widlund J. Xu R. Kornhuber, R. Hoppe, editor, *Domain Decomposition Methods in Science and Engineering*, pages 631–638. LNCSE, 2004.

[Li] M. Lintner. The eigenvalue problem for the 2d Laplacian in $\mathcal{H}$-matrix arithmetic and application to the heat and wave equation. *Computing*, 72:293–323, 2004.

[WGH] C. Wolters, L. Grasedyck and W. Hackbusch. Efficient Computation of Lead Field Bases and Influence Matrix for the FEM-based EEG and MEG Inverse Problem. Part I: Complexity Considerations. *Inverse Probems*, 20:1099–1116, 2004.

[Wo] C. Wolters, M. Kuhn, A. Anwander, and S. Reitzinger. A parallel algebraic multigrid solver for finite element method based source localization in the human brain. *Comp. Vis. Sci.*, 5(3):165–177, 2002.

$\mathcal{H}^2$-matrices

Steffen Börm

Hierarchical matrices [17, 13, 6] use local low-rank approximations in order to treat large dense matrices efficiently. $\mathcal{H}^2$-matrices [18, 7, 3] impose additional restrictions on the choice of the low-rank approximations in order to improve the efficiency. While hierarchical matrices are the algebraic counterparts of panel-clustering techniques [19] and multipole expansions [15, 16], $\mathcal{H}^2$-matrices use hierarchical expansion systems, similar to multilevel and wavelet methods [11], in order to reach the optimal order of complexity. Due to their purely algebraic construction, they can not only speed up matrix-vector multiplications, but also provide efficient algorithms for the approximation of far more complicated operations like multiplication or inversion of matrices.

All hierarchical matrix techniques subdivide a matrix $M \in \mathbb{R}^{\mathcal{I}\times\mathcal{J}}$ into a hierarchical partition of submatrices $M|_{t\times s}$ for $t \subseteq \mathcal{I}$ and $s \subseteq \mathcal{J}$. The subsets t and s are not arbitrary, but picked from a *row cluster tree* $\mathcal{T}_{\mathcal{I}}$ or a *column cluster tree* $\mathcal{T}_{\mathcal{J}}$, which provide us with a hierarchy of partitions of the row and column index sets $\mathcal{I}$ and $\mathcal{J}$.

Among the blocks $t \times s$ of the hierarchical partition, some are marked as *admissible*, which means that we expect to be able to approximate them by low-rank matrices. Typically, the admissibility of a block is related to its distance from the diagonal, since diagonal blocks of a matrix will typically be invertible, i.e., of full rank.

For standard hierarchical matrices, each admissible block $t \times s$ is approximated by a rank-k-matrix $\widetilde{M}|_{t\times s}$ which can be expressed by the factorization $\widetilde{M}|_{t\times s} = AB^\top$, where A and B have k columns. For $\mathcal{H}^2$-matrices, a different type of factorization is used: we fix matrices V_t and W_s with k columns for all row clusters $t \in \mathcal{T}_\mathcal{I}$ and for all column clusters $s \in \mathcal{T}_\mathcal{J}$. The admissible blocks are then represented in the form $\widetilde{M}|_{t\times s} = V_t S_{t,s} W_s^\top$ for a k-by-k matrix $S_{t,s}$. Obviously, the admissible blocks will still be of low rank, therefore each $\mathcal{H}^2$-matrix is also a hierarchical matrix. In order to reach the optimal order of complexity, we have to require that the *cluster bases* V_t and W_s are nested, i.e., that we can find k-by-k *transfer matrices* $E_{t'}$ and $F_{s'}$ for all $t' \in \operatorname{sons}(t)$ and $s' \in \operatorname{sons}(s)$ which satisfy

$$(V_t)_{i\nu} = (V_{t'} E_{t'})_{i\nu}, \qquad (W_s)_{j\mu} = (W_{s'} E_{s'})_{j\mu}$$

for all $i \in t'$, $j \in s'$ and $\nu, \mu \in \{1, \ldots, k\}$.

The nested structure of the cluster bases is crucial for the efficiency of $\mathcal{H}^2$-matrix techniques, because it allows us to re-use results prepared on lower levels of the hierarchy when treating its higher levels, much as in other multilevel schemes [3]: the cluster tree can be seen as a generalization of a grid hierarchy, the cluster bases correspond to trial and test spaces on the different levels, the transfer matrices play the role of prolongation and restriction operators.

In some situations, e.g., if asymptotically smooth integral operators are approximated, the construction of a nested cluster basis is straightforward [12, 8, 10], but in general situations, even the question of its existence can prove challenging. A general criterion [4] can be used to establish the existence of nested cluster bases for the approximation of integral operators and for the approximation of the solution operators of elliptic partial differential equations.

The numerical results in Table 1 demonstrate the efficiency of the $\mathcal{H}^2$-matrix representation: on the left side, the classical double layer potential operator, a boundary integral operator involving the normal derivative of an asymptotically smooth kernel function, has been discretized and approximated by an $\mathcal{H}^2$-matrix

n	Build	MVM	DoF
2048	11	0.01	3.7
8192	51	0.11	4.4
32768	210	0.45	4.6
131072	883	2.07	4.7
524288	3818	9.77	5.2

n	Build	MVM	DoF
1024	1	< 0.01	1.6
4096	10	< 0.01	2.0
16384	80	0.07	2.5
65536	595	0.34	2.8
262144	4127	1.51	3.0
1048576	26178	6.64	3.1

TABLE 1. Approximation of integral and solution operators by $\mathcal{H}^2$-matrices up to a relative precision of 10^{-3}

using the algorithms presented in [9, 1]. On the right side, Poisson's equation was discretized, its solution operator computed by $\mathcal{H}$-matrix arithmetics [14] and the result converted into an $\mathcal{H}^2$-matrix. The parameters are adjusted to guarantee a relative precision of 10^{-3}. Table 1 gives the time in seconds for the construction, the time in seconds for the matrix-vector multiplication and the storage requirements in KB per degree of freedom. We can see that the storage requirements, the time for the matrix-vector multiplication and the time for the construction of the integral operator scale linearly [1].

In order to construct the approximant of a solution operator efficiently, arithmetic operations like matrix addition and multiplication can be used. These operations can also be employed to perform other matrix operations like finding a Cholesky or LU factorization or even solving matrix equations.

If the cluster bases are prescribed *a priori*, it is possible to compute the best approximations of sums and products of $\mathcal{H}^2$-matrices in optimal complexity [2] by preparing suitable data-sparse approximations of all matrix blocks in advance and then re-using these precomputed quantities in order to avoid unnecessary recursions. If the cluster bases are not known in advance, as it is typically the case when treating partial differential operators, we compute the product in a suitable $\mathcal{H}$-matrix format and then construct suitable cluster bases *a posteriori*. Due to the detour via standard hierarchical matrices, this approach reaches only a log-linear complexity in the number of degrees of freedom, but can guarantee a prescribed precision.

Table 2 compares the performance of the different matrix-matrix multiplication algorithms: the classical single layer potential operator is discretized by Galerkin's method, and the resulting matrix multiplied by itself, an operation which corresponds to a convolution of the kernel function. We can see that the a priori algorithm is significantly faster than the a posteriori and the $\mathcal{H}$-matrix algorithm and that its computational complexity scales linearly. The a posteriori algorithm reaches a better accuracy than the a priori algorithm and is still significantly faster than the $\mathcal{H}$-matrix method.

[1]The experiments were carried out using the HLib [5] package on one UltraSPARC IIIcu processor with 900 MHz in a SunFire 6800 system.

n	$\mathcal{H}^2$ a priori		$\mathcal{H}^2$ a posteriori		$\mathcal{H}$	
	Time	Err.	Time	Err.	Time	Err.
512	0.3	7.5_{-5}	0.4	5.9_{-6}	0.7	5.3_{-6}
2048	9.4	1.0_{-4}	12.5	5.6_{-6}	35.2	4.6_{-6}
8192	54.5	2.5_{-3}	100.0	5.1_{-5}	794.8	3.1_{-5}
32768	245.7	8.1_{-4}	546.1	7.3_{-5}	1560.7	3.9_{-5}
131072	1020.4	6.8_{-4}	2769.8	7.1_{-5}	9022.8	3.9_{-5}

TABLE 2. Comparison between a priori, a posteriori and $\mathcal{H}$-matrix multiplication algorithms

The application of these $\mathcal{H}^2$-matrix arithmetic operations to the inversion and LU factorization of FEM and BEM matrices is the topic of ongoing research.

References

[1] S. Börm, *Approximation of integral operators by $\mathcal{H}^2$-matrices with adaptive bases*, Preprint 18/2004, Max Planck Institute for Mathematics in the Sciences, 2004. To appear in Computing.

[2] ———, *$\mathcal{H}^2$-matrix arithmetics in linear complexity*, Preprint 47/2004, Max Planck Institute for Mathematics in the Sciences, 2004. Submitted to Computing.

[3] ———, *$\mathcal{H}^2$-matrices — multilevel methods for the approximation of integral operators*, Comput. Visual. Sci., 7 (2004), pp. 173–181.

[4] ———, *Data-sparse approximation of non-local operators by $\mathcal{H}^2$-matrices*, Tech. Rep. 44/2005, Max Planck Institute for Mathematics in the Sciences, 2005.

[5] S. Börm and L. Grasedyck, HLib – *a library for $\mathcal{H}$- and $\mathcal{H}^2$-matrices*, 1999. Available at `http://www.hlib.org/`.

[6] S. Börm, L. Grasedyck, and W. Hackbusch, *Hierarchical Matrices*. Lecture Note 21 of the Max Planck Institute for Mathematics in the Sciences, 2003.

[7] S. Börm and W. Hackbusch, *Data-sparse approximation by adaptive $\mathcal{H}^2$-matrices*, Computing, 69 (2002), pp. 1–35.

[8] ———, *$\mathcal{H}^2$-matrix approximation of integral operators by interpolation*, Applied Numerical Mathematics, 43 (2002), pp. 129–143.

[9] ———, *Approximation of boundary element operators by adaptive $\mathcal{H}^2$-matrices*, Foundations of Computational Mathematics, 312 (2004), pp. 58–75.

[10] S. Börm and J. Ostrowski, *Fast evaluation of boundary integral operators arising from an eddy current problem*, Journal of Computational Physics, 193 (2003), pp. 67–85.

[11] W. Dahmen and R. Schneider, *Wavelets on manifolds I: Construction and domain decomposition*, SIAM Journal of Mathematical Analysis, 31 (1999), pp. 184–230.

[12] K. Giebermann, *Multilevel approximation of boundary integral operators*, Computing, 67 (2001), pp. 183–207.

[13] L. Grasedyck, *Theorie und Anwendungen Hierarchischer Matrizen*, PhD thesis, Universität Kiel, 2001.

[14] L. Grasedyck and W. Hackbusch, *Construction and arithmetics of $\mathcal{H}$-matrices*, Computing, 70 (2003), pp. 295–334.

[15] L. Greengard and V. Rokhlin, *A fast algorithm for particle simulations*, Journal of Computational Physics, 73 (1987), pp. 325–348.

[16] ———, *A new version of the fast multipole method for the Laplace in three dimensions*, in Acta Numerica 1997, Cambridge University Press, 1997, pp. 229–269.

[17] W. Hackbusch, *A sparse matrix arithmetic based on $\mathcal{H}$-matrices. Part I: Introduction to $\mathcal{H}$-matrices*, Computing, 62 (1999), pp. 89–108.

[18] W. Hackbusch, B. Khoromskij, and S. Sauter, *On $\mathcal{H}^2$-matrices*, in Lectures on Applied Mathematics, H. Bungartz, R. Hoppe, and C. Zenger, eds., Springer-Verlag, Berlin, 2000, pp. 9–29.

[19] W. Hackbusch and Z. P. Nowak, *On the fast matrix multiplication in the boundary element method by panel clustering*, Numerische Mathematik, 54 (1989), pp. 463–491.

Efficient Operator Calculus Based on Data-Sparse Tensor-Product Decompositions

Boris N. Khoromskij
(joint work with W. Hackbusch)

Coupling the hierarchical and tensor-product formats allows an opportunity for efficient data-sparse approximation of integral and more general nonlocal operators in higher dimensions (cf. [2], [3], [1], [4]). Examples of such nonlocal mappings are solution operators of elliptic, parabolic and hyperbolic boundary value problems, Lyapunov and Riccati solution operators in control theory, spectral projection operators associated with the matrix *sign* function of the Fock matrix in solving the Hartree-Fock equation (many-particle models), collision integrals in the deterministic Boltzmann equation (dilute gas) as well as the convolution integrals in the Ornstein-Zernike equation (disordered matter).

We discuss how the $\mathcal{H}$-matrix techniques combined with the low-rank Kronecker tensor-product approximation allow to represent a function $\mathcal{F}(A)$ of a discrete elliptic operator A in a hypercube $(0,1)^d \in \mathbb{R}^d$ in the case of a high spatial dimension $d \geq 3$. Along with integral operators, we focus on the functions A^{-1} and $sign(A)$. Applying the analytic approximation tools based on Sinc-quadratures or fitting by exponential sums, we prove that the asymptotic complexity of our representations can be estimated by $O(N^{p/d} \log^q N)$ with $p = 1, 2$, where N is the discrete problem size. Numerical results confirm our approximation theory.

References

[1] W. Hackbusch, B.N. Khoromskij: *Low-Rank Kronecker-Product Approximation to Multi-Dimensional Nonlocal Operators.* Parts I,II. Preprints 29/30, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig 2005; (Computing, to appear).

[2] W. Hackbusch, B.N. Khoromskij, and E. Tyrtyshnikov: *Hierarchical Kronecker tensor-product approximation*, Preprint 35, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 2003; J. Numer. Math. 13 (2005), 119-156.

[3] I. P. Gavrilyuk, W. Hackbusch and B. N. Khoromskij: *Tensor-Product Approximation to Elliptic and Parabolic Solution Operators in Higher Dimensions.* Computing 74 (2005), 131-157.

[4] B.N. Khoromskij: *Structured data-sparse approximation to high order tensors arising from the deterministic Boltzmann equation.* Preprint 4, Max-Planck-Institut für Mathematik in den Naturwissenschaften, 2005 (submitted).

Fast Solvers for Non-Newtonian Flow Models

Jinchao Xu
(joint work with Youngju Lee et al)

In the design of fast solvers for partial differential equations, it is desirable to give integrated considerations of issues related to discretizations, grid adaptation and algebraic iterative methods. In this talk, we report our recent studies of fast solvers for a class of non-Newtonian models.

A new finite element scheme. Most existing discretization methods for non-Newtonian models such as Johnson-Segalman model are known to be numerically unstable when the Weissenberg number reaches to a critical value. This phenomenon, known as "the high Weissenberg number problem" in the literature (see [8]), is believed to be related to the fact that the so-called conformation tensor is difficult to be kept positive definite on the discrete level[8]. In Lee and Xu[6], we recently designed a new finite element discretization scheme for a class of rate-type non-Newtonian models by combining many analytic and numerical techniques, including the use of Lie derivatives, the reformulation of the constitutive relation as a generalized Riccati equation in terms of Lie derivatives, Eulerian-Lagrangian discretization, special positivity preserving for temporal varialbe, special positivity preserving for spatial variables, special stable finite element spaces for velocity and pressure, and volume preserving schemes for the characteristic feet. The new scheme is proven to preserve the positivity property of the conformation tensore on each time step and to satisfy some discrete energy estimates which assure the numerical stability of the new scheme for any size of Weissenberg number. Hence the new scheme provides a solution to the long-standing *high Weissenberg number problem*[8].

Fast iterative methods for the discretized systems. One great advantage of our new discretization scheme is that at each time-step only a linearized Stokes like system need to be solved together with numerous independent nonlinear ordinary different equations that can be solved in parallel. For the Stokes like system, we report a new preconditioned MINRES method [7] with preconditioner given by multigrid methods. The preconditioned iterative method is proven to be uniform with respect to all physical and discretization parameters. In order to more easily combine our preconditioned methods with adaptive finite element method which often leads to unstructured grids, we developed a new efficient algebraic multigrid methods for high order finite element systems in Shu, Sun and Xu [10]. For a given sparse stiffness matrix from a quadratic Lagrangian finite element discretization, an algebraic approach is carefully designed to recover the stiffness matrix associated with the linear finite element discretization on the same underlying (but nevertheless unknown to the user) finite element grid. With any given classic algebraic multigrid solver for linear finite element stiffness matrix, a corresponding algebraic multigrid method can then be designed for quadratic or higher order finite element stiffness matrix by combining with a standard smoother for the original system. This method is designed under the assumption that the sparse matrix to be solved is associated with a specific higher order, quadratic for example, finite element discretization on a finite element grid but the geometric data for the underlying grid is unknown. The resulting new algebraic multigrid method is shown, by numerical experiments, to be much more efficient than the classic algebraic multigrid method that is directly applied to the high order finite element matrix. Some theoretical analysis is also provided for the convergence of the new method.

Grid adaptation. For the new scheme, we further report how to apply some new grid adaptation techniques. The new techniques we recently developed are based on the work of Bank and Xu [1, 2] for linear elements. In Huang and Xu [4], we obtained superconvergence results for quadratic finite element on mildly structured grids for second order elliptic equations. In Bank, Xu and Zheng [3], we developed averaging and smoothing techniques (that are problem independent) for superconvergence recovery of Hessian matrix for general quadratic finite element methods on general unstructured grids. All these new methods can be used for grid adaptation for our new finite element method for non-Newtonian models.

We would like to emphasis that our new finite element scheme for non-Newtonian models is based on semi-Langrangian method or method of characteristic [5, 9]. The efficiency of this type of method can be much enhanced if proper grid adaptation methods are used.

References

[1] Randolph E. Bank and Jinchao Xu, *Asymptotically Exact A Posteriori Error Estimators, Part I: Grids with Superconvergence*, SIAM J. Numer. Anal., V. 41, 2003(6), pp. 2294-2312.

[2] Randolph E. Bank and Jinchao Xu, *Asymptotically Exact A Posteriori Error Estimators, Part II: General Unstructured Grids*, SIAM J. Numer. Anal., V. 41, 2003(6), pp. 2313-2332.

[3] Randolph E. Bank, Jinchao Xu and Bing Zheng, *Postprocessing techniques for quadratic finite element methods on unstructured grids* (in preparation).

[4] Yunqing Huang and Jinchao Xu, *Superconvergence for quadratic finite element methods on mildly structured grids* (preprint)

[5] Jr J. Douglas and T.F. Russell, Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures. *SIAM J. Numer. Anal.*, 19(5):871–885, 1982.

[6] Youngju Lee an Jinchao Xu, *New formulations, positivity preserving disretizations and stability analysis for non-Newtonian flow models*, Computer methods in applied mechanics and engineering (in press)

[7] Youngju Lee an Jinchao Xu, *Fast iterative methods for the discrete systems arising from discretization of non-Newtonian flow models*, (in preparation)

[8] R.G. Owens and T.N. Phillips, *Computational Rheology.* London : Imperial College Press, 2002.

[9] O. Pironneau, On the transport-diffusion algorithm and its applications to the navier-stokes equations. *Numer. Math.*, 38, 1982.

[10] Shi Shu, Dudu Sun and Jinchao Xu, *An algebraic multigrid method based on geometric considerations*, (submitted to Computing)

Kernel Preserving Multigrid Methods for Convection Dominated Problems

Justin W.L. Wan
(joint work with Randolph E. Bank and Zhenpeng Qu)

In this talk, we consider the steady state solution of the model equation on a domain $\Omega \subset \mathbb{R}^2$:

$$\begin{aligned} -\epsilon\,\Delta u + a(x,y)\,u_x + b(x,y)\,u_y &= f \qquad \text{in } \Omega \\ \alpha\,u + \gamma\,\frac{\partial u}{\partial n} &= g \qquad \text{on } \partial\Omega, \end{aligned}$$

where ϵ is a small diffusion parameter, the vector (a, b) represents the convection velocity, and α, γ determine the inflow and outflow boundary conditions. The algorithms and analysis presented will be mainly in 1D and 2D, but extension to 3D is possible in most cases. We are interested in the convection dominated limit where $\epsilon \to 0$.

The equation can be discretized by upwinding finite difference methods [8], finite element methods [9] and finite volume methods [1]. In any case, it will result in a linear system of the form

$$A^h u^h = f^h.$$

When $\epsilon \gg 1$, the linear system can be solved efficiently using, for instance, fast Fourier transform, preconditioned conjugate gradient, multigrid and domain decomposition methods. For small ϵ, however, A^h is a highly nonsymmetric matrix, and most of these solvers become less efficient.

Multigrid methods have been widely used for solving elliptic partial differential equations (PDEs) since the convergence rates are often independent of mesh size. For nonelliptic PDEs, in particular, convection diffusion equations, the multigrid convergence deteriorates with increasing convection. One reason is that the elliptic multigrid approaches do not generally take into account the hyperbolicity of the convection diffusion operator. Thus, modifications need to be made in the smoother and coarse grid correction processes to improve convergence.

Different smoothing techniques have been developed, for instance, Gauss-Seidel with downwind ordering [4], smoothers based on time-stepping schemes [7], line smoothers [10], and ILU smoothers [13]. Although often effective, all these smoothers are relatively expensive to compute and apply, especially in 3D. Thus, in this talk, we primarily consider relaxation smoothers, and focus on the choice and construction of the interpolation and restriction operators.

Coarse grid correction leads to more subtle issues. For a model constant coefficient problem, the two-level convergence factor can be as low as 0.5 [5]. A recent phase error analysis [11] also leads to a similar result. A number of techniques have been proposed to improve multigrid convergence, for instance, applying artificial viscosity on coarse grid matrices [16], Galerkin coarsening [15], Petrov-Galerkin coarsening [3, 6], and higher order coarse grid operators [14].

In this talk, we propose a kernel preserving multigrid approach for solving convection-diffusion equations. The multigrid methods use Petrov-Galerkin coarse grid correction and linear interpolation. The restriction operator is constructed by preserving the kernel of the convection-diffusion operator. The construction considers constant and variable coefficient problems as well as cases where the convection term is not known explicitly. For constant convection, the kernel functions are known analytically. More precisely, they are constant and exponential functions of the form, $e^{-\beta x}$, where β is the convection vector. Then, the restriction weights in one dimension can be easily computed as:

$$\mu = \frac{1}{1+e^{\beta h}}, \quad \nu = \frac{1}{1+e^{-\beta h}}.$$

The restriction in higher dimensions can be constructed similarly as long as the fine grid is a regular refinement of a coarse grid. Note that when $\beta = 0$, i.e. pure diffusion, we recover full-weighting restriction (i.e. transpose of the linear interpolation). When β is large, however, it becomes an upwind biased piecewise constant restriction. One may view this as a generalization of the full-weighting restriction to convection-diffusion equations. We remark that the interpolation weights given above have also been considered in [2]. For nonconstant convection, however, the kernel functions are not known. We thus approximate the kernel locally. One approach is to assume the convection is locally constant and it then reduces to the constant convection case. Another approach is to assume the kernel functions are still constant and exponential functions, $e^{-\beta x}$, where $\beta = \beta(x)$. Finally, if the convection is not given explicitly or the fine grid is not a regular refinement of a coarse grid, we construct the restriction and interpolation operators by solving a minimization problem with constraints given by preserving the left and right null vectors of the matrix A^h. More precisely, let $\{\phi_i^H\}$ and $\{\psi_i^H\}$ be the coarse grid basis functions corresponding to interpolation and restriction, respectively. Our approach is to compute $\{\phi_i^H\}$ and $\{\psi_i^H\}$ at the same time using the minimization problem:

$$\min \quad \sum_{i=1}^{M} (\psi_i^H, \phi_i^H)_A \tag{1}$$

$$\text{subject to} \quad \begin{cases} \sum_{i=1}^{M} \phi_i^H(x_j^h) = 1 \\ \sum_{i=1}^{M} e^{-\beta \cdot x_i^H} \psi_i^H(x_j^h) = e^{-\beta \cdot x_j^h} \end{cases} \qquad j = 1, \ldots, N.$$

When $\beta = 0$, A^h becomes the standard Laplace operator and is symmetric positive definite. Then $\{\psi_i^H\} = \{\phi_i^H\}$ and $(\psi_i^H, \phi_i^H)_A = \|\phi_i^H\|_A^2$, and hence reduces to the elliptic formulation. Thus, it generalizes the energy minimization approach [12] to the convection diffusion case.

The main objective of the restriction operator construction is to ensure that the coarse grid correction process is accurate and stable. We show that although the coarse grid matrix has a phase error of $1/2$ which shifts waves of any frequency

by one grid point, the kernel preserving restriction has the same but opposite effect that counteracts the shifting caused by the coarse grid matrix. As a result, the coarse grid correction is accurate. Specifically, the accuracy of the Petrov-Galerkin coarse grid correction is much better than the direct discretization approach. Moreover, we also prove that the Petrov-Galerkin coarse grid matrix is stable in the sense that it is asymptotically an M-matrix for large convection, if the fine grid matrix is an M-matrix. In contrast, the Galerkin coarse grid matrix (using linear interpolation and full weighting restriction) is unstable operator on the coarse grid, although it has small phase errors like the Petrov-Galerkin approach.

To demonstrate the effectiveness of the proposed multigrid method, we will apply it to solve a real application problem: pricing Asian options. The price of an Asian option can be found by solving a PDE in 2D based on the Black-Scholes equations [17] with appropriate initial and boundary conditions. The resulting PDE is a convection-diffusion equation which has no diffusion in one direction, leading to many numerical difficulties. It is a particularly interesting test case for multigrid since it is very convection dominated (in fact, pure hyperbolic) in the direction with no diffusion and the convection is not constant. We will apply our multigrid with point GS smoothing to solve the zero strike call option, a case where the analytic solution is known. Other numerical results, including entering and recirculating flow problems, will also be presented. We will show that the multigrid convergence rate is independent of the mesh size and insensitive to the convection term.

References

[1] R. E. Bank, W. M. Coughran, and L. C. Cowsar. The finite volume Scharfetter-Gummel method for steady convection diffusion equations. *Comput. Visual. Sci.*, 1:123–136, 1998.

[2] R. E. Bank and S. Gutsch. Hierarchical basis for the convection-diffusion equation on unstructured meshes. In P. Bjorstad, M. Espedal, and D. Keyes, editors, *Ninth International Conference on Domain Decomposition Methods*, pages 251–265. John Wiley & Son, 1998.

[3] A. Brandt. Multigrid solvers for non-elliptic and singular-perturbation steady-state problems. Department of Applied Mathematics, The Weizmann Institute of Science, 76100 Rehovot, Israel, 1981.

[4] A. Brandt and I. Yavneh. On multigrid solution of high-Reynolds incompressible entering flows. *J. Comput. Phys.*, 101:151–164, 1992.

[5] A. Brandt and I. Yavneh. Accelerated multigrid convergence and high-Reynolds recirculating flows. *SIAM J. Sci. Comput.*, 14:607–626, 1993.

[6] J. E. Dendy, Jr. Black box multigrid for nonsymmetric problems. *Appl. Math. Comput.*, 13:261–283, 1983.

[7] A. Jameson. Solution of the Euler equations for two dimensional transonic flow by a multigrid method. *Appl. Math. Comp.*, 13:327–355, 1983.

[8] R. LeVeque. *Numerical Methods for Conservation Laws*. Birkhäuser, Zürich, 1992.

[9] K. W. Morton. *Numerical Solution of Convection-Diffusion Problems*. Chapman & Hall, London, 1996.

[10] C. W. Oosterlee, F. J. Gaspar, T. Washio, and R. Wienands. Multigrid line smoothers for high order upwind discretization of convection-dominated problems. *J. Comp. Phys.*, 139:274–307, 1998.

[11] W. L. Wan and T. F. Chan. A phase error analysis of multigrid methods for hyperbolic equations. *SIAM J. Sci. Comput.*, 25:857–880, 2003.

[12] W. L. Wan, T. F. Chan, and B. Smith. An energy-minimizing interpolation for robust multigrid. *SIAM J. Sci. Comput.*, 21:1632–1649, 2000.
[13] P. Wesseling. *An Introduction to Multigrid Methods*. Wiley, Chichester, 1992.
[14] I. Yavneh. Coarse-grid correction for nonelliptic and singular perturbation problems. *SIAM J. Sci. Comput.*, 19:1682–1699, 1998
[15] P. M. De Zeeuw. Matrix-dependent prolongations and restrictions in a blackbox multigrid solver. *J. Comp. Appl. Math.*, 33:1–27, 1990.
[16] P. M. De Zeeuw and E. J. Van Asselt. The convergence rate of multi-level algorithms applied to the convection-diffusion equations. *SIAM J. Sci. Stat. Comput.*, 6:492–503, 1985.
[17] R. Zvan, P. A. Forsyth, and K. R. Vetzel. Robust numerical methods for PDE models of Asian options. *J. Comp. Finance*, 1:39–78, 1998.

Machnumber independent multigrid convergence for low Machnumber flows

Achim Gordner

Aeroacoustic noise becomes more and more an issue in science and technology. One can perform aeroacoustic simulations either using the popular Hybrid approach or solving the compressible Navier-Stokes equations on one grid [3]. For flows with Machnumbers lower than one $M < 1$, a multiscale problem results, where the relation between the local Strouhalnumber $St = \frac{Lf}{|\mathbf{v}|}$ of the dynamic pressure oscillations in the flow with velocity $\mathbf{v}$ and frequency f and the Helmholtznumber $He = \frac{Lf}{a}$ of the acoustic pressure oscillations is given by the ratio

$$M = \frac{He}{St}. \tag{1}$$

Hereby L denotes a given reference length and a denotes the speed of sound. Hence the ratio of the acoustic wave length λ_a and the dynamic pressure oscillations λ_d is proportional to the Machnumber as well. Therefore, in the hybrid approach, the acoustic grid is coarser than the grid used to calculate the flow solution. To account for the multiscale properties of the wavelengths in pressure variations if the compressible Navier-Stokes equations are calculated on one grid only, one can use an unstructured grid. In the regions, where the fluid flow has to be resolved accurately, the grid becomes sufficiently fine, while in the far field, where only the acoustic dominates, the grid can become much coarser in order to reduce the number of unknowns.

However for low Machnumbers $M << 1$ the grid becomes extremely unstructured which gives raise to a new problem, the limiting time step size due to the CFL-number if someone is using an explicit time stepping scheme. On an optimal designed grid, the ratio between the smallest grid size h_{min} and the largest grid size in the acoustic far-field h_{max} would be

$$M = \frac{h_{min}}{h_{max}}. \tag{2}$$

An optimal relation between the order of the discretization and the gridsize would lead to a constant cutoff frequency f_{max} on the domain Ω, for which frequencies in the velocity field $f_V < f_{max}$ and in the acoustic field $f_A < f_{max}$ can be resolved

accurately with almost no dispersion and diffusion error. With the relevant local CFL-number $\mathrm{CFL}(x) = \frac{a\Delta t}{h(x)}, \quad x \in \Omega$, one get a different cutoff frequency $f_{max} = \frac{1}{\#p\Delta t} = \frac{a}{h\#pCFL_{max}}$, with $CFL_{max} = \max_{x\in\Omega}(CFL(x))$, for the acoustic far field and the velocity field

$$f_{max_V} = \frac{a}{h_{max}\#p\, CFL_{max}} = \frac{|\mathbf{v}|}{h_{min}\#p\, CFL_{max}} \tag{3}$$

and for the acoustic near field

$$f_{max_A} = \frac{a}{h_{min}\#p\, CFL_{max}} \tag{4}$$

$\#p$ denotes the number grid point to be used to resolve a periodic time with a dispersion- and diffusion error lower than ϵ. For a given time-step Δt, the local CFL-number varies

$$CFL(x) \in [C, \frac{C}{M}[\quad \forall x \in \Omega. \tag{5}$$

For explicit methods C has to be smaller than M which results into a relation $f_{max_V} = M f_{max_A}$. The optimal condition, where the cutoff frequency $f_{max} = \min_{x\in\Omega}(f_{max_V}, f_{max_A})$ is constant on the domain Ω, is fulfilled for $C = 1$, resulting into local CFL-numbers greater than 1, which can be solved in general with implicit methods.

However, then for each time-step, after linearization of the nonlinear compressible Navier-Stokes equations, a linear system of equation in the form

$$Jq = b \tag{6}$$

have to be solved, for which a geometric multigrid procedure is used. It is essential for an robust method, that the convergence rate is independent of the Machnumber M. It turned out, theoretical and numerically, that classical iterative methods, like Jacobi or Gauss-Seidel, have to be damped with $\omega \sim M^2$ to be used as a smoother $S = I - \omega W^{-1} J$ within the multigrid process. W^{-1} denotes the approximate inverse of J that is used in the iterative solver. Hence, these are not robust for low Machnumbers [1]. However, ILU_0 showed without damping a Machnumber independent convergence and can be used as a smoother in multigrid to solve the compressible Navier-Stokes equations for low Machnumbers $M < 1$.

In addition, to guarantee also a Machnumber independent coarse grid correction, the injection j has to be used as restriction r within the multigrid process to obtain a robust multigrid convergence with respect to the Machnumber and the discretization used. If someone takes the adjoint of the bilinear prolongation p for the restriction step together with an upwind dominated discretization for the convective parts of the Navier-Stokes equations, the coarse grid correction scales at the boundaries proportional to $\frac{1}{M^2}$, which deteriorate the convergence rate of the multigrid methods for Machnumbers $M < 1$.

Once the Two-grid method is robust against small Machnumber, it can be shown in [1], based on a theorem found in [2], that this holds also for the Multigrid method.

References

[1] A. Gordner, Numerische Simulation nichtlinearer Aeroakustik bei kleinen Machzahlen, Dissertation, University of Heidelberg, 2004.
[2] P. Wesseling, An Introduction to Multigrid Methods, Teubner. 2. edition, 1993.
[3] S.K. Lele, Computational Aeroacoustics: A Review AIAA paper, 97-0018:1ff, 1997.

New Smoothers for the Stokes Problem

Susanne C. Brenner

(joint work with Li-yeng Sung)

We consider the two-dimensional Stokes problem:
Find $(\boldsymbol{u},p)\in[H_0^1(\Omega)]^2\times L_2^0(\Omega)$ such that

$$\mathcal{S}\big((\boldsymbol{u},p),(\boldsymbol{v},q)\big)=(\boldsymbol{f},\boldsymbol{v})_{L_2(\Omega)}\qquad\forall\,(\boldsymbol{v},q)\in[H_0^1(\Omega)]^2\times L_2^0(\Omega), \tag{1}$$

where $\Omega\subset\mathbb{R}^2$ is a bounded polygon, $\boldsymbol{f}\in[L_2(\Omega)]^2$, $L_2^0(\Omega)$ is the subspace of $L_2(\Omega)$ whose members have zero mean, and the bilinear form $\mathcal{S}(\cdot,\cdot)$ is defined by

$$\mathcal{S}\big((\boldsymbol{u},p),(\boldsymbol{v},q)\big)=\int_\Omega\Big[\nabla\boldsymbol{u}:\nabla\boldsymbol{v}+(\nabla\cdot\boldsymbol{v})p+(\nabla\cdot\boldsymbol{u})q\Big]\,dx.$$

Let $\mathcal{T}_k$ $(k=0,1,2,\ldots)$ be a sequence of triangulations of Ω generated by uniform subdivision from an initial mesh $\mathcal{T}_0$. We assume that $\boldsymbol{V}_k\times Q_k\subset[H_0^1(\Omega)]^2\times L_2^0(\Omega)$ is a stable pair of finite element spaces [BF] associated with $\mathcal{T}_k$, i.e., the Ladyzhenskaya-Babuška-Brezzi inf-sup condition

$$\inf_{q\in Q_h}\sup_{\boldsymbol{v}\in\boldsymbol{V}_k}\int_\Omega(\nabla\cdot\boldsymbol{v})q\,dx/(|\boldsymbol{v}|_{H^1(\Omega)}\|q\|_{L_2(\Omega)})\geq\beta>0 \tag{2}$$

holds for a constant β which is independent of k.

Furthermore we assume that the finite element spaces are nested:

$$\boldsymbol{V}_{k-1}\times Q_{k-1}\subset\boldsymbol{V}_k\times Q_k\qquad\text{for}\quad k=1,2,\ldots.$$

Consequently we can use the natural injection as the coarse-to-fine intergrid transfer operator $I_{k-1}^k:\boldsymbol{V}_{k-1}\times Q_{k-1}\longrightarrow\boldsymbol{V}_k\times Q_k$, and then take the fine-to-coarse operator $I_k^{k-1}:\boldsymbol{V}_k\times Q_k\longrightarrow\boldsymbol{V}_{k-1}\times Q_{k-1}$ to be the transpose of I_{k-1}^k with respect to the weighted L_2 inner product on $\boldsymbol{V}_k\times Q_k$ defined by

$$\big((\boldsymbol{v}_1,q_1),(\boldsymbol{v}_2,q_2)\big)_k=(\boldsymbol{v}_1,\boldsymbol{v}_2)_{L_2(\Omega)}+h_k^2(q_1,q_2)_{L_2(\Omega)}, \tag{3}$$

where h_k denotes the mesh size of $\mathcal{T}_k$.

The discrete problem for (1) can be written as

$$S_k(\boldsymbol{u}_k,p_k)=\boldsymbol{f}_k, \tag{4}$$

where $S_k:\boldsymbol{V}_k\times Q_k\longrightarrow\boldsymbol{V}_k\times Q_k$ is defined by

$$\big(S_k(\boldsymbol{v},q),(\boldsymbol{w},r)\big)_k=\mathcal{S}\big((\boldsymbol{v},q),(\boldsymbol{w},r)\big)\quad\forall\,(\boldsymbol{v},q),(\boldsymbol{w},r)\in\boldsymbol{V}_k\times Q_k$$

and $\boldsymbol{f}_k$ is the L_2-orthogonal projection of $\boldsymbol{f}$ in $\boldsymbol{V}_k$.

Different W-cycle multigrid algorithms [H] for the solution of (4) can be constructed using different smoothers. However, all the known convergence results [V, W, BSa, Z, SZ] are established under the assumption that Ω is convex and for norms other than the energy norm $\|\cdot\|_1$ defined by

$$\|(\boldsymbol{v},q)\|_1^2 = |\boldsymbol{v}|_{H^1(\Omega)}^2 + \|q\|_{L_2(\Omega)}^2.$$

Note that the energy norm is the norm where the Stokes problem is well-posed. Indeed the LBB condition (2) implies that

$$\sup_{(\boldsymbol{w},r)\in \boldsymbol{V}_k\times Q_k} \mathcal{S}\big((\boldsymbol{v},q),(\boldsymbol{w},r)\big)/\|(\boldsymbol{w},r)\|_1 \approx \|(\boldsymbol{v},q)\|_1. \tag{5}$$

Our goal is to design multigrid algorithms that can be shown to converge in the energy norm for general Ω. Towards this end we introduce two new smoothers for the generalized Stokes problem $S_k(\boldsymbol{\zeta},\eta) = (\boldsymbol{g},\rho)$.

The first one is defined by

$$(\boldsymbol{\zeta}_j,\eta_j) = (\boldsymbol{\zeta}_{j-1},\eta_{j-1}) + \gamma_k S_k C_k^{-1}\big((\boldsymbol{g},\rho) - S_k(\boldsymbol{\zeta}_{j-1},\eta_{j-1})\big),$$

where the operator $C_k : \boldsymbol{V}_k\times Q_k \longrightarrow \boldsymbol{V}_k\times Q_k$ is symmetric positive-definite with respect to $(\cdot,\cdot)_k$ and satisfies

$$\big(C_k(\boldsymbol{v},q),(\boldsymbol{v},q)\big)_k \approx |\boldsymbol{v}|_{H^1(\Omega)}^2 + \|q\|_{L_2(\Omega)}^2 \qquad \forall\,(\boldsymbol{v},q)\in \boldsymbol{V}_k\times Q_k, \tag{6}$$

and $\gamma_k = (\text{constant})\,h_k^2$ is a damping factor. In practice the construction of C_k^{-1} involves an optimal preconditioner for the discrete Laplace operator where $C_k^{-1}(\boldsymbol{v},q)$ can be computed at a cost proportional to the dimension of $\boldsymbol{V}_k\times Q_k$.

The definition of this smoother is motivated by the relation

$$\big(S_k C_k^{-1} S_k(\boldsymbol{v},q),(\boldsymbol{v},q)\big)_k \approx \|(\boldsymbol{v},q)\|_1^2 \qquad \forall\,(\boldsymbol{v},q)\in \boldsymbol{V}_k\times Q_k, \tag{7}$$

which follows from (5) and (6). From (3) and (7) we see that the constant in the definition of γ_k can be chosen so that

$$\text{the spectral radius of } \gamma_k S_k C_k^{-1} S_k \le 1. \tag{8}$$

In view of (7), it is natural to introduce the following scale of discrete norms on $\boldsymbol{V}_k\times Q_k$:

$$|\!|\!|(\boldsymbol{v},q)|\!|\!|_{s,k}^2 = \big((S_k C_k^{-1} S_k)^s(\boldsymbol{v},q),(\boldsymbol{v},q)\big)_k \qquad \text{for} \quad 0\le s\le 1. \tag{9}$$

Observe that (7) and (9) imply

$$|\!|\!|(\boldsymbol{v},q)|\!|\!|_{1,k} \approx \|(\boldsymbol{v},q)\|_1 \approx |\boldsymbol{v}|_{H^1(\Omega)} + \|q\|_{L_2(\Omega)} \tag{10}$$

and hence, by interpolation,

$$|\!|\!|(\boldsymbol{v},q)|\!|\!|_{s,k} \approx \|\boldsymbol{v}\|_{H^s(\Omega)} + h_k^{1-s}\|q\|_{L_2(\Omega)} \qquad \forall\,(\boldsymbol{v},q)\in \boldsymbol{V}_k\times Q_k. \tag{11}$$

Let $R_k = Id_k - \gamma_k S_k C_k^{-1} S_k$, where Id_k is the identity operator on $\boldsymbol{V}_k$, be the error propagation operator of one smoothing step. It follows from (8) and (9) that R_k has the smoothing properties

$$|\!|\!|R_k^m(\boldsymbol{v},q)|\!|\!|_{1,k} \lesssim h_k^{-t} m^{-t/2} |\!|\!|(\boldsymbol{v},q)|\!|\!|_{1-t,k} \qquad \text{for} \quad 0\le t\le 1. \tag{12}$$

The second smoother is defined by

$$(\boldsymbol{\zeta}_j, \eta_j) = (\boldsymbol{\zeta}_{j-1}, \eta_{j-1}) + \gamma_k C_k^{-1} S_k\big((\boldsymbol{g}, \rho) - S_k(\boldsymbol{\zeta}_{j-1}, \eta_{j-1})\big)$$

and the corresponding error propagation operator is $R_k^* = Id_k - \gamma_k C_k^{-1} S_k^2$. This smoother is motivated by the relation

$$\mathcal{S}\big(R_k(\boldsymbol{v}, q), (\boldsymbol{w}, r)\big) = \mathcal{S}\big((\boldsymbol{v}, q), R_k^*(\boldsymbol{w}, r)\big) \qquad \forall\, (\boldsymbol{v}, q), (\boldsymbol{w}, r)\big) \in \boldsymbol{V}_k \times Q_k, \tag{13}$$

which implies the following smoothing properties through duality:

$$|\!|\!|(R_k^*)^m(\boldsymbol{v}, q)|\!|\!|_{1+t,k} \lesssim h_k^{-t} m^{-t/2} |\!|\!|(\boldsymbol{v}, q)|\!|\!|_{1,k} \qquad \text{for} \quad 0 \le t \le 1, \tag{14}$$

provided that the scale of norms $|\!|\!| \cdot |\!|\!|_{s,k}$ for $1 \le s \le 2$ is defined by

$$|\!|\!|(\boldsymbol{v}, q)|\!|\!|_{s,k} = \sup_{(\boldsymbol{w}, r) \in \boldsymbol{V}_k \times Q_k} \mathcal{S}\big((\boldsymbol{v}, q), (\boldsymbol{w}, r)\big) / |\!|\!|(\boldsymbol{w}, r)|\!|\!|_{2-s,k}. \tag{15}$$

Note that we have, because of (5),

$$|\!|\!|(\boldsymbol{v}, q)|\!|\!|_{1,k} \approx \|(\boldsymbol{v}, q)\|_{1,k} \qquad \forall\, (\boldsymbol{v}, q) \in \boldsymbol{V}_k \times Q_k. \tag{16}$$

On the other hand, using (11), elliptic regularity [D] and duality arguments, we have the following approximation property:

$$|\!|\!|(Id_k - I_{k-1}^k P_k^{k-1})(\boldsymbol{v}, q)|\!|\!|_{1-\alpha,k} \lesssim h_k^{2\alpha} |\!|\!|(\boldsymbol{v}, q)|\!|\!|_{1+\alpha,k}, \tag{17}$$

where $P_k^{k-1} : \boldsymbol{V}_k \times Q_k \longrightarrow \boldsymbol{V}_{k-1} \times Q_{k-1}$ is the Ritz projection operator with respect to the Stokes bilinear form $\mathcal{S}(\cdot, \cdot)$, and $\alpha \in (1/2, 1]$ is the index of elliptic regularity.

The error propagation operator for the two-grid algorithm, where we apply the second smoother m_1 times in the pre-smoothing step and the first smoother m_2 times in the post-smoothing step, is given by $R_k^{m_2}(Id_k - I_{k-1}^k P_k^{k-1})(R_k^*)^{m_1}$. We have, by (10), (12), (14), (16) and (17),

$$\|R_k^{m_2}(Id_k - I_{k-1}^k P_k^{k-1})(R_k^*)^{m_1}(\boldsymbol{v}, q)\|_1 \lesssim (m_1 m_2)^{-\alpha/2} \|(\boldsymbol{v}, q)\|_1. \tag{18}$$

In particular, when Ω is convex, we can take $\alpha = 1$ and the contraction number of the two-grid algorithm decreases at the rate of $(m_1 m_2)^{-1/2}$. The convergence of the W-cycle in the energy norm for a sufficiently large number of smoothing steps follows from (18) and a standard perturbation argument [BD].

Detailed proofs for the results outlined here can be found in [BSu], where we address general saddle point problems [B] and discuss the convergence of W-cycle algorithms in both the energy norm and lower order norms.

Acknowledgement This work is supported in part by the National Science Foundation under Grant No. DMS-03-11790.

References

[BD] R.E. Bank, T.F. Dupont, An optimal order process for solving finite element equations, Math. Comp., 36, 1981, 35–51.

[BSa] D. Braess, R. Sarazin, An efficient smoother for the Stokes equation, Appl. Numer. Math., 23, 1996, 3–19.

[B] S.C. Brenner, Multigrid methods for parameter dependent problems, Math. Modell. Anal. Numer., 30, 1996, 265–297.

[BSu] S.C. Brenner, Li-yeng Sung, New smoothers for saddle point problems, in preparation, 2005.
[BF] F. Brezzi, M. Fortin, Mixed and Hybrid Finite Element Methods, Springer-Verlag, 1991.
[D] M. Dauge, Elliptic Boundary Value Problems on Corner Domains, Springer-Verlag, 1988.
[H] W. Hackbusch, Multi-grid Methods and Applications. Springer-Verlag, 1985.
[SZ] J. Schöberl, W. Zulehner, On Schwarz-type smoothers for saddle point problems, Numer. Math., 95, 2003, 377–399.
[V] R. Verfürth, A multilevel algorithm for mixed problems, SIAM J. Numer. Anal., 21, 1984, 264–271.
[W] G. Wittum, On the convergence of multigrid methods with transforming smoothers, Numer. Math., 57, 1990, 15–38.
[Z] W. Zulehner, A class of smoothers for saddle point problems, Computing, 65, 2000, 227–246.

Meshless Multilevel Methods - Some Analytic Concepts

Wolfgang Dahmen
(joint work with Shai Dekel, Pencho Petrushev)

Meshless methods are currently attracting increasing attention in the computational engineering community. They help avoiding complicated mesh connectivities when dealing with problems of higher spatial dimension and facilitate a painless realization of locally high order of resolution. A unified approach to the main variants such as hp-clouds, radial basis functions or generalized finite elements is given in [BBO]. Nevertheless, the theoretical foundation of the meanwhile acquired substantial computational experience is still at its infancy. This refers, in particular, to the analysis of fast methods for the solution of resulting systems of equations. An account of the state of the art of multigrid solvers can be found in [GS1, S, GS2]. In this lecture, as a conceptual foundation for a better theoretical backup of such methods, a scale of nonlinear smoothness spaces is proposed that is capable among other things of capturing anisotropic features. It is based on multiscale collections of atoms that are products of polynomials and smooth compactly supported cutoff functions forming on each scale a partition of unity. It is indicated under which circumstances representations in terms of such atoms characterize the above mentioned smoothness classes and related best N-term approximation. Possible applications concern meshless methods for the numerical treatment of elliptic boundary value problems based on such collections of atoms. The obtained norm equivalences provide stable splittings for typical energy spaces arising in this context. This allows one to formulate multivariate Schwarz preconditioners that yield uniformly bounded condition numbers and support adaptive updating techniques.

References

[BBO] I. Babuska, U. Banerjee, J.E. Osborn, Survey of meshless and generalized finite element methods,: A unified approach, Acta Numerica, Cambridge University Press, 2003, 1–125.
[GS1] M. Griebel, M.A. Schweitzer, Meshfree Methods for Partial Differential Equations, Lecture Notes in Computational Sciences and Engineering, Springer Verlag, Vol. 26, 2002.

[S] M.A Schweitzer, A Parallel Multilevel Partition of Unity Method for Elliptic Partial Differential Equations, Lecture Notes in Computational Sciences and Engineering, Springer Verlag, Vol. 29, 2003.

[GS2] M. Griebel, M.A. Schweitzer, Meshfree Methods for Partial Differential Equations II, Lecture Notes in Computational Sciences and Engineering, Springer Verlag, Vol. 26, 2004.

Upscaling and multigrid for flow in heterogeneous porous media

Jens P. Eberhard

(joint work with S. Attinger, G. Wittum)

Many scientific problems involve multiple scales and, therefore, multi-scale phenomena. A prominent example for this problem class is the subsurface of the earth. Flow through the subsurface shows a multi-scale behaviour. The system can be modeled by a flow equation for heterogeneous porous media. The fine-scale structure significantly influences here the coarse-scale properties of the system. Consequently, the computational effort to resolve the fine scale often exceeds the power of computers.

We have developed and analyzed a multi-scale upscaling method for flow in heterogeneous porous media. The new upscaling method, called Coarse graining method, is based on filtering procedures introduced in [1]. The main idea is to derive an upscaled flow equation using the Fourier transformation. This is achieved by using projections and Green's function in Fourier space. By cutting-off high frequency modes the upscaled equation brings the small scale information to the large scales through a scale-dependent permeability coefficient. Using perturbative expansions and renormalization group techniques we can derive an explicit function for the upscaled permeability [2]. The advantages of the Coarse graning method are: (1) Upscaling for stochastic media with a continuous scale parameter, (2) The method is easy to compute numerically, (3) It provides a general framework for upscaling of partial differential equations with stochastic coefficients, and (4) Using a perturbative expansion the upscaled coefficients can be evaluated.

The Coarse graining method has been extended to a numerical upscaling which computes the upscaled coefficients locally. We have compared the method with other existing upscaling methods by evaluating fluxes and the solutions of the flow equation for varying scales. In all cases the numerical Coarse graining proves best. Further, the upscaling can be extended to an iterative upscaling which utilizes only the previous upscaled variables for the next upscaling step. The new upscaling method is also powerful to be applicable for other types of processes considered in heterogeneous media, e.g., time-dependent transport in heterogeneous media.

We have also used the results of the upscaling in a multigrid solver to generate the coarse grid operators which are adapted to the problem. We discuss such an (algebraic) multgrid method and give numerical convergence results. For moderate coefficient jumps or variances up to three, the new Coarsening multigrid method is competitive with the algebraic Ruge-Stueben multigrid method and other Galerkin-type multigrid methods with matrix-dependent prolongations [3].

References

[1] S. Attinger, J. Eberhard, N. Neuss, Filtering procedures for flow in heterogeneous porous media: Numerical results, Comput. Visual. Sci., 5, 2002, 67–72.

[2] J. Eberhard, S. Attinger, G. Wittum, Coarse graining for upscaling of flow in heterogeneous porous media. Multiscale Model. Simul., 2(2), 2004, 269–301.

[3] J. Eberhard, G. Wittum, A coarsening multigrid method for flow in heterogeneous porous media, In B. Engquist and P. Lötstedt, editors, *Computational Science and Engineering*, Springer Lecture Notes. Springer, Heidelberg, New York, 2005.

[Co] A. Cohen, Numerical Analysis of Wavelet Methods, Studies in Mathematics and its Applications 32, Elsevier, 2003.

[CDD] A. Cohen, W. Dahmen, R. DeVore, Adaptive wavelet scheme for nonlinear variational problems, SIAM J. Numer. Anal., 41 (5), 2003, 1785–1823.

[DK] W. Dahmen, A. Kunoth, Adaptive wavelet methods for linear–quadratic elliptic control problems: Convergence rates, Preprint # 46, SFB 611, Universität Bonn, December 2002, submitted for publication, revised, November 2003.

Fast methods for simulation based optimization

Volker Schulz

After successfully building up a simulation tool for PDE models within a certain problem class, one is often confronted with the problem of computing optimal shapes, controls, parameters etc. such that the states of the PDE model behave in a desired way. In particular, one is looking for optimization strategies, which enable the re-use of as much of the simulation tool as possible, but have on the other hand a low relative computational complexity, which means $\frac{\text{optimization effort}}{\text{simulation effort}} < \text{const.}$ with a small constant.

In this talk, recent results on a collaborative project with DLR Braunschweig on shape optimization of aircrafts with respect to drag are presented. The underlying flow solver is based on a semi-iterative strategy (so-called pseudo-timestepping in engineering terminology). A simultaneous optimization approach, updating state, adjoint and design variables jointly in each step of the semi-iterative method is shown to lead to a relative computational complexity of const.=4 up-to const.=10, depending on the absence/presence of typical state constraints (lift, pitching moment). First results for the simultaneous optimization strategy applied to a model problem have been presented in [HS]. Practical 2D-results for wing profiles have been published in [HSBG]. The 3D-results presented in the talk will be published soon.

References

[HS] S. B. Hazra, V. Schulz: Simultaneous Pseudo-timestepping for PDE-model based optimization problems. Bit Numerical Mathematics, Vol. 44, No. 3, pp. 457-472, 2004.

[HSBG] S. B. Hazra, V. Schulz, J. Brezillon, N. Gauger: Aerodynamic shape optimization using simultaneous pseudo-timestepping. Journal of Computational Physics, Vol. 204, No.1, pp. 46-64, 2005.

Monotone Multigrid Methods Based on B–Splines

Angela Kunoth
(joint work with Markus Holtz)

We consider on a domain $\Omega \subset \mathbb{R}^d$ an elliptic variational inequality

$$\text{find } u \in \mathcal{K}: \;\; a(u, v-u) \geq f(v-u) \;\; \text{ for all } v \in \mathcal{K},$$

involving a continuous, symmetric and $H_0^1(\Omega)$– elliptic bilinear form $a(\cdot,\cdot)$ and a linear functional $f : H_0^1(\Omega) \to \mathbb{R}$. The inequality is to be solved on a closed convex subspace

$$\mathcal{K} := \{v \in H_0^1(\Omega): \; v(x) \leq g(x) \;\; \text{ for all } x \in \Omega\} \subset H_0^1(\Omega),$$

where $g \in H_0^1(\Omega)$ represents a given upper obstacle.

For the efficient numerical solution of such variational inequalities, multigrid methods in different variants based on piecewise linear finite elements have been investigated over the past decades, see, e.g., [BC, HM, Hp, M]. However, not all of them have assured that on coarser grids the obstacle criterion is met, which is essential for the success of these methods. A systematic discussion of this issue can be found in [Ko1, Ko2] in which context the terminology *monotone multigrid (MMG) methods* was introduced. For piecewise finite elements as basis functions, the appropriate approximation of the obstacle on coarser grids can be based on geometric considerations employing point values. For higher order basis functions, working with function evaluations does no longer yield admissible obstacle approximations so that an extension of the multigrid method to higher order basis functions is not so obvious.

On the other hand, there are a number of problems which profit from higher order approximations. Among these is the problem of prizing American options, formulated in a standard model as a parabolic boundary value problem involving Black–Scholes' equation with a free boundary which indicates when the option is to be exerted. In addition to computing this free boundary, of particular importance are pointwise derivatives of the solution, the value of the stock option, up to order two to high precision, the so–called Greek letters.

In this talk based on [HK], a monotone multigrid method was presented for discretizations in terms of B–splines of arbitrary order to solve variational inequalities of the above form. In order to maintain monotonicity (upper bound) and quasi–optimality (lower bound) of the coarse grid corrections for the equivalent linear complementary problem, we have proposed an optimized coarse grid correction (OCGC) algorithm which is based on B–spline evaluation coefficients. The OCGC scheme was formulated by solving a linear constrained optimization problem. For the solution process, we have exploited essential properties of B–Splines, namely, positivity of B–Splines and total positivity of their refinement matrices. We have proved that the OCGC algorithm is of optimal complexity of the degrees of freedom of the coarse grid. Moreover, the resulting monotone multigrid method was shown to be of optimal multigrid complexity and converges with an optimal rate independent of the discretization. Using tensor products, the construction of the

OCGC scheme can be shown to be immediately extensible to the multivariate case, yielding also an MMG method of optimal complexity.

Finally, the method was applied to the valuation of American options. It was shown that a discretization based on B–Splines of order four in particular meets the requirement of computing the pointwise error of the second derivative of the value of the stock option up to high precision. Further results for the prizing of options applying monotone multigrid methods can be found in [Hz].

References

[BC] A. Brandt, C.W. Cryer, *Multigrid algorithms for the solution of linear complementary problems arising from free boundary problems*, SIAM J. Sci. Stat. Comput. 4, 655–684, 1983.

[HM] W. Hackbusch, H.D. Mittelmann, *On multigrid methods for variational inequalities*, Numer. Math. 42, 65–76, 1983.

[Hz] M. Holtz, *On the computation of American option price sensitivities via multigrid schemes*, Manuscript, October 2004, submitted for publication.

[HK] M. Holtz, A. Kunoth, *Construction of B–spline based higher order monotone multigrid methods*, Manuscript, September 2004, submitted for publication.

[Hp] R.H.W. Hoppe, *Multigrid algorithms for variational inequalities*, SIAM J. Numer. Anal. 24, 1046–1065, 1987.

[Ko1] R. Kornhuber, *Monotone multigrid methods for elliptic variational inequalities I*, Numer. Math. 69, 167–184, 1994.

[Ko2] R. Kornhuber, *Adaptive Monotone Multigrid Methods for Nonlinear Variational Problems*, Teubner, 1997.

[M] J. Mandel, *A multilevel iterative method for symmetric, positive definite linear complementarity problems*, Appl. Math. Optimization 11, 77–95, 1984.

Balancing Domain Decomposition by Constraints – New Results

Olof B. Widlund

(joint work with Jing Li)

The often very large linear systems of algebraic equations which arise in finite element analysis of linear elasticity and other applications have traditionally been solved directly using a Cholesky factorization in engineering software systems. Considerable and steady progress is being made in the deployment of efficient solvers of this kind. In this talk, an alternative approach is explored, which has been proven quite successful even on massively parallel computers.

Domain decomposition methods are preconditioned iterative methods often using conjugate gradients. The preconditioners are often built from direct Cholesky solvers for problems on the subdomains and a global component which is necessary to ensure scalability, i.e., a convergence rate which is independent of the number of subdomains into which the original elastic body, etc., has been divided and which deteriorates very slowly with the number of degrees of freedom of the individual subdomains. In a BDDC or FETI–DP domain decomposition algorithm, the global component is given in terms of a set of constraints on the continuity of the finite element solution across the interfaces of the decomposition. We demonstrate

that FETI-DP and BDDC algorithms, see [FDP, SDP, NIE, CBD], can be built from a few simple components of which a Cholesky solver is the most important. This framework also highlights the close relationship between these two families of algorithms; in fact the iteration operators of a pair of FETI–DP and BDDC algorithms, with the same set of constraints, have the same eigenvalues with the possible exception of 0 and 1; see [ATP]. Their rates of convergence are therefore virtually identical and the choice of one method over another can be based on other considerations. It appears that the BDDC algorithms often have certain advantages over the FETI-DP methods, e.g., when developing multi-level algorithms; see [TLB, TLB2] for recent work on three-level BDDC methods motivated by the introduction of very powerful parallel computing systems with very many processors.

With Jing Li, the speaker has recently rederived the BDDC and FETI–DP algorithms, see [FBC], and provided a much shorter proof of the main result of [ATP]. One of the main ideas behind this work is an explicit change of variables which also is described in [FDP] and which appears to lead to a greater robustness of the FETI–DP algorithms; see [PID].

There has also been recent, relatively extensive work on BDDC and FETI–DP algorithms for mixed finite element methods and the resulting saddle point problems. A pioneering effort was carried out by Jing Li in his doctoral dissertation, [FSS]. More recent work is due to Dohrmann [NIE] and Li and the speaker [BAS] in which the same close connection between the spectra of the FETI–DP and BDDC algorithms is established under a certain assumption on the constraints. Xuemin Tu has also completed two papers, [PMF, PMH], on BDDC algorithms for the equations of flow in porous media.

References

[PSC] Clark R. Dohrmann, A preconditioner for substructuring based on constrained energy minimization, SIAM J. Sci. Comput., 25 (1), 2003, 246–258.

[NIE] Clark R. Dohrmann, A Substructuring Preconditioner for Nearly Incompressible Elasticity Problems, technical report SAND2004-539, SANDIA National Laboratories, October 2004.

[FDP] Charbel Farhat, Michel Lesoinne, Patrick Le Tallec, Kendall Pierson, Daniel Rixen, FETI-DP: A Dual-Primal Unified FETI Method – Part I: A Faster Alternative to the Two-Level FETI Method, Internat. J. Numer. Methods Engrg., 50, 2001, 1523–1544.

[SDP] Charbel Farhat, Michel Lesoinne, Kendall Pierson, A scalable dual-primal domain decomposition method, Numer. Linear Algebra Appl., 7 (7–8), 2000, 687–714.

[FDP] Axel Klawonn, Olof B. Widlund, Dual-Primal FETI Methods for Linear Elasticity, technical report TR2004-855, Department of Computer Science, Courant Institute of Mathematical Sciences, September 2004, submitted for publication.

[PID] Axel Klawonn, Oliver Rheinbach, A parallel implementation of Dual-Primal FETI methods for three dimensional linear elasticity using a transformation of basis, technical report University of Duisburg–Essen, SM-E-601, February 2005.

[FSS] Jing Li, Dual-Primal FETI Methods for Stationary Stokes and Navier-Stokes Equations, PhD thesis, Courant Institute, technical report TR2002-830, Department of Computer Science, Courant Institute of Mathematical Sciences, September, 2002.

[FBC] Jing Li, Olof B. Widlund, FETI–DP, BDDC, and Block Cholesky Methods, technical report TR2004-857, Department of Computer Science, Courant Institute of Mathematical Sciences, December 2004, submitted for publication.

[BAS] Jing Li, Olof B. Widlund, BDDC Algorithms for Incompressible Stokes Equations, technical report TR2005-861, Department of Computer Science, Courant Institute of Mathematical Sciences, April 2005, submitted for publication.

[CBD] Jan Mandel, Clark R. Dohrmann, Convergence of a Balancing Domain Decomposition by Constraints and Energy Minimization, Numer. Linear Algebra Appl., 10, 2003, 639–659.

[ATP] Jan Mandel, Clark R. Dohrmann, Radek Tezaur, An Algebraic Theory for Primal and Dual Substructuring Methods by Constraints, Appl. Numer. Math., 2005, to appear.

[TLB] Xuemin Tu, Three-level BDDC in Two Dimensions, technical report TR2004-856, Department of Computer Science, Courant Institute of Mathematical Sciences, November 2004, submitted for publication.

[TLB2] Xuemin Tu, Three-level BDDC in Three Dimensions, technical report TR2005-862, Department of Computer Science, Courant Institute of Mathematical Sciences, April 2005, submitted for publication.

[PMF] Xuemin Tu, A BDDC Algorithm for a Mixed Formulation for Flow in Porous Media, technical report TR2005-864, Department of Computer Science, Courant Institute of Mathematical Sciences, May 2005, submitted for publication.

[PMH] Xuemin Tu, A BDDC Algorithm for Flow in Porous Media with a Hybrid Finite Element Discretization, technical report TR2005-865, Department of Computer Science, Courant Institute of Mathematical Sciences, May 2005, submitted for publication.

A Simple Projected Multigrid Algorithms for Locally Refined Meshes

Peter K. Jimack
(joint work with Alison C. Jones)

This work is concerned with the fast solution of partial differential equations (PDEs) where the solution may vary rapidly in some parts of the domain yet be smooth and slowly varying elsewhere. In such cases it is natural to use some form of adaptivity to ensure that the resolution of the solution is sufficiently fine to obtain a solution that is accurate everywhere, whilst avoiding the use of an excessive number of degrees of freedom. Examples of this type of PDE are numerous and include convection-dominated problems, whose solution may contain steep fronts or boundary layers, and phase-change or free-boundary problems for which the interface geometry should be resolved to a high accuracy [PGD]. In this work we focus on the use of adaptivity based upon hierarchical local mesh refinement. In two space dimensions this typically involves the use of a quad-tree mesh data structure to organise the local refinement and coarsening of triangular or quadrilateral mesh elements, e.g. [PGD] (in three dimensions, not explicitly considered here, the corresponding data structure is an oct-tree with tetrahedral or octahedral mesh elements, e.g. [SB]).

In addition to using mesh refinement in order to improve efficiency it is also important to use the best possible solution algorithms for the discrete systems of equations that arise on these grids. For many time-dependent problems this means the use of an implicit time-stepping algorithm combined with a fast algebraic solver such as multigrid, [Bra]. It is clear that multigrid algorithms should fit

naturally into the framework of a numerical code which is built around hierarchical mesh refinement. Indeed numerous authors have considered such a combination with great success, including [Bra, HMO] for example. Perhaps the main practical issue that needs to be overcome in order to efficiently implement a multigrid solver on a locally refined sequence of grids is the need to decide what action to take at the boundary of locally refined regions. Numerous possibilities exist, including: treating such boundaries as Dirichlet conditions for the refined regions, [Bra]; undertaking additional local refinement with special temporary elements that remove the *hanging nodes* that lie on edges which have refined elements on one side and a non-refined element on the other (this is often referred to as *green refinement*, [Riv, SB]), and; modifying the usual finite element basis to ensure that the trial space remains continuous everywhere, [Wan].

Here we present an alternative approach for the implementation of multigrid on a locally refined sequence of meshes based upon a minor modification of the full approximation scheme (FAS) algorithm. It is motivated by the work of Meyer [Mey] in which constraints are imposed on the solution values at hanging nodes only after the finite element system has been assembled for a class of linear problems: these constraints appearing simply as a minor modification to the usual preconditioned conjugate gradient algorithm. To illustrate the approach we consider a simple linear elliptic model problem and then indicate the generalization to the nonlinear case.

Poisson's equation, with Dirichlet boundary conditions $u|_{\partial\Omega} = 0$, on a square domain $\Omega \in \Re^2$ is given by:

$$\text{find} \quad u \in H_0^1(\Omega) \quad \text{such that} \quad a(u,v) = b(v) \;\; \forall v \in H_0^1(\Omega) \tag{1}$$

where

$$a(u,v) = \int_\Omega \underline{\nabla} u \cdot \underline{\nabla} v \; d\underline{x} \quad \text{and} \quad b(v) = \int_\Omega f v \; d\underline{x} \; .$$

The standard finite element (FE) approach prescribes a conforming mesh, of rectangles say, and a space $S^h \subset H_0^1(\Omega)$, of piecewise bilinears say, such that:

$$\text{find} \quad u^h \in S^h \quad \text{such that} \quad a(u^h, v^h) = b(v^h) \;\; \forall v^h \in S^h \; .$$

Selecting a basis $\{\phi_1, ..., \phi_n\}$ for S^h, the usual FE "hat" functions say, leads to a linear algebraic system:

$$A\underline{u} \; = \; \underline{b} \, . \tag{2}$$

Here $A \in \Re^{n\times n}$, $\underline{u} \in \Re^n$, $\underline{b} \in \Re^n$ and

$$A_{ij} = a(\phi_i, \phi_j) = \sum_{e=1}^{E} a^e(\phi_i, \phi_j), \quad b_i = b(\phi_i) = \sum_{e=1}^{E} b^e(\phi_i), \quad u^h = \sum_{j=1}^{n} u_j \phi_j \; ,$$

where the superscript e indicates that integration is restricted to element e.

Now suppose that the FE mesh is locally refined and contains some *hanging nodes*: $\overline{n}$ nodes in total (excluding the Dirichlet boundary) of which m are hanging nodes (and let $n = \overline{n} - m$). For each node $i = 1, ..., \overline{n}$ define $\overline{\phi}_i$ to be:

- zero on each element that does not have node i as a vertex,

- bilinear on remaining elements with value 1 at node i and 0 at the other vertices.

Now, let $\overline{S}^h = \text{Span}\{\overline{\phi}_1, ..., \overline{\phi}_{\overline{n}}\}$ and let $\overline{u}^h \in \overline{S}^h$ be given by $\overline{u}^h = \sum_{j=1}^{\overline{n}} \overline{u}_j \overline{\phi}_j$. Note that when $m \geq 1$ this is not a subspace of $H^1(\Omega)$. Furthermore, define $S^h \subset \overline{S}^h$ to be the n-dimensional space given by

$$\begin{aligned} S^h \quad = \quad & \{\sum_{j=1}^{\overline{n}} u_j \overline{\phi}_j : \text{at each hanging node, } k \text{ say, } u_k = \tfrac{1}{2}(u_{k(1)} + u_{k(2)}) \text{ where} \\ & k(1) \text{ and } k(2) \text{ are the two neighbours of node } k\} \ . \end{aligned}$$

We will seek a finite element solution to (1) from S^h.

Rather than working with a basis for S^h directly however we propose an alternative which is designed lead to a more straightforward implementation of the multigrid solver. To achieve this consider assembling the FE equations on each element of the non-conforming mesh, using the non-conforming basis, to obtain

$$\overline{A}\underline{\overline{u}} = \underline{\overline{b}} \ , \tag{3}$$

where $\overline{A} \in \Re^{\overline{n} \times \overline{n}}$, $\underline{\overline{u}} \in \Re^{\overline{n}}$, $\underline{\overline{b}} \in \Re^{\overline{n}}$ and

$$\overline{A}_{ij} = \sum_{e=1}^{E} a^e(\overline{\phi}_i, \overline{\phi}_j) \ , \quad \overline{b}_i = \sum_{e=1}^{E} b^e(\overline{\phi}_i) \ .$$

Let $U^n \subset \Re^{\overline{n}}$ such that: $\underline{u} \in U^n \Leftrightarrow \sum_{j=1}^{\overline{n}} u_j \overline{\phi}_j \in S^h$. Also define $P \in \Re^{\overline{n} \times \overline{n}}$ such that

$$(P\underline{u})_k = \begin{cases} \frac{1}{2}(u_{k(1)} + u_{k(2)}) & \text{when } k \text{ is a } \textit{hanging node}, \\ u_k & \text{otherwise.} \end{cases}$$

Note that $P : \Re^{\overline{n}} \to U^n$. Although we assemble (3) we really wish to solve

$$P^T \overline{A} P \underline{u} \ = \ P^T \underline{\overline{b}} \tag{4}$$

which represents n independent equations for n degrees of freedom (since $(P^T \underline{\overline{u}})_k = 0$ for each k corresponding to a *hanging node*). To apply a smoothing step of Jacobi iteration we should use a solution update vector of the form:

$$\underline{\delta} = P(\text{diag}(P^T \overline{A} P))^{-1}(P^T \underline{\overline{b}} - P^T \overline{A} \underline{u}^{\text{old}}) \ ,$$

ensuring that the initial guess $\underline{u}^0 \in U^n$ (hence $\underline{u}^{\text{old}} \in U^n$ and therefore $P\underline{u}^{\text{old}} = \underline{u}^{\text{old}}$). In fact we may still obtain the required smoothing property if the diagonal matrix is simplified to $(\text{diag}(A))^{-1}$ and a relaxation parameter, ω, is incorporated in the update.

The generalization of the above idea to a nonlinear elliptic problem is straightforward.

- Discretize the problem by taking the FE approximation on each element and then assemble as normal (i.e. without regard for hanging nodes).

- Apply the projected version of *nonlinear* Jacobi iteration, say, as above to "solve" the non-conforming system $\overline{\underline{b}} - \overline{\underline{A}}(\overline{\underline{u}}) = \underline{0}$. This gives $\underline{\delta} = \omega P \overline{\underline{\delta}}$ where

$$\overline{\delta}_j = \left(P^T \overline{\underline{b}} - P^T \overline{\underline{A}}(\underline{u}^{\text{old}}) \right)_j / \left(\frac{\partial \overline{\underline{A}}}{\partial u_j}(\underline{u}^{\text{old}}) \right)_j .$$

In practice this smoother is applied as part of a nonlinear multigrid scheme and it is demonstrated that the FAS scheme requires only minor modification to ensure that at every stages the latest estimate of the solution lies within the conforming subspace: by applying the projections P and P^T at appropriate stages in the update procedure [JJ]. This works naturally in the FAS context since this algorithm always maintains and updates an approximation to the solution itself.

Some examples are presented to illustrated the optimal performance of this PFAS (projected FAS) approach for nonlinear elliptic PDEs and systems of nonlinear parabolic equations discretized implicitly in time. The optimal behaviour is as expected however the contribution of this work is to present a simpler implementation of the adaptive multigrid approach than is currently available elsewhere.

References

[Bra] A. Brandt, Multi-level adaptive solutions to boundary-value problems, Math. Comp., 31, 1977, 333–390.

[HMO] L. Hart, S. McCormick, A. O'Gallagher, The fast adaptive composite-grid method (FAC): algorithms for advanced computers, Appl. Math. Comp., 19, 1986, 103–125.

[JJ] A.C. Jones, P.K. Jimack, An adaptive multigrid tool for elliptic and parabolic systems, Int. J. Numer. Meth. Fluids, 47, 2005, 1123–1128.

[Mey] A. Meyer, Projection techniques embedded in the PCGM for handling hanging nodes and boundary restrictions, in Engineering Computational Technology, Topping B.H.V, Bittnar Z (eds). Saxe-Coburg Publications, Stirling, Scotland, 2002, 147–165.

[PGD] N. Provatas, N. Goldenfeld, J. Dantzig, Adaptive mesh refinement computation of solidification mircostructures using dynamic data structures, J. Comp. Phys., 148, 1999, 265–290.

[Riv] M.-C. Rivara, A grid generator based upon 4-traingles conforming mesh-refinement algorithm, Int. J. Numer. Meth. Engrg., 24, 1987, 1343–1354.

[SB] W. Speares, M. Berzins, A 3-d unstructured mesh adaption algorithm for time-dependent shock dominated problems, Int. J. Num. Meth. Fluids, 25, 1997, 81-104.

[Wan] W. Wang, Special bilinear quadrilateral elements for locally refined finite element grids, SIAM J. Sci. Comp., 22, 2001, 2029–2050.

Asymptotically Exact Functional Error Estimators on Meshes with Superconvergence

Jeffrey S. Ovall

The use of dual/adjoint problems for approximating functionals of solutions of PDEs with great accuracy or to merely drive a goal-oriented adaptive refinement scheme has become well-accepted, and it continues to be an active area of research [EHL, GS, HR, OP]. The traditional approach involves dual residual weighting (DRW). In this work we present two new functional error estimators based on

gradient recovery results of Bank and Xu [BX1, BX2] and give conditions under which we can expect them to be asymptotically exact. The first of these estimators is of the DRW type, but the second involves dual error estimate weighting (DEW) and uses the original stiffness matrix in its computation.

We consider second order linear elliptic problems on a bounded domain $\Omega \subset \mathbb{R}^2$, with weak formulation

$$B(u,v) \equiv \int_\Omega a\nabla u \cdot \nabla v + (\mathbf{b}\cdot\nabla u + cu)v\,dx = \int_\Omega fv\,dx \equiv F(v),$$

where B and F are bounded and B is coercive. In [BX1], Bank and Xu show that

$$\|\nabla u - Q\nabla u_h\|_{1,\Omega} \lesssim h^{1+\min(1,\sigma)}|\log h|\|u\|_{3,\infty,\Omega},$$

where u_h is the piecewise linear finite element solution, Q is the (componentwise) global L^2-projector into the space of piecewise linear polynomials on the mesh, and σ is a measure of the violation of an $\mathcal{O}(h^2)$ approximate parallelogram assumption on the mesh. Here we also show that

$$\|\nabla u - \nabla\varepsilon_h\|_{1,\Omega} \lesssim h^{1+\min(1,\sigma)}|\log h|\|u\|_{3,\infty,\Omega},$$

where ε_h satisfies the residual equation $B(\varepsilon_h, v) = F(v) - B(u_h, v)$ on the space of quadratic "bump" functions on the mesh. These two estimates form the basis for the two functional error estimators.

Let G be a given functional of interest and $B^*(w,v) \equiv B(v,w)$ denote the dual bilinear form. We take ω_h to be the piecewise linear finite element solution of the dual equation $B^*(\omega_h, v) = G(v)$, and ε_h to be the solution of the dual residual equation $B^*(\varepsilon_h, v) = G(v) - B^*(\omega_h, v)$ on the space of quadratic bump functions. The two functional error estimators which we propose are

$$\mathcal{G}_1 = F(\varepsilon_h) - B(u_h, \varepsilon_h) \quad \text{and} \quad \mathcal{G}_2 = \int_\Omega a(Q-I)\nabla u_h \cdot (Q-I)\nabla\omega_h\,dx,$$

and we show that

$$\begin{aligned} |G(u-u_h) - \mathcal{G}_1| &\lesssim h^{2+2\min(1,\sigma)}|\log h|^2\|u\|_{3,\infty,\Omega}\|\omega\|_{3,\infty,\Omega} \\ |G(u-u_h) - \mathcal{G}_2| &\lesssim h^{2+\min(1,\sigma)}|\log h|\|u\|_{3,\infty,\Omega}\|\omega\|_{3,\infty,\Omega}. \end{aligned}$$

The functional error estimator $\mathcal{G}_1$ is of DRW type, and $\mathcal{G}_2$ is representative of a new class of estimators, of DEW type, which employ gradient recovery techniques. If the functional error satisfies $h^2 \lesssim |G(u-u_h)|$, for example, then both $\mathcal{G}_1$ and $\mathcal{G}_2$ are asymptotically exact estimators of $G(u-u_h)$. We demonstrate the accuracy of the estimator $\mathcal{G}_2$ and the usefulness of the corresponding local error indicators for refinement on several examples - with functionals including weighted averages, point values, and approximate local norms.

References

[BX1] R. E. Bank, J. Xu, Asymptotically exact a posteriori error estimators. I. Grids with superconvergence, SIAM J. Numer. Anal., 41 (6), 2003, 2294–2312 (electronic).

[BX2] R. E. Bank, J. Xu, Asymptotically exact a posteriori error estimators. II. General unstructured grids, SIAM J. Numer. Anal., 41 (6), 2003, 2313–2332 (electronic).

[EHL] D. J. Estep, M. J. Holst, M. Larson, Generalized Green's Functions and the Effective Domain of Influence, SIAM J. Sci. Comput., 26 (4), 2005, 1314–1339.
[GS] M. Giles, E. Süli, Adjoint methods for PDEs: *a posteriori* error analysis and postprocessing by duality, Acta Numerica vol. 11, Cambridge University Press, 2002, 145–236.
[HR] V. Heuveline, R. Rannacher, Duality-based adaptivity in the *hp*-finite element method, J. Numer. Math., 121 (2), 2003, 95–113.
[Ov] J. S. Ovall, Asymptotically exact functional error estimators based on gradient recovery, Numer. Math., submitted, 2005.
[OP] S. Prudhomme, J. T. Oden, On goal-oriented error estimation for elliptic problems: application to control of pointwise errors, Comput. Methods Appl. Mech. Engrg., 1-4, 1999, 313-331.

Multilevel Solvers for Partition of Unity Methods

Marc Alexander Schweitzer
(joint work with Michael Griebel, Peter Oswald)

1. Partition of Unity Method

The particle–partition of unity method (PUM) [1, 2, 3, 4, 5, 6, 8] is a meshfree Galerkin method for the numerical treatment of partial differential equations (PDE). In essence, it is a generalized finite element method (GFEM) which employs piecewise rational shape functions rather than piecewise polynomial functions. The PUM shape functions, however, make up a basis of the discrete function space unlike other GFEM approaches which allows us to construct fast multilevel solvers in a similar fashion as in the finite element method (FEM).

In the following, we shortly review the construction partition of unity spaces and the meshfree Galerkin discretization of an elliptic PDE. Furthermore, we give a summary of the efficient multilevel solution of the arising linear block-system.

1.1. **Construction of Partition of Unity Spaces.** In a partition of unity method, we define a global approximation u^{PU} simply as a weighted sum of local approximations u_i, i.e. $u^{\mathrm{PU}}(x) := \sum_{i=1}^{N} \varphi_i(x) u_i(x)$. These local approximations u_i are completely independent of each other, i.e., the local supports $\omega_i := \mathrm{supp}(u_i)$, the local basis $\{\psi_i^n\}$ and the order of approximation p_i for every single $u_i := \sum u_i^n \psi_i^n \in V_i^{p_i}$ can be chosen independently of all other u_j. Here, the functions φ_i form a partition of unity (PU). They are used to splice the local approximations u_i together in such a way that the global approximation u^{PU} benefits from the local approximation orders p_i yet it still fulfills global regularity conditions. Hence, the global approximation space on Ω is defined as

$$V^{\mathrm{PU}} := \sum_i \varphi_i V_i^{p_i} = \sum_i \varphi_i \,\mathrm{span}\langle\{\psi_i^n\}\rangle = \mathrm{span}\langle\{\varphi_i \psi_i^n\}\rangle.$$

The starting point for any meshfree method is a collection of N independent points $P := \{x_i \in \mathbb{R}^d \,|\, x_i \in \overline{\Omega}, i = 1, \ldots, N\}$. In the PU approach we need to construct a partition of unity $\{\varphi_i\}$ on the domain of interest Ω to define an approximate solution where the union of the supports $\mathrm{supp}(\varphi_i) = \overline{\omega_i}$ covers the

domain $\overline{\Omega} \subset \bigcup_{i=1}^{N} \omega_i$ and $u_i \in V_i^{p_i}(\omega_i)$ is some locally defined approximation of order p_i to u on ω_i. Thus, the first (and most crucial) step in a PUM is the efficient construction of an appropriate cover $C_\Omega := \{\omega_i\}$. We use a tree-based construction algorithm for d-rectangular covers C_Ω presented in [2, 8]. Here, the cover patches ω_i are products of intervals $(x_i^l - h_i^l, x_i^l + h_i^l)$ for $l = 1, \ldots, d$. With the help of weight functions W_k defined on these cover patches ω_k we can easily generate a partition of unity by *Shepard's method*, i.e., we define

$$\varphi_i(x) = \frac{W_i(x)}{\sum_{\omega_k \in C_\Omega^i} W_k(x)},$$

where $C_i := \{\omega_j \in C_\Omega \,|\, \omega_i \cap \omega_j \neq \emptyset\}$ is the set of all geometric neighbors of a cover patch ω_i. Due to the use of d-rectangular patches ω_i, the most natural choice for a weight function W_i is a product of one-dimensional functions, i.e., $W_i(x) = \prod_{l=1}^{d} W_i^l(x^l) = \prod_{l=1}^{d} \mathcal{W}(\frac{x - x_i^l + h_i^l}{2h_i^l})$ with $\mathrm{supp}(\mathcal{W}) = [0, 1]$ such that $\mathrm{supp}(W_i) = \overline{\omega_i}$. It is sufficient for this construction to choose a one-dimensional weight function $\mathcal{W}$ with the desired regularity which is non-negative. The partition of unity functions φ_i inherit the regularity of the generating weight function $\mathcal{W}$.

In general, a partition of unity $\{\varphi_i\}$ can only recover the constant function on the domain Ω. Hence, we need to improve the approximation quality to use the method for the discretization of a PDE. To this end, we multiply the partition of unity functions φ_i locally with polynomials ψ_i^n. Since we use d-rectangular patches ω_i only, a local tensor product space is the most natural choice. Here, we use products of univariate Legendre polynomials as local approximation spaces $V_i^{p_i}$, i.e., we choose $V_i^{p_i} = \mathrm{span}\langle\{\psi_i^n \,|\, \psi_i^n = \prod_{l=1}^{d} \mathcal{L}_i^{\hat{n}_l}, \|\hat{n}\|_1 = \sum_{l=1}^{d} \hat{n}_l \leq p_i\}\rangle$, where $\hat{n}$ is the multi-index of the polynomial degrees $\hat{n}_l$ of the univariate Legendre polynomials $\mathcal{L}_i^{\hat{n}_l} : [x_i^l - h_i^l, x_i^l + h_i^l] \to \mathbb{R}$, and n is the index associated with the product function $\psi_i^n = \prod_{l=1}^{d} \mathcal{L}_i^{\hat{n}_l}$.

1.2. **Galerkin Discretization.** Consider the elliptic boundary value problem

$$Lu = f \quad \text{in } \Omega \subset \mathbb{R}^d, \qquad Bu = g \quad \text{on } \partial\Omega,$$

where L is a symmetric partial differential operator of second order and B expresses suitable boundary conditions. The imposition of essential boundary conditions within meshfree methods is more involved than in the FEM for a number of reasons and many different approaches have been proposed. We use Nitsche's method [7] to enforce Dirichlet boundary conditions. The main advantages of this approach are that it does not require a second function (or multiplier) space and that it leads to a positive definite linear system, see [5, 8] for a more detailed discussion of Nitsche's method in the PUM context. Here, we just state resulting weak formulation $a(u, v) = l(v)$ of the simple Poisson problem

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega \subset \mathbb{R}^d, \\ u &= g_D && \text{on } \Gamma_D \subset \partial\Omega, \\ u_n &= g_N && \text{on } \Gamma_N = \partial\Omega \setminus \Gamma_D, \end{aligned}$$

with mixed boundary conditions which reads as

$$(1)\quad \int_\Omega \nabla u \nabla v + \int_{\Gamma_D} u(\beta v - v_n) - u_n v = \int_\Omega fv + \int_{\Gamma_D} g_D(\beta v - v_n) + \int_{\Gamma_N} g_N v,$$

where the subscript n denotes the normal derivative and β is the Nitsche regularization parameter which depends on the employed PUM space but can be precomputed without much additional cost. Finally, for the Galerkin discretization of (1) we have to compute the stiffness matrix

$$A = (A_{(i,n),(j,m)})\,,\ \text{with } A_{(i,n),(j,m)} = a\,(\varphi_j\psi_j^m, \varphi_i\psi_i^n) \in \mathbb{R}\,,$$

and the right-hand side vector

$$\hat{f} = (f_{(i,n)})\,,\ \text{with } f_{(i,n)} = \langle f, \varphi_i\psi_i^n\rangle_{L^2} = \int_\Omega f\varphi_i\psi_i^n \in \mathbb{R}\,.$$

The stable approximation of these integrals is somewhat more involved than in the FEM. Due to the meshfree construction given above the shape functions $\varphi_i\psi_i^n$ are piecewise rational functions only so that the respective integrands have a number of jumps within the integration domain which need to the resolved. For the stable numerical integration of the weak form we use a tree-based decompostion scheme together with efficient sparse grid integration rules, see [2, 8].

1.3. **Multilevel Solution of Resulting Linear System.** In a multilevel method we need a sequence of discretization spaces V_k with $k = 0, \ldots, J$ where J denotes the finest level. To this end we construct a sequence of PUM spaces V_k^{PU} with the help of a tree-based algorithm developed in [2, 3]. As a first step we generate a sequence of point sets P_k and covers C_Ω^k from a given initial point set $\tilde{P}$ with this algorithm. Following the construction given in §1.1 we can then define an associated sequence of PUM spaces V_k^{PU}. Note that these spaces are nonnested, i.e., $V_{k-1}^{\mathrm{PU}} \not\subset V_k^{\mathrm{PU}}$, and that the shape functions $\varphi_{i,k}\psi_{i,k}^n$ are non-interpolatory. Thus, we need to construct appropriate transfer operators $I_{k-1}^k : V_{k-1}^{\mathrm{PU}} \to V_k^{\mathrm{PU}}$ and $I_k^{k-1} : V_k^{\mathrm{PU}} \to V_{k-1}^{\mathrm{PU}}$. With such transfer operators I_{k-1}^k, I_k^{k-1} and the stiffness matrices A_k coming from the Galerkin discretization on each level k we can then set up a standard multiplicative multilevel iteration to solve the linear system $A_J\tilde{u}_J = \hat{f}_J$. To this end, we have developed a special localized L^2-projection which exploits the product structure of the shape functions as well as our tree-based coarsening scheme for the interlevel transfer. The remaining ingredient for our multilevel solver is a block-smoothing scheme. Our numerical experiments indicate that the $V(1,1)$-cycle based on our localized L^2-projections together with an overlapping multiplicative Schwarz smoother converges with a rate which is independent of the number of patches N as well as the employed polynomial degree p. The overall complexity of the multilevel solver is $O(Np^{3d})$ whereas the number of nonzeros of the stiffness matrix is $O(Np^{2d})$. Hence the proposed solver is optimal up to a factor p^d.

References

[1] M. Griebel and M. A. Schweitzer, *A Particle-Partition of Unity Method for the Solution of Elliptic, Parabolic and Hyperbolic PDE*, SIAM J. Sci. Comput., 22 (2000), pp. 853–890.

[2] M. Griebel and M. A. Schweitzer, *A Particle-Partition of Unity Method—Part II: Efficient Cover Construction and Reliable Integration*, SIAM J. Sci. Comput., 23 (2002), pp. 1655–1682.

[3] M. Griebel and M. A. Schweitzer, *A Particle-Partition of Unity Method—Part III: A Multilevel Solver*, SIAM J. Sci. Comput., 24 (2002), pp. 377–409.

[4] M. Griebel and M. A. Schweitzer, *A Particle-Partition of Unity Method—Part IV: Parallelization*, in Meshfree Methods for Partial Differential Equations, M. Griebel and M. A. Schweitzer, eds., vol. 26 of Lecture Notes in Computational Science and Engineering, Springer, 2002, pp. 161–192.

[5] M. Griebel and M. A. Schweitzer, *A Particle-Partition of Unity Method—Part V: Boundary Conditions*, in Geometric Analysis and Nonlinear Partial Differential Equations, S. Hildebrandt and H. Karcher, eds., Springer, 2002, pp. 517–540.

[6] M. Griebel, P. Oswald, and M. A. Schweitzer, *A Particle-Partition of Unity Method—Part VI: A p-robust Multilevel Solver*, in Meshfree Methods for Partial Differential Equations II, M. Griebel and M. A. Schweitzer, eds., vol. 43 of Lecture Notes in Computational Science and Engineering, Springer, 2004, pp. 71–92.

[7] J. Nitsche, *Über ein Variationsprinzip zur Lösung von Dirichlet-Problemen bei Verwendung von Teilräumen, die keinen Randbedingungen unterworfen sind*, Abh. Math. Sem. Univ. Hamburg, 36 (1970–1971), pp. 9–15.

[8] M. A. Schweitzer, *A Parallel Multilevel Partition of Unity Method for Elliptic Partial Differential Equations*, vol. 29 of Lecture Notes in Computational Science and Engineering, Springer, 2003.

Operator Preconditioning

Ralf Hiptmair

1. Theoretical Foundations

On two reflexive Banach spaces V, W we consider two continuous sesqui-linear forms $a \in L(V \times V, \mathbb{C})$ and $b \in L(W \times W, \mathbb{C})$. Let $V_h \subset V$ and $W_h \subset W$ be finite-dimensional subspaces, on which the sesqui-linear forms fulfill the inf-sup-conditions

$$\sup_{v_h \in V_h} \frac{|a(u_h, v_h)|}{\|v_h\|_V} \geq c_A \|u_h\|_V \quad \forall u_h \in V_h \,, \tag{1}$$

$$\sup_{w_h \in W_h} \frac{|b(q_h, w_h)|}{\|w_h\|_W} \geq c_B \|q_h\|_W \quad \forall q_h \in W_h \,. \tag{2}$$

Further, there is a stable pairing connecting the spaces V_h and W_h: we assume the existence of a continuous sesqui-linear form $d \in L(V \times W, \mathbb{C})$ that satisfies another inf-sup-condition

$$\sup_{w_h \in W_h} \frac{|d(v_h, w_h)|}{\|w_h\|_W} \geq c_D \|v_h\|_V \quad \forall v_h \in V_h \,. \tag{3}$$

Picking bases $\{b_1,\dots,b_N\}$, $N := \dim V_h$, of V_h and $\{q_1,\dots,q_M\}$, $M := \dim W_h$, of W_h, we can introduce the Galerkin-matrices

$$\mathbf{A} := (a(b_i,b_j))_{i,j=1}^{N} \quad , \quad \mathbf{D} := (d(b_i,q_j))_{i,j=1}^{N,M} \quad , \quad \mathbf{B} := (b(q_i,q_j))_{i,j=1}^{M} .$$

Theorem 1 (*cf.* [6])**.** *If, besides* (1), (2), *and* (3), $\dim V_h = \dim W_h$, *then*

$$\kappa(\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-T}\mathbf{A}) \le \frac{\|a\|\,\|b\|\,\|d\|^2}{c_A c_B c_D^2} ,$$

where $\kappa(\cdot)$ *stands for the spectral condition number of a square matrix.*

Proof. Denote by $A_h : V_h \mapsto V_h'$, $B_h : W_h \mapsto W_h'$, and $D_h : V_h \mapsto W_h'$ the bounded linear operators associated with the sesqui-linear forms a, b, and d. Writing $D_h^* : W_h \mapsto V_h'$ for the adjoint operator of D_h, we immediately conclude

$$\begin{aligned} \|A_h\|_{V_h\mapsto V_h'} = \|a\| , \quad \left\|A_h^{-1}\right\|_{V_h'\mapsto V_h} \le c_A^{-1} , \\ \|B_h\|_{W_h\mapsto W_h'} = \|b\| , \quad \left\|B_h^{-1}\right\|_{W_h'\mapsto W_h} \le c_B^{-1} , \\ \|D_h\|_{V_h\mapsto W_h'} = \|D_h^*\|_{W_h\mapsto V_h'} = \|d\| \quad , \quad \left\|D_h^{-1}\right\|_{W_h'\mapsto V_h} = \left\|D_h^{-*}\right\|_{V_h'\mapsto W_h} \le c_D^{-1} . \end{aligned}$$

$$\Rightarrow \quad \begin{aligned} \left\|D_h^{-1}B_hD_h^{-*}A_h\right\|_{V\mapsto V} &\le c_D^{-2}\|a\|\,\|b\| , \\ \left\|A_h^{-1}D_h^*B_h^{-1}D_h\right\|_{V\mapsto V} &\le \|d\|^2 c_A^{-1}c_b^{-1} . \end{aligned}$$

Recall that the Galerkin matrix corresponding to D_h^* is $\mathbf{D}^T$. Thus, equipping $\mathbb{C}^N$ with a norm $\|\cdot\|_V$ inherited from the space V_h via the coefficient isomorphism w.r.t to the basis $\{b_1,\dots,b_N\}$, we find

$$\begin{aligned} |\lambda_{\max}(\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-T}\mathbf{A})| &\le \left\|\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-T}\mathbf{A}\right\|_{V\mapsto V} \le c_D^{-2}\|a\|\,\|b\| , \\ |\lambda_{\min}(\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-T}\mathbf{A})^{-1}| &\le \left\|\mathbf{A}^{-1}\mathbf{D}^T\mathbf{B}\mathbf{D}\right\|_{V\mapsto V} \le \|d\|^2 c_A^{-1}c_b^{-1} . \end{aligned}$$

□

Remark. The bound of Thm. 1 is completely independent of the choice of bases for V_h and W_h. The choice of Galerkin spaces V_h and W_h only enters through the constants c_A, c_B, and c_D.

2. Finite Element Applications

Now, the role of the space V of Sect. 1 is played by a Hilbert space H with inner product $(\cdot,\cdot)_H$. As before, a is a bounded sequi-linear form on H that satisfies (1) on a finite-dimensional subspace $H_h \subset H$.

Specializing the generic setting on Sect 1, we choose W as the dual space H'. A suitable finite dimensional subspace $W_h \subset H'$ with $\dim W_h = \dim H_h$ is furnished by the polar set of the orthogonal complement of H_h in H.

The role of the sesqui-linear form $b \in L(W,W)$ will be played by the inner product of H'. In other words, the associated operator $B : W' \mapsto W'' = W$ boils down to the inverse of the isometric Riesz-isomorphism $R : H \mapsto H'$. It is immediate that $\|b\| = 1$ and (2) holds with $c_B = 1$.

Finally, the sesqui-linear pairing $d \in L(V \times W, \mathbb{C})$ will agree with the natural duality pairing $\langle\cdot,\cdot\rangle_{H'\times H}$. Given any basis $\{b_1,\dots,b_N\}$, $N := \dim H_h$, of H_h, we

can find $\beta_1, \ldots, \beta_N \in H'$ such that $\langle \beta_i, b_j \rangle_{H' \times H} = \delta_{ij}$. This gives a basis for W_h, for which the Galerkin matrix associated with $d(\cdot,\cdot)$ becomes the identity matrix. Further, the Galerkin matrix $\mathbf{B}$ for $b(\cdot,\cdot)$ with respect to these bases is the inverse of the Riesz matrix $\mathbf{R} := ((b_i, b_j)_H)_{i,j=1}^N$. The bottom line is that we can conclude from Thm. 1 that

$$\kappa(\mathbf{R}^{-1}\mathbf{A}) \leq \|a\| {c_A}^{-1} . \tag{4}$$

Saddle point problems [1]**.** Consider the mixed variational formulation of second-order elliptic boundary value problems with Dirichlet boundary conditions [3, Ch. 3]. Here we have $H = \boldsymbol{H}(\mathrm{div};\Omega) \times L^2(\Omega)$ and the Galerkin matrix induced by the corresponding inner product can serve as a preconditioner for the indefinite saddle point matrix, if stable pairs of conforming finite element spaces are used.

Another example is the variational formulation of the Stokes problem [2, III.§ 5], where $H = H_0^1(\Omega) \times L_0^2(\Omega)$. The indefinite matrix arising from a stable conforming finite element method can be preconditioned by the block-diagonal s.p.d. matrix related to the inner product of H.

Complex variational problems. We target the sesqui-linear form

$$a(\boldsymbol{u},\boldsymbol{v}) := (\mathbf{curl}\,\boldsymbol{u}, \mathbf{curl}\,\boldsymbol{v})_{L^2(\Omega)} + i\,(\boldsymbol{u},\boldsymbol{v})_{L^2(\Omega)} \ , \quad \boldsymbol{u},\boldsymbol{v} \in \boldsymbol{H}(\mathbf{curl};\Omega) .$$

Since,

$$|a(\boldsymbol{u},\boldsymbol{u})| \geq \frac{1}{\sqrt{2}}(\|\mathbf{curl}\,\boldsymbol{u}\|^2_{L^2(\Omega)} + \|\boldsymbol{u}\|^2_{L^2(\Omega)}) \tag{5}$$

we conclude that $c_A \geq \frac{1}{2}\sqrt{2}$ and $\|a\| \leq 1$ is evident.

When splitting a variational problem for the sesqui-linear form $a(\cdot,\cdot)$ into real and imaginary parts, we end up with a saddle point problem on $H := \boldsymbol{H}(\mathbf{curl};\Omega) \times \boldsymbol{H}(\mathbf{curl};\Omega)$ related to the bi-linear form (subscripts tag real/imaginary parts)

$$\widetilde{a}\left(\begin{pmatrix}\boldsymbol{u}_R\\ \boldsymbol{u}_I\end{pmatrix}, \begin{pmatrix}\boldsymbol{v}_R\\ \boldsymbol{v}_I\end{pmatrix}\right) := a(\boldsymbol{u}_R,\boldsymbol{v}_R) + a(\boldsymbol{u}_I,\boldsymbol{v}_R) + a(\boldsymbol{u}_R,\boldsymbol{v}_I) - a(\boldsymbol{u}_I,\boldsymbol{v}_I) .$$

It goes without saying that $\widetilde{a}$ inherits stability and continuity constants from a. Writing $\mathbf{R} \in \mathbb{R}^{N,N}$ for the Galerkin matrix associated with the inner product of $\boldsymbol{H}(\mathbf{curl};\Omega)$, we thus find $\kappa\left(\begin{pmatrix}\mathbf{R}^{-1} & \\ & \mathbf{R}^{-1}\end{pmatrix}\widetilde{\mathbf{A}}\right) \leq \frac{1}{2}\sqrt{2}$. Using MINRES and replacing $\mathbf{R}^{-1}$ by a multigrid cycle will yield a robust iterative solver for the complex variational problem.

3. Boundary Element Applications

The weak forms of boundary integral equations of the first kind on a surface $\Gamma := \Omega$, $\Omega \subset \mathbb{R}^3$, naturally involve sesqui-linear forms defined on trace spaces. Prominent examples are the single layer boundary integral equation [7, Ch. 3] with

$$a(u,v) := \int_\Gamma \int_\Gamma \frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\, u(\boldsymbol{x})\, \bar{v}(\boldsymbol{y})\, \mathrm{d}S(\boldsymbol{x},\boldsymbol{y}) \ , \quad u,v \in H^{-\frac{1}{2}}(\Gamma) \ , \tag{6}$$

and the electric field boundary integral equation [5] posed on $H^{-\frac{1}{2}}(\mathbf{curl}_\Gamma, \Gamma)$, for which

$$a(\boldsymbol{u}, \boldsymbol{v}) = \int_\Gamma \int_\Gamma \frac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|} \left(\boldsymbol{u}(\boldsymbol{y})\bar{\boldsymbol{v}}(\boldsymbol{x}) - \frac{1}{k^2} \operatorname{curl}_\Gamma \boldsymbol{u}(\boldsymbol{y}) \operatorname{curl}_\Gamma \bar{\boldsymbol{v}}(\boldsymbol{x}) \right) \mathrm{d}S(\boldsymbol{y}, \boldsymbol{x}) \, .$$

Operator preconditioning for these boundary integral equation, *cf.* [9], is suggested by

- the availability of a continuous, bijective hypersingular boundary integral operator $W : H_*^{\frac{1}{2}}(\Gamma) \mapsto (H_*^{\frac{1}{2}}(\Gamma))'$ and the duality $(H^{-\frac{1}{2}}(\Gamma))' \cong H^{\frac{1}{2}}(\Gamma)$.
- the self-duality of $H^{-\frac{1}{2}}(\mathbf{curl}_\Gamma, \Gamma)$ w.r.t. to the pairing $(\boldsymbol{u}, \boldsymbol{v}) \mapsto \int_\Gamma \boldsymbol{u} \cdot (\bar{\boldsymbol{v}} \times \boldsymbol{n}) \, \mathrm{d}S$ (Hodge duality).

The construction of pairs of conformig boundary element spaces that play the role of V_h and W_h in Thm. 1 makes use of pairs of *dual meshes*. For instance, in the case of (6) we may use piecewise constants as $H^{-\frac{1}{2}}(\Gamma)$-conforming boundary elements on Voronoi cells to get V_h, and piecewise linear continuous boundary elements on the corresponding Delauney triangulation to build $W_h \subset H^{\frac{1}{2}}(\Gamma)$. Under weak assumptions on shape regularity O. Steinbach [8] showed that $d(u, v) := \int_\Gamma u \, \bar{v}$ is a h-uniformly stable discrete pairing. A related contruction for surface edge elements has been proposed by A. Buffa and S. Christiansen in [4] and can be used for the operator preconditioning approach to the electric field integral equation.

References

[1] D. Arnold, R. Falk, and R. Winther, *Preconditioning in H(*div*) and applications*, Math. Comp., 66 (1997), pp. 957–984.

[2] D. Braess, *Finite Elements*, Cambridge University Press, 2nd ed., 2001.

[3] F. Brezzi and M. Fortin, *Mixed and hybrid finite element methods*, Springer, 1991.

[4] A. Buffa and S. Christiansen, *A dual finite element complex on the barycentric refinement*, C.R. Acad. Sci Paris, Ser I, 340 (2005), pp. 461–464.

[5] A. Buffa and R. Hiptmair, *Galerkin boundary element methods for electromagnetic scattering*, in Topics in Computational Wave Propagation. Direct and inverse Problems, M. Ainsworth, P. Davis, D. Duncan, P. Martin, and B. Rynne, eds., vol. 31 of Lecture Notes in Computational Science and Engineering, Springer, Berlin, 2003, pp. 83–124.

[6] S. Christiansen and J.-C. Nédélec, *Des préconditionn eurs pour la résolution numérique des équations intégrales de frontiére de l'acoustique*, C.R. Acad. Sci. Paris, Ser. I Math, 330 (2000), pp. 617–622.

[7] S. Sauter and C. Schwab, *Randelementmethoden*, BG Teubner, Stuttgart, 2004.

[8] O. Steinbach, *On a generalized L_2 projection and some related stability estimates in Sobolev spaces*, Numer. Math., 90 (2002), pp. 775–786.

[9] O. Steinbach and W. Wendland, *The construction of some efficient preconditioners in the boundary element method*, Adv. Comput. Math., 9 (1998), pp. 191–216.

Underlying Parallel Algorithm for Numerical Solution of PDEs Based on Acyclic Directed Graph

Zeyao Mo

In recent two decades, various parallel algorithms have been successfully designed for a wide range of numerical computations especially arising from the grid-based simulations of partial differential equation where a discrete solution is defined on a grid [3]. The grid consists of a set of disjoint polyhedrons called zones. Most of cases, the data dependent relationship between neighboring two zones is often symmetric and can be accurately depicted by undirected graphs [9]. In sequence, the graph can be partitioned for zones distribution for load balance. Then, the underlying parallel algorithms can be designed in the concept of supersteps as defined in the Bulk Synchronous Parallel (BSP) programming model [10].

However, such symmetric relationship doesn't hold for another kind of grid-based numerical computations where zones should be updated in the behavior of downstream dataflow depicted by directed graph (digraph) [4]. Those numerical computations vary from the computational challenging application of radiation or neutron transport [2][5] on the unstructured grid to many numerical cores on the rectangular grid. Many works have applied the well known pipelining techniques [11] to parallelize the downstream sweeping out of the framework of BSP model. On rectangular grid, Baker et.al. discuss the neutron transport [1], Mo et.al. [6] discuss the solution of implicitly upwind stencils or downstream smoothers for convection dominated fluids, zhang [12] address the solution of a group of independent tridiagonal linear system arising from compact difference stencil for incompressible Navier-Stokes equation. On the unstructured grid, Plimpton and Hendrickson et.al.[8] and Mo et.al.[7] addressed the particle transport problems in Cartesian geometry and in cylindrical geometry respectively. On the unstructured grid, however, the realization is essentially more tricky because regular pipelines are not possible to be predefined owing to the irregular data dependent relationship between neighboring zones.

Nevertheless, these parallel pipelining algorithms depends severely on the characteristics of applications such as types of grid, shapes of zone, discrete stencil, number of sweeping directions, and so on. Is it possible to design a uniformed underlying parallel algorithm independent of applications but also suitable for parallel realization of such kinds of grid-based numerical computations where the data dependent relationship is non-symmetric and can be accurately depicted by digraph? This report tries to find a solution.

Firstly, we construct a universe model of acyclic digraph for the description of data dependent relationship among zones from a wide range of grid-based numerical computations. So, the underlying data flowchart of those numerical computations can be equivalently transformed to the computation of this digraph. The acyclic digraph is written as follows

$$D = (V(D), A(D), U(D)) \tag{1}$$

Here, D is the digraph, $V(D)$ and $A(D)$ are the set of vertices and arcs respectively, and $U(D)$ is the underlying supergraph. Each vertex relates to each pair of zone and sweeping direction, and each arc represents the data dependent relationship between the neighboring two vertices. The underlying supergraph is a undirected graph representing the geometric connectivity of all zones. Each vertex called supervertex relates to a geometric zone and it includes all these vertices of the digraph who having the same zone. This model is highly abstract and universe independent of concrete characteristics of grid-based applications. This digraph is computable if and only if it is acyclic. If a digraph includes a cycle, we should break it using some application-specific methods while the digraph is constructed.

Based on this digraph, we present a underlying parallel algorithm suitable for the parallel computation of acyclic digraph, or more aggressively, suitable for these numerical computations. This algorithm consists of three components such as digraph partitioning, parallel sweeping and vertices priority strategies.

The most natural idea for partitioning of an acyclic digraph D is the application of many undirected graph partitioning methods [9] on the underlying supergraph $U(D)$. The set of vertices of each supervertex will be distributed to the same processor to which the supervertex belongs. For these methods, loads can be well balanced and vertices are connected. However, we also present a universe partitioning method towards better performance for single sweeping direction.

Given the digraph partitioning, a parallel sweeping scheme is presented in this report for the parallel computation of this digraph. The parallel sweeping can extremely mine the parallelism for sweeping across digraph vertices only if it is coupled with an optimal vertices priority strategy for vertex selection in the case of many vertices are locally waiting for computation. In fact, we give an optimal priority strategy with the idea of that each vertex is assigned a priority equal to the length of shortest path away from the processor boundaries. The optimal property is coincident with the philosophy of that a vertex should be inserted into the waiting list satisfying that the current vertex located at the head is the most welcome for the release of downstream vertices located at neighboring processors. Thus, the parallel downstream sweeping algorithm presented in this report is optimal for any given digraph partitioning.

The numerical results show that our new parallel algorithm can improve algorithm speedup or realistic speedup by 10% compared with original results in work [7]. Here, the algorithm speedup is the theoretical speedup under the assumption of that message passing has zero overhead. Obviously, we wish our realistic speedup will be close to the algorithm speedup. For a realistic particle transport application on a massively parallel computer, this algorithm can achieve speedup 400 using 512 processors each having the peak performance of 1GFLOPS. The new digraph partitioning method can improve the algorithm speedup by 50% for single sweeping direction.

We prospect more and more realistic applications apart from the particle transport and some numerical cores, especially prospect the application for robust and

scalable parallel solver for linear or nonlinear convection dominated fluids on unstructured grid. Of course, we prospect the applications for mesh free computations or non-numerical computations where similar data dependent relationship exits.

In this report, we always assume that the diagraph can be well constructed in advance. However, it is impossible for those applications where the downstream sweeping directions depend on the swept solution itself. The digraph can only be constructed in accordance with the realistic computation. Particularly, we denote such digraphs by dynamically increasing digraphs. In fact, our underlying parallel algorithm can be generalized to be suitable for such digraphs only if we modify the priority strategy based on the shortest path away from the processor boundaries. We look forward to realistic application of underlying parallel algorithm for such digraphs.

In computer science, the underlying parallel algorithm and its realistic applications also bring forward a basic problems, i.e., is there a more practical parallel programming model suitable for such kinds of parallel sweeping computing? We can't make sure.

References

[1] R.S.Baker, K.R.Koch, An Sn algorithm for the massively parallel CM-200 computer,Nucl.Sci.Eng.,128(1998):312-320.
[2] R.L.Bowers, J.R.Wilson, Numerical modeling in applied physics and astrophysics, Jones and Bartlett publishers, 1991.
[3] J.Dongarra, K.Kennedy, L.Torczon, et.al, Sourcebook of parallel computing, Morgan Kaufmann Publisher, California, 2003.
[4] B.J.Jorgen,G.Gregory, Digraphs: theory, algorithms and applications, Springer-Verlag, London, 2001.
[5] E.E.Lewis, W.F.Miller, Computational Methods of Neutron Transport, John Wiley & Sons Publisher, 1984.
[6] Z.Mo,X.Li, On the Jacobi components at pseudo-boundaries for parallel multigrid computations, Mathematica Numerica Sinica, 21(1999):9-18.
[7] Z.Mo,L.Fu, Parallel flux sweeping algorithm for neutron transport on unstructured grid, Journal of Supercomputing, 30(1)(2004):5-17.
[8] S.Plimpton, B.Hendrickson, S.Burns, W.McLendon, Parallel algorithms for radiation transport on unstructured grids, in Proceeding of SuperComputing'2000, Dallas, Nov.4-10, 2000.
[9] K.Schloegel, G.Karypis, V.Kumar, Graph partitioning techniques for high performance scientific simulations, Chapter 18, Sourcebook of Parallel Computing, edited by J.Dongarra, K.Kennedy, L.Torczon, et.al., Morgan Kaufmann Publisher, California, 2003.
[10] L.G.Valiant, A bridging model for parallel computation, Communications of the ACM, 33:8(1990):108-111.
[11] B.Wilkinson, M.Allen, Parallel programming : Techniques and applications using networked workstations and parallel computers, Prentice Hall, 2002.
[12] L.Zhang, Pipelining parallelization of a cluster of recursive formulae, Chinese J. Numer. Math. & Comput. Appl., 20:3(1999):184-191.

Convergence estimates for preconditioned GMRES using element-by-element bounds on the field of values

Martin van Gijzen
(joint work with Daniel Loghin and Eline Jonkers)

1. Introduction

Preconditioned GMRES [SS] is among the most popular methods for solving non-symmetric linear systems of equations. To analyse the convergence of GMRES several upper bounds on the residual norm have been proposed. A class of such bounds is based on the field of values of the (preconditioned) matrix, see e.g. [E]. These bounds are quite useful in the analysis of preconditioners, for example to establish mesh-independence or to determine an optimal value for a tuning parameter.

To apply these bounds knowledge of the field of values is necessary. In the recent paper [LGJ] bounds on the field of values of a preconditioned global Finite Element matrix are derived based on the fields of values of the element matrices. These bounds are easy to compute and are applicable to general matrices. The preconditioner, however, needs to be Hermitian positive definite.

The GMRES-convergence estimates and bounds for the field of values can be combined in order to analyse and predict the performance of a preconditioner. To illustrate this we will analyse two problems. We will show that for a wide class of convection-diffusion-reaction problems the number of iterations is mesh-independent if the matrix is preconditioned with the symmetric part of the operator. For the damped Helmholtz equation that is preconditioned with a shifted Laplacian we will show how a quasi optimal (real) shift can be determined.

2. Element-by-element bounds on the field of values

In [LGJ] a bound is formulated on the field of values $FOV(\mathbf{A},\mathbf{B})$ of the matrix pair $(\mathbf{A},\mathbf{B})$, with $\mathbf{A}$ general and $\mathbf{B}$ Hermitian positive definite. $FOV(\mathbf{A},\mathbf{B})$ is defined by

$$FOV(\mathbf{A},\mathbf{B}) = \left\{ \frac{\mathbf{x}^H\mathbf{A}\mathbf{x}}{\mathbf{x}^H\mathbf{B}\mathbf{x}}, \mathbf{x} \in \mathbb{C}^n, \mathbf{x} \neq 0 \right\}$$

Furthermore, a bound is given on the numerical radius $r(\mathbf{A},\mathbf{B})$ which is defined by

$$r(\mathbf{A},\mathbf{B}) = \max\left\{ |z| : z \in FOV(\mathbf{A},\mathbf{B}) \right\}.$$

These bounds are based on the fields of values of the element matrices and hence are easy to compute.

The element-by-element bound on the field of values $FOV(\mathbf{A},\mathbf{B})$ is summarised as follows. Let $\mathbf{A}^e, e = 1,\cdots,n_e$ be (possibly non-Hermitian) element matrices and $\mathbf{B}^e, e = 1,\cdots,n_e$ be Hermitian positive definite element matrices and let $\mathbf{A}$

and $\mathbf{B}$ be the global matrices that are assembled from these element matrices. Then the following bounds hold for $z \in FOV(\mathbf{A}, \mathbf{B})$:

$$\min_e \lambda_{min}^{\Re(\mathbf{A}^e),\mathbf{B}^e} \leq Re(z) \leq \max_e \lambda_{max}^{\Re(\mathbf{A}^e),\mathbf{B}^e} \tag{1}$$

$$\min_e \lambda_{min}^{\Im(\mathbf{A}^e),\mathbf{B}^e} \leq Im(z) \leq \max_e \lambda_{max}^{\Im(\mathbf{A}^e),\mathbf{B}^e}. \tag{2}$$

Here $\Re(\mathbf{A}^e) = \frac{1}{2}(\mathbf{A}^e + \mathbf{A}^{eH})$ and $\Im(\mathbf{A}^e) = \frac{1}{i2}(\mathbf{A}^e - \mathbf{A}^{eH})$. $\lambda^{\Re(\mathbf{A}^e),\mathbf{B}^e}$ and $\lambda^{\Im(\mathbf{A}^e),\mathbf{B}^e}$ are eigenvalues of the generalised element eigenproblems $\Re(\mathbf{A}^e)\mathbf{x}^e = \mathbf{B}^e\mathbf{x}^e$, and $\Im(\mathbf{A}^e)\mathbf{x}^e = \mathbf{B}^e\mathbf{x}^e$, respectively.

The numerical radius $r(\mathbf{A}, \mathbf{B})$ can be bounded from above as follows. Let $\mathbf{A}^e, e = 1, \cdots, n_e$ be (possibly non-Hermitian) element matrices and $\mathbf{B}^e, e = 1, \cdots, n_e$ be Hermitian positive definite element matrices and let $\mathbf{A}$ and $\mathbf{B}$ be the global matrices that are assembled from these element matrices. Let ν be defined by

$$\nu = \max \left\{ |z| : z \in \bigcup_{e=1}^{n_e} FOV(\mathbf{A}^e, \mathbf{B^e}) \right\},$$

then

$$r(\mathbf{A}, \mathbf{B}) \leq \nu \ .$$

3. Combination with upper bounds on the GMRES-residual norm

The element-by-element bounds on the field of values can be combined with some of the classical bounds on the GMRES residual norm. To illustrate this we will consider two different test problems: a family of convection-diffusion-reaction equations and a damped Helmholtz equation.

3.1. **Convection-diffusion-reaction equation.**

We consider the following family of convection-diffusion-reaction equations

$$-\epsilon\Delta u + \mu u + \beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} = f \ . \tag{3}$$

with homogeneous Neumann boundary conditions. We assume that the parameters ϵ (diffusion), μ (reaction), and β_x and β_y (convection) are constant, and that $\epsilon > 0$ and $\mu \geq 0$. Discretisation of equation (3) using linear triangular elements on a uniform mesh with mesh-size h yields a global matrix that we will denote with $\mathbf{A}$. As a preconditioner we take the matrix $\mathbf{P}$ that corresponds to the symmetric part of the partial differential operator, i.e., to $-\epsilon\Delta + \mu$.

To derive an upper bound on the number of GMRES iterations we apply the bound on the GMRES-residual norm that is given in [G], page 56. This bound states that if $FOV(\mathbf{A}, \mathbf{P})$ is contained in a disk $D = \{z \in \mathbb{C} : |z - c| \leq s\}$ which does not contain the origin, then the GMRES-residual norm after k iterations satisfies

$$\|\mathbf{r}^k\| / \|\mathbf{r}^0\| \leq 2 \left(\frac{s}{|c|} \right)^k \ .$$

Since $FOV(\mathbf{A},\mathbf{P}) = 1 - FOV(\mathbf{A}-\mathbf{P},\mathbf{P})$, $FOV(\mathbf{A},\mathbf{P})$ is enclosed by a circle centered at 1 and with radius $r(\mathbf{A}-\mathbf{P},\mathbf{P})$. An upper bound for $r(\mathbf{A},\mathbf{P})$ can be derived using (2). It can be shown that the numerical radius of the element matrices is given by

$$\nu = r(\mathbf{A}^e - \mathbf{P}^e, \mathbf{P}^e) = \frac{1}{2}\sqrt{\frac{(\beta_x-\beta_y)^2}{2\epsilon\mu + \frac{2}{3}h^2\mu^2} + \frac{(\beta_x+\beta_y)^2}{2\epsilon\mu + \frac{2}{9}h^2\mu^2}}.$$

Since $\lim_{h\to 0}\gamma = \frac{\|\beta\|}{2\sqrt{\epsilon\mu}}$ we have derived an upper bound on the GMRES-residual norm that is *independent* of the mesh-size h. This is also confirmed by extensive numerical experiments.

3.2. **Damped Helmholtz equation.** As a second example we consider the damped Helmholtz equation

$$-\Delta u + (i\gamma - k^2)u = f \ .$$

on the unit square with Neumann boundary conditions. In this equation γ represents the damping parameter and k the wave number. The problem is discretised with 16 x 16 x 2 linear triangular elements. The wavenumber is $k = 10$.

As a preconditioner we take the discretisation of a shifted Laplace operator $-\Delta + s^2$, in which s^2 is a positive shift. The question is how to chose s^2 for optimal performance.

To answer this question we use the techniques outlined in the previous section to determine a lower bound for the distance between the field of values and the origin, which we denote by θ, and for the numerical radius Θ. These values can be combined with the upper bound on the GMRES-residual norm proposed by Elman [E]:

$$\|\mathbf{r}^k\|/\|\mathbf{r}^0\| \leq (1 - \frac{\theta^2}{\Theta^2})^{k/2}.$$

The upper bound that is obtained in this way shows that the minimum number of iterations is achieved for the following choice of s^2:

$$s^2_{opt} = \frac{\frac{3}{2}|z|}{|\frac{3}{2} + \frac{h^2}{6}z| - |\frac{h^2}{6}z|} \qquad\qquad z = i\gamma k - k^2$$

Numerical experiments confirm that the number of iterations is indeed (almost) minimised for this value for s^2 for a large class of problems.

4. Concluding remarks

We have discussed two examples for which the combination of element-by-element bounds on the field of values and bounds on the GMRES-residual norm provides a useful approach to analyse a given preconditioner. This approach works well for problems where the preconditioner is symmetric positive definite and where the fields of values of the element matrices do not include the origin. Further research aims to generalise our approach to problems with a nonsymmetric preconditioner.

References

[E] H.C. Elman, Iterative methods for large sparse non-symmetric systems of linear equations, PhD thesis, Yale University, New Haven, 1982.

[G] A. Greenbaum, Iterative Methods for Solving Linear Systems, SIAM Press, 1997.

[LGJ] D. Loghin, M.B. van Gijzen, E. Jonkers, Bounds on the eigenvalue range and on the Field of Values of non-Hermitian and indefinite finite element matrices, CERFACS Technical Report TR/PA/04/86, to appear in: Journal of Computational and Applied Mathematics.

[SS] Y. Saad and M.H. Schultz, GMRES: A Generalized Minimal Residual Algorithm for Solving Non-Symmetric Linear Systems, SIAM J. Sci. Stat. Comp. 7 (1986) 856–869.

Adaptive FEM for crack propagation and quick solvers

Arnd Meyer

(joint work with M.Kuna, M.Scherzer)

We consider the numerical simulation of crack growth in mechanical structures. While the model of (slow) crack propagation is well understood in fracture mechanics, the efficient numerical simulation requires some modern tools in numerical analysis [MRS04, MRS05]. One is adaptive finite elements for accurate but simple approximating the displacement field of a structure with existing crack from the inherent strong singularities. Another important ingredient is the need of quick solvers for the resulting series of single finite element computations along the crack propagation. Both is contained in an efficient way using hierarchical meshes (as they are directly obtained from the adaptive mesh–refinement) and multilevel techniques for the preconditioner of the preconditioned conjugate gradient method (PCGM) for each of the linear systems.

The mesh refinement of the standing crack produces hierarchical meshes, where the hierarchy in the nodes is contained in the "'edge–tree"' of refined edges and can be used efficiently for the hierarchical preconditioner [Ys] or more sophisticated methods such as Multi–Grid. After crack propagation, we have inserted some new extra edges along the crack line, which possess its hierarchical information as well, but the nodes along the crack carry "'double"' number of degrees of freedom for the new crack opening. These are not directly contained in the hierarchical information, hence an efficient preconditioner of the next PCG–run is to be constructed expecially.

If we consider a transformation of the usual basis of f.e. ansatz functions along the crack into one full hat function and one jump function per crack–node, we are able to find an efficient domain decomposition–like preconditioner for the resulting transformed stiffness matrix from its block–structure of a main block as usual stiffness matrix without crack and another block of fixed low bandwidth.

Some experiments yield about 30 iterations on all successive meshes for all the PCG–iteration with this new preconditioner [Mey].

References

[MRS04] A. Meyer, F. Rabold, M. Scherzer, Efficient finite element simulation of crack propagation, Prepr. SFB393 04-01, TU Chemnitz.

[MRS05] A. Meyer, F.Rabold, M.Scherzer, Efficient Finite Element Simulation of Crack Propagation Using Adaptive Iterative Solvers, Commun.Numer.Meth Engng, 2005, to appear.

[Mey] A. Meyer A New Efficient Preconditioner for Crack Growth Problems, Prepr. SFB393 05-06, TU Chemnitz.

[Ys] H. Yserentant, Two Preconditioners Based on the Multilevel Splitting of Finite Element Spaces, Numerische Mathematik 58, pp. 163–184, 1990.

Reporter: Babett Lemke

Participants

Prof. Dr. Randolph E. Bank
rbank@ucsd.edu
Dept. of Mathematics
University of California, San Diego
9500 Gilman Drive
La Jolla, CA 92093-0112
USA

Dr. Steffen Börm
sbo@mis.mpg.de
Steffen.Boerm@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Prof. Dr. Dietrich Braess
braess@num.ruhr-uni-bochum.de
Fakultät für Mathematik
Ruhr-Universität Bochum
44780 Bochum

Prof. Dr. James H. Bramble
James.Bramble@math.tamu.edu
Department of Mathematics
Texas A & M University
College Station, TX 77843-3368
USA

Prof. Dr. Susanne C. Brenner
brenner@math.sc.edu
Dept. of Mathematics
University of South Carolina
Columbia, SC 29208
USA

Prof. Dr. Wolfgang Dahmen
dahmen@igpm.rwth-aachen.de
Institut für Geometrie und
Praktische Mathematik
RWTH Aachen
Templergraben 55
52056 Aachen

Prof. Dr. Peter Deuflhard
deuflhard@zib.de
Konrad-Zuse-Zentrum für
Informationstechnik Berlin (ZIB)
Takustr. 7
14195 Berlin

Prof. Dr. Maksymilian Dryja
dryja@hydra.mimuw.edu.pl
M.Dryja@mimuw.edu.pl
Dept. of Mathematics, Informatics
and Mechanics
University of Warsaw
ul. Banacha 2
02-097 Warszawa
POLAND

Dr. Jens P. Eberhard
eberhard@techsim.org
Institute f. Scientific Computation
Texas A&M University
612 Blocker Bldg.
College Station TX 77843-3404
USA

Dr. Robert D. Falgout
rfalgout@llnl.gov
Centre of Applied and Scientific
Computing
Lawrence Livermore National Lab.
P.O.Box 808, L-561
Livermore, CA 94551
USA

Dr. Martin van Gijzen
m.b.vangijzen@ewi.tudelft.nl
Delft University of Technology
Kluyverweg 1
P.O. Box 5058
NL-2600 GB Delft

Achim Gordner
achim.gordner@iwr.uni-heidelberg.de
Institut für Informatik
Ruprecht-Karls-Universität
Heidelberg
Im Neuenheimer Feld 368
69120 Heidelberg

Prof. Dr. Lars Grasedyck
lgr@numerik.uni-kiel.de
lgr@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr.22-26
04103 Leipzig

Univ.-Prof. Dr. Gundolf Haase
ghaase@numa.uni-linz.ac.at
Institut für Mathematik und
wissenschaftliches Rechnen
Karl-Franzens-Universität Graz
Heinrichstr. 36
A-8010 Graz

Prof. Dr. Wolfgang Hackbusch
wh@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Prof. Dr. Ralf Hiptmair
hiptmair@sam.math.ethz.ch
Seminar für Angewandte Mathematik
ETH-Zentrum
Rämistr. 101
CH-8092 Zürich

Dr. Michael Holst
mholst@math.ucsd.edu
Dept. of Mathematics
University of California, San Diego
9500 Gilman Drive
La Jolla, CA 92093-0112
USA

Prof. Dr. Ronald H.W. Hoppe
hoppe@math.uni-augsburg.de
rohop@math.uh.edu
Lehrstuhl für Angewandte
Mathematik I
Universität Augsburg
Universitätsstr. 14
86159 Augsburg

Prof. Dr. Peter Jimack
pkj@comp.leeds.ac.uk
The School of Computing
University of Leeds
GB-Leeds LS2 9JT

Dr. Klaus Johannsen
Klaus.Johannsen@iwr.uni-heidelberg.de
mail@klaus-johannsen.net
ICES
The University of Texas at Austin
1 University Station, C0200
Austin TX 78712-0027
USA

Dr. Boris N. Khoromskij
bokh@mis.mpg.de
Boris.Khoromskij@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Prof. Dr. Angela Kunoth
kunoth@iam.uni-bonn.de
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 6
53115 Bonn

Prof. Dr. Ulrich Langer
ulanger@numa.uni-linz.ac.at
Institut für Numerische Mathematik
Johannes Kepler Universität Linz
Altenbergstr. 69
A-4040 Linz

Dr. Babett Lemke
Babett.Lemke@iwr.uni-heidelberg.de
Mathematisches Institut
Universität Heidelberg
Im Neuenheimer Feld 288
69120 Heidelberg

Prof. Dr. Arnd Meyer
a.meyer@mathematik.tu-chemnitz.de
Fakultät für Mathematik
TU Chemnitz
09107 Chemnitz

Prof. Dr. Hans D. Mittelmann
mittelmann@math.asu.edu
Dept. of Mathematics and Statistics
Arizona State University
Box 871804
Tempe, AZ 85287-1804
USA

Prof. Dr. Zeyao Mo
zeyao_mo@mail.iapcm.ac.cn
Institute of Applied Physics and
Computational Mathematics
P.O.Box 8009
Beijing 100088
P.R.China

Arne Nägel
arne.naegel@kurz.uni-heidelberg.de
IWR Technische Simulation
Universität Heidelberg
Im Neuenheimer Feld 368
69120 Heidelberg

Dr. Nicolas Neuss
Nicolas.Neuss@iwr.uni-heidelberg.de
Interdisziplinäres Zentrum
für Wissenschaftliches Rechnen
Universität Heidelberg
Im Neuenheimer Feld 368
69120 Heidelberg

Dr. Jeffrey Ovall
ovall@mis.mpg.de
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Dr. Christoph Reisinger
christoph.reisinger@iwr.uni-heidelberg.de
reisinge@maths.ox.ac.uk
Mathematical Institute
Oxford University
24-29, St. Giles
GB-Oxford OX1 3LB

Prof. Dr. Arnold Reusken
reusken@igpm.rwth-aachen.de
Institut für Geometrie und
Praktische Mathematik
RWTH Aachen
Templergraben 55
52062 Aachen

Prof. Dr. Thomas F. Russell
trussell@nsf.gov
Division of Mathematical Sciences
National Science Foundation
4201 Wilson Blvd
Arlington, VA 22230
USA

Prof. Dr. Stefan A. Sauter
stas@math.unizh.ch
Institut für Mathematik
Universität Zürich
Winterthurerstr. 190
CH-8057 Zürich

Prof. Dr. Volker Schulz
Volker.Schulz@uni-trier.de
Fachbereich IV - Mathematik
Numerik - Optimierung, partielle Differentialgleichungen
Universität Trier
54286 Trier

Dr. Marc Alexander Schweitzer
m.a.schweitzer@ins.uni-bonn.de
schweitz@iam.uni-bonn.de
Institut für Numerische Simulation
Universität Bonn
Wegelerstr. 6
53115 Bonn

Dr. Rob Stevenson
stevenso@math.uu.nl
Department of Mathematics
Utrecht University
P.O.Box 80.010
NL-3508 TA Utrecht

Dr. Klaus Stüben
Klaus.Stueben@scai.fraunhofer.de
Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen (SCAI)
Schloss Birlinghoven
53754 Sankt Augustin

Prof. Dr. Justin W.L. Wan
jwlwan@uwaterloo.ca
Department of Computer Science
University of Waterloo
200 University Avenue West
Waterloo ONT N2L 3G1
Canada

Prof. Dr. Mary Fanett Wheeler
mfw@ticam.utexas.edu
Department of Mathematics
University of Texas at Austin
1 University Station C1200
Austin, TX 78712-1082
USA

Prof. Dr. Olof B. Widlund
widlund@cs.nyu.edu
Courant Institute of Mathematical Sciences
New York University
251, Mercer Street
New York, NY 10012-1110
USA

Prof. Dr. Christian Wieners
wieners@math.uni-karlsruhe.de
Institut für Praktische Mathematik
Universität Karlsruhe
76128 Karlsruhe

Prof. Dr. Gabriel Wittum
wittum@iwr.uni-heidelberg.de
wittum@techsim.org
IWR Technische Simulation
Universität Heidelberg
Im Neuenheimer Feld 368
69120 Heidelberg

Prof. Dr. Jinchao Xu
xu@math.psu.edu
Department of Mathematics
Pennsylvania State University
University Park, PA 16802
USA

Prof. Dr. Harry Yserentant
yserentant@math.tu-berlin.de
Institut für Mathematik
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin

Prof. Dr. Christoph Zenger
Zenger@in.tum.de
Institut für Informatik
TU München
Boltzmannstr. 3
85748 Garching