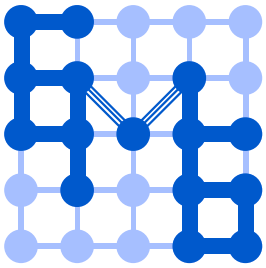

2014 European Multigrid Conference

September 9–12

Leuven, Belgium

Sponsors

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Foreword

The European Multigrid Conference (EMG2014) provides a forum for researchers to present and discuss recent research on the development, theory, and application of multigrid, multilevel, and multiscale methods. Previous EMG meetings took place in Cologne (1981 and 1985), Bonn (1990), Amsterdam (1993), Stuttgart (1996), Ghent (1999), Hohenwart (2002), Scheveningen (2005), Bad Herrenhalb (2008), Ischia (2010) and Schwetzingen (2012).

The 2014 edition in the EMG series of conferences is held in Leuven, Belgium, in the historical setting of the Irish College. Central topics of the conference are algebraic multigrid, multigrid for systems of PDEs, parallel multigrid, non-PDE applications, industrial applications, multilevel optimization, Schwarz and domain decomposition methods, multiscale modeling, data-sparse representations, sparse grids approaches.

The conference brings together around 85 participants from all over the world : Germany (27), Belgium (21), The Netherlands (5), United Kingdom (5), United States (5), Austria (4), Italy (4), Israel (3), Spain (3), Canada (2), France (2), Czech Republic (1), Ecuador (1), Norway (1), Saudi Arabia (1). Of those participants, 20 are PhD-students.

Plenary speakers

- Hans De Sterck, *University of Waterloo*, Canada
- Wolfgang Hackbusch, *Max Planck Institute*, Leipzig, Germany
- Arne Nägel, *Ghoete-Universität Frankfurt am Main*, Germany
- Luke Olson, *University of Illinois at Urbana-Champaign*, USA
- Dorit Ron, *Weizmann Institute of Science*, Rehovot, Israel
- Giovanni Samaey, *KU Leuven - University of Leuven*, Belgium
- Robert Scheichl, *University of Bath*, UK
- Klaus Stüben, *Fraunhofer Institute*, Sankt Augustin, Germany
- Philippe Toint, *Université de Namur*, Belgium
- Wim Vanroose, *Antwerp University*, Belgium
- Jinchao Xu, *Penn State University*, USA

Organisation committee

- Artem Napov, *Université Libre de Bruxelles* (local organiser)
- Yvan Notay, *Université Libre de Bruxelles* (local organiser)
- Stefan Vandewalle, *KU Leuven - University of Leuven* (local organiser)
- Erik Dick, *Ghent University*
- Wolfgang Hackbusch, *Max Planck Institute*, Leipzig
- Cornelis Oosterlee, *Delft University of Technology*
- Annick Sartenaer, *Université de Namur*
- Gabriel Wittum, *Ghoete-Universität Frankfurt am Main*

Programme

Monday, September 8, 2014
Registration **17h00–19h00**
Welcome reception **18h00–19h00**

Tuesday, September 9, 2014		
Welcoming remarks **8h45–9h00**		
	Auditorium, Chair : *Stefan Vandewalle*	
9h00–9h45	Solution of linear systems for boundary value problems in high spatial dimensions, *Wolfgang Hackbusch* p.9	
9h45–10h30	Multigrid for far and near field maps of the Helmholtz equation, *Wim Vanroose* p.13	
Coffee break		
	LFA for MG Auditorium, Chair : *Artem Napov*	**Parallel-in-time MG** Conference Room 1, Chair : *Stefan Vandewalle*
11h00–11h25	Finite element multigrid framework for mimetic finite difference discretizations, *Carmen Rodrigo* p.36	Parallel time integration with multigrid for parabolic problems, *Stephanie Friedhoff* .. p.23
11h25–11h50	Local Fourier analysis for ILU smoothers on triangular grids, *Marcio Augusto Villela Pinto* p.32	Time-parallelism using inexact PFASST, *Robert Speck* p.39
11h50–12h15	Local Fourier Analysis of Pattern Structured Operators, *H. Rittich* p.35	A parallel space-time multigrid solver for the Navier-Stokes equations, *Martin Neumüller* p.31
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	Auditorium, Chair : *Yvan Notay*	
14h00–14h45	A Review on AMG: From Academia to Industry, *Klaus Stüben* p.12	
	AMG Auditorium, Chair : *Yvan Notay*	**Nonlinear MG** Conference Room 1, Chair : *Francisco Gaspar*
14h50–15h15	BootCMatch: an alpha-AMG solver based on Compatible Weighted Matching, *Pasqua D'Ambra* p.20	Newton-Multigrid or Nonlinear Multigrid?, *Keeran Brabazon* p.17
15h15–15h40	Theoretical Advances in non-Galerkin Algebraic Multigrid, *Eran Treister* p.42	Truncated Nonsmooth Newton multigrid methods for vector valued minimization problems, *Carsten Gräser* p.25
15h40–16h05	Parallel Filtering Algebraic Multigrid for Linear Elasticity Problems, *Martin Rupp* p.36	Multigrid Method for Systems of Nonlinear Equations arising from Poroelasticity Problem, *Peiyao Luo* p.30
Coffee break		
	Helmholtz Auditorium, Chair : *Wim Vanroose*	**Applications** Conference Room 1, Chair : *Luke Olson*
16h30–16h55	A multigrid based iterative solver for the frequency domain elastic wave equation, *Gabrio Rizzuti* p.36	A Fast Method for Modeling Water Infiltration in Porous Media, *Craig Douglas* p.21
16h55–17h20	A new level-dependent coarse grid correction scheme for indefinite Helmholtz problems, *Siegfried Cools* p.19	Mechanistic dynamics of Hepatitis C virus replication in single liver cells, *Markus M. Knodel* p.28
17h20–17h45	A hybrid multigrid-domain decomposition method for the Helmholtz equation, *Chris Stolk* p.41	Three-stage multiscale algebraic preconditioner for highly heterogeneous diffusion subsurface problem on unstructured mesh, *Davide Baroli* p.17
17h45–18h10	Coarse-grid-correction preconditioner for the Helmholtz Equation, *A. H. Sheikh* p.38	Condition number estimates for higher order NURBS discretizations, *Krishan Gahalaut* p.23
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9h45–10h30	Three decades of multilevel optimization strategies, *Dorit Ron* p.11	
Coffee break		
	Structured preconditioners Auditorium, Chair : *Wolfgang Hackbusch*	**MG for special discretizations** Conference Room 1, Chair : *Stefan Vandewalle*
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11h25–11h50	H2-matrix preconditioners, *Steffen Börm* . p.18	Multigrid algorithms for high-order Discontinuous Galerkin discretizations, *Marco Sarti* . p.37
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Excursion to Brussels **Departure from the Irish College at 14h30** **Departure from the Leuven train station at 15h00**		

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9h45–10h30	Adaptive Algebraic Multigrid for Singular Value and Tensor Decompositions, *Hans De Sterck* p.9	
Coffee break		
	Multilevel approaches Auditorium, Chair : *Robert Scheichl*	**Parallel MG** Conference Room 1, Chair : *Bram Reps*
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11h25–11h50	Multigrid Method for Solving Elliptic Monge-Ampere Equation Arising from Image Registration, *Justin Wan* p.43	On a highly scalable infrastructure for massively parallel multigrid solvers, *Sebastian Reiter* p.33
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	Auditorium, Chair : *Craig Douglas*	
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	High-performance MG Auditorium, Chair : *Craig Douglas*	**MG and neurons** Conference Room 1, Chair : *Arne Nägel*
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15h15–15h40	Multigrid method on Intel Xeon Phi (MIC), *Kab Seok Kang* p.27	A Multiscale Model of Synaptic Contacts between Brain Cells, *Gillian Queisser* p.33
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17h45–18h10	Algebraic Multigrid Methods for Velocity Pressure Coupling in CFD, *Sarah Engleder* ... p.22	MGOPT Methods for Optimization Problems Arising in Non-Newtonian Fluids Simulation, *Sergio González-Andrade* p.24
Conference dinner **19h00–22h00, KU Leuven - University of Leuven Faculty Club**		

Friday, September 12, 2014		
	Auditorium, Chair : *Irad Yavneh*	
9h00–9h45	Efficient solvers for coupled problems in geophysics, *Arne Nägel* p.10	
9h45–10h30	A micro-macro parareal algorithm for slow-fast systems with applications to molecular dynamics, *Giovanni Samaey* p.11	
Coffee break		
	MG for special and coupled PDEs Auditorium, Chair : *Artem Napov*	**Applications and optimization** Conference Room 1, Chair : *Hans De Sterck*
11h00–11h25	Challenges in multigrid for mixed elliptic/hyperbolic problems in radiation transport, *Steven Dargaville* p.21	Adaptive fracture approximation, *Sabine Stichel* p.41
11h25–11h50	A multigrid preconditioner for the Hellan-Herrmann-Johnson mixed method for biharmonic problems, *Walter Zulehner* p.45	A simulation technique for density-driven flow in porous media with complicated fracture networks, *Dmitry Logashenko* p.29
11h50–12h15	A new multigrid strategy for Stokes problems, *Yvan Notay* p.31	Multigrid methods for boundary control problems, *Dirk Abbeloos* p.17
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Plenary sessions

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Adaptive Algebraic Multigrid for Singular Value and Tensor Decompositions

Hans De Sterck
Department of Applied Mathematics
University of Waterloo

An adaptive algebraic multigrid (AMG) method is presented for the rank-K canonical tensor decomposition problem, which aims to approximate a data tensor by a sum of K rank-one terms. This canonical tensor decomposition is widely used in a variety of application areas that include chemometrics, signal processing, neuroscience, and social network analysis. An adaptive version of AMG is required for this problem to ensure that error components that converge slowly during relaxation lie approximately in the range of interpolation. The method uses the bootstrap adaptive AMG approach and is derived by first considering an adaptive AMG method for the singular value decomposition, which is the matrix version of canonical tensor decomposition.

Solution of linear systems for boundary value problems in high spatial dimensions

Wolfgang Hackbusch
Max-Planck-Institut
Mathematik in den Naturwissenschaften

Consider an elliptic boundary value problem in the domain D1 x D2 x ... x Dd, where the spatial dimension d may be much larger than 3. In such a case, standard methods lead to linear systems of a size too huge for any computer. Because of the Cartesian product domain, tensor methods can be applied. We show how iterative methods with a good preconditioner can be constructed. Even multigrid ideas can be applied.

Efficient solvers for coupled problems in geophysics

Arne Nägel
Goethe-Center for Scientific Computing
Goethe University Frankfurt a.M.

Many problems in geophysics comprise interactions of processes, and are typically formulated as a system of coupled PDEs. In most cases this systems are transient and often also non-linear. Hence, developing efficient solvers is often a delicate task and must include combining suitable schemes for (i) time integration, (ii) linearization, and (iii) geometric and algebraic multigrid solvers. In this presentation we take an application oriented approach and focus on the problem classes of density-driven-flow and poroelasticity problems. For these two examples, we first comment on similarities and differences, and then provide details on their respective solution strategy:

For density-driven-flow problems, the fluid flow is density dependent and coupled non-linearly to a second quantity such as a substance concentration or heat, which is transported as well. For this problem class we investigate different non-linear solvers and decoupling strategies. In benchmark computations, an iterative coupling (single step nonlinear Gauss-Seidel) outperforms a partial Newton method (single step non-linear Jacobi). This effect is less pronounced for the iterative coupling, and mitigates after the first simulation phase when the velocity profile has stabilized. In the latter case corrections are computed independently, thus, this scheme shows to be inappropriate for this highly nonlinear problem class. The fully coupled Newton method, requiring a monolithic linear solver, however, proofs being superior to both approaches.

The poroelasticity problems considered in the second part of the talk are linear and are known to be decoupled efficiently by iterative coupling strategies. Since the mechanics sub-system can be considered as time-independent constraint, this the problem perfectly suited for (algebraic) multigrid solvers. We provide scalability results and also comment on the monolithic (fully coupled) solution.

Improving Convergence and Reducing Complexity in Algebraic Multigrid through a Root-node Method

Luke Olson
Computer Science
University of Illinois at Urbana-Champaign

Recent approaches to improving multigrid convergence through modified coarsening and enhanced interpolation have shown to be effective in a general setting (e.g. complex, non-Hermitian, and indefinite). Yet, the the resulting multigrid hierarchies may exhibit higher complexities than necessary. In this talk we outline a root-node based approach to multigrid, which can be viewed as a hybrid of classical and aggregation based multigrid methods. This allows both point-wise decisions in the setup while retaining the framework of aggregation. We give an overview of root-node multigrid using interpolation based on energy minimization and show how the complexity of the multigrid cycle is controlled through selective filtering by utilizing a root-node. The method yields improved interpolation (and convergence), while limiting the total work of the cycle with minimal tuning of parameters. We present several numerical results in support and discuss directions for further theoretical and numerical development.

Three decades of multilevel optimization strategies

Dorit Ron
Department of Computer Science and Applied Mathematics
Weizmann Institute of Science

Multilevel approach has become common in many applications involving optimization problems. Many of these problems may consist of millions of discrete state variables and are known to be NP-hard. In many theoretical and industrial fields, this class of problems is often addressed and actually poses a computational bottleneck, e.g., graph visualization, facility location problem, VLSI layout, etc. We have developed fast multilevel solvers for a variety of such combinatorial optimization problems including graph and hypergraph problems. In particular, we suggest a local measure, the algebraic distance, for the graph coarsening process yielding a multiscale graph organization. Another problem we introduce is an optimization problem of continuous state variables under non-linear global constraints describing the movement of a soft robotic arm inspired by the octopus extension and fetching movements.

A micro-macro parareal algorithm for slow-fast systems with applications to molecular dynamics

Giovanni Samaey
Dept. Computer Science
KU Leuven
joint work with Frederic Legoll, Tony Lelievre

We introduce a micro-macro parareal algorithm for the time-parallel integration of multiscale-in-time systems. The algorithm first computes a cheap, but inaccurate, solution using a coarse propagator (simulating an approximate slow macroscopic model), which is iteratively corrected using a fine-scale propagator (accurately simulating the full microscopic dynamics). This correction is done in parallel over many subintervals, thereby reducing the wall-clock time needed to obtain the solution, compared to the integration of the full microscopic model. We provide a numerical analysis of the algorithm for a prototypical example of a micro-macro model, namely singularly perturbed ordinary differential equations. We show that the computed solution converges to the full microscopic solution (when the parareal iterations proceed) only if special care is taken during the coupling of the microscopic and macroscopic levels of description. The convergence rate depends on the modeling error of the approximate macroscopic model. We illustrate these results with numerical experiments, including a non-trivial model inspired by molecular dynamics.

Multilevel Uncertainty Quantification Methods

Robert Scheichl
Mathematical Sciences
University of Bath

The coefficients in mathematical models of physical processes are often impossible to determine fully or accurately, and are hence subject to uncertainty. It is of great importance to quantify the uncertainty in the model outputs based on the (uncertain) information that is available on the model inputs. This invariably leads to very high dimensional quadrature problems associated with the computation of statistics of quantities of interest, such as the time it takes a pollutant plume in an uncertain subsurface flow problem to reach the boundary of a safety region or the buckling load of an airplane wing. Higher order methods, such as stochastic Galerkin or polynomial chaos methods, suffer from the curse of dimensionality and when the physical models themselves are complex and computationally costly, they become prohibitively

expensive in higher dimensions. Instead, some of the most promising approaches to quantify uncertainties in continuum models are based on Monte Carlo sampling and the "multigrid philosophy". Multilevel Monte Carlo (MLMC) Methods have been introduced recently and successfully applied to many model problems, producing significant gains. In this talk I want to recall the classical MLMC method and then show how the gains can be improved further (significantly) by using quasi-Monte Carlo (QMC) sampling rules. More importantly the dimension independence and the improved gains can justified rigorously for an important model problem in subsurface flow. In the final part of my talk I will move away from the simple problem of uncertainty propagation from model inputs to model outputs and discuss how multilevel methods can also be used very successfully in Bayesian inference, i.e. stochastic inverse problems incorporating also some measurements of model outputs.

A Review on AMG: From Academia to Industry

Klaus Stüben
NUSO
Fraunhofer Institut SCAI

The development of algebraic multigrid (AMG) started over 30 years ago, driven by the attempt to automate and generalize geometric multigrid for the efficient solution of elliptic partial differential equations. The original AMG approach was effectively restricted to particular classes of problems, an important one being the class of linear algebraic systems with matrices close to rowsum zero M-matrices. In such cases, the original AMG is very mature and can handle large linear systems much more efficiently than any one-level method. While geometric multigrid solvers, when available, are generally still faster than their algebraic counterpart, the strengths of AMG-based solvers are its robustness and ease of use, its applicability in complex geometric situations with unstructured grids, and its capability to even solve certain (non-PDE) problems which are beyond the reach of geometric multigrid.

In spite of its potential, it took until around 1995 before there was a remarkable increase of interest in AMG, essentially caused by two facts: First, on the scientific side, the increasing geometrical complexity of applications, discretized on large and unstructured grids, technically limited the immediate use of geometric multigrid. Here AMG-based techniques appeared to be a promising alternative to tackle such problems. Second, in industrial simulation, models have been rapidly growing in geometric complexity, heterogeneity and size, causing the computational time required to solve linear systems of equations to become the major bottleneck. The classical one-level solvers used in industrial software packages seriously limited the practicability of numerical simulation. The potential of AMG-based solvers – their numerical efficiency, robustness and scalability – together with their ease-of-use as "plug-in" solvers have caused a growing industrial interest in such solvers.

Fostered by this situation, R&D on AMG-based and related methods has become a significant part of the general R&D on multigrid. Various extensions of the original AMG approach have been introduced, aiming at increasing its range of applicability. Several other possibilities to generalize AMG have been investigated; research on various new and related approaches has started and is still ongoing today. Most important from a practical point of view, substantial progress has been achieved regarding the efficient treatment of coupled systems of PDEs.

In this presentation we will give a review on the history of AMG in general and its impact on various branches of industrial simulation in particular. In contrast to geometric multigrid methods, AMG methods have found their way into many industrial and commercial simulation programs. We will summarize on our experiences and difficulties to bridge the gap between academia and industry.

Ideas in multilevel optimization

Philippe Toint
Mathematics
University of Namur
joint work with S. Gratton, A. Sartenaer, D. Tomanos, M. Mouffe

A review of some recent ideas for exploiting the multilevel structure in nonlinear optimization will be discussed. In many case, optimization problems involve variables which correspond to a discretization of an underlying continuous problem, and more than one level of discretization may be considered. We will briefly discuss three approaches which attempt to exploit this structure, in different algorithmic contexts. The first is that of trust-region methods for (possibly bound-constrained) optimization and the second is that of variable-metric methods for unconstrained problems. The third is simpler (a more standard mesh refinement scheme) but operates in the observation space of large-scale data fitting problems.

Multigrid for far and near field maps of the Helmholtz equation

Wim Vanroose
Mathematics and Computer Science
Universiteit Antwerpen
joint work with Siegfried Cools, Bram Reps

The Helmholtz equation desribes the scattering of electrons in small microscopic systems such a molecules. These problems are high-dimensional and are characterized by a smoothly varying wave number in contrast to typical engineering problems where the wave number has material jumps. Understanding these scattering process is important to basic sciences such as chemistry and biology.

In this talk we show that the far and near field scattering amplitudes for these Helmholtz equations can be efficiently be calculated using multigrid. Indeed, these amplitudes are integral expressions over the solution of the Helmholtz equation solved on a finite numerical box with absorbing boundary conditions covering the object of interest. A typical calculation has two steps. The first step is to solve the high-dimensional Helmholtz equation, which is a computationally very expensive and requires supercomputer infrastructure for the most challenging problems. The second step is to integrate over the solution to obtain the far field or near field amplitude. The latter is cheap can be done as a post processing step on a laptop.

By deforming the contour of integration into complex plane in the second step, the Helmholtz problem in the first step becomes much easier. Indeed, we show that the deformation of the contour turns the Helmholtz into a Complex shifted Laplacian problem, known to be solvable in a scalable way.

We validate the method for some benchmark problems and show the $\mathcal{O}(n)$ scalability on 3D Helmholtz and Schrödinger equations.

References

[1] Cools, S., Reps, B., and Vanroose, W. *An Efficient Multigrid Calculation of the Far Field Map for Helmholtz and Schrödinger Equations*, SIAM Journal on Scientific Computing **36** p267-395 (2014).

A unified study of geometric and algebraic multigrid methods

Jinchao Xu
Department of Mathematics
Penn State University

In this talk, I will report on a unified study of a number of multilevel methods including geometric and algebraic methods and upscaling methods. Emphasis will be on two classes of algebraic multigrid methods: one optimizing the coarsening with a fixed smoother, and the other optimizing the smoother with a fixed coarsening.

Regular sessions

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Multigrid methods for boundary control problems

Dirk Abbeloos
Department of Computer Science
University of Leuven
joint work with Stefan Vandewalle

In this talk we give an overview of multigrid methods designed for parabolic boundary control problems, i.e. a class of optimization problems where right-hand sides of the boundary conditions needs to be found in order to minimize an objective. We present multigrid components, e.g smoother and coarse grid operator, designed for Dirichlet and Robin type of boundary control problems. Numerical results are presented and illustrated through a half-space analysis, which is a mode analysis based on a half-space domain where the effect of only one boundary condition at a time can be included.

Three-stage multiscale algebraic preconditioner for highly heterogeneous diffusion subsurface problem on unstructured mesh

Davide Baroli
Departement of Mathematics, Laboratory for Modeling and Scientific Computing
Politecnico di Milano
joint work with Luca Formaggia

In subsurface problem, diffusion flow with multiscale coefficients and nature of media properties pose significant challenges for numerical methods. We investigate a novel multiscale domain decomposition preconditioner for solving the Darcian flow characterized by highly heterogeneous and highly anisotropic permeability field. Among multiscale domain decomposition framework, we present a three-stage multiscale algebraic preconditioner that yield condition number bound independent of the contrast in the media properties, extending the recent two-scale additive Schwarz preconditioner based on spectral coarse space introduced by Efendiev. In this work the third stage of multiscale solver is provided by auxiliary coarse space based on variational subgrid correction, which is able to capture the high oscillatory energy modes inside and across the coarse-grid block. We also present different synthetic test cases of porous media problem with high degree of variability due to presence of barrier, inclusion, and salt triangular layers to validate the robustness of the multiscale solver proposed.

Newton-Multigrid or Nonlinear Multigrid?

Keeran Brabazon
School of Computing
University of Leeds
joint work with Peter Jimack and Matthew Hubbard

Nonlinear multigrid methods such as the Full Approximation Scheme (FAS) and Newton-multigrid (Newton-MG) are well established as fast solvers for nonlinear PDEs of elliptic and parabolic type. In this presentation Newton-MG and FAS iterations are considered in a general setting and a theoretical approximation of the execution time of the algorithms is derived, which is shown to be sharp, that clearly demonstrates that Newton-MG is a faster iteration for finite element discretisations. Results are provided for elliptic and parabolic problems, demonstrating a faster execution time as well as greater stability of the

Newton-MG iteration. Results are tied in with current theory for the convergence of multigrid methods, giving a qualitative insight into how the nonlinear multigrid methods can be expected to perform in practice.

Simulating ion dynamics in neurons

Markus Breit
Goethe-Center for Scientific Computing
University of Frankfurt
joint work with Gillian Queisser

The neurosciences are a very active field of research. Numerical simulation, however, has not (yet) been broadly used where the experimental approach is costly or otherwise difficult. A key system to a huge variety of processes (such as maintenance and development of neurons in the context of learning or degenerative disease) is the regulation of intracellular calcium dynamics. Many players are involved, especially ion channel and pump activities in the cell membrane and the membranes of cell organelles are of interest and often have quite complex behaviour. We have developed a model including diffusion and reaction processes of calcium and other species as well as highly nonlinear membrane fluxes that can be applied in simulations for various neuroscientific purposes.

H2-matrix preconditioners

Steffen Börm
Department of Computer Science
University of Kiel
joint work with Knut Reimer

Generalised regularity results imply that the solution operators of strongly elliptic PDEs are rank-structured, i.e., that the interaction between well-separated subdomains can be approximated by low-rank operators. This holds true even for differential operators with discontinuous and anisotropic coefficients. The $\mathcal{H}^2$-matrix representation takes advantage of this property in order to find efficient preconditioners or solve eigenvalue problems.

In this talk, we consider new algorithms for constructing $\mathcal{H}^2$-matrix approximations of products, inverses and factorisations of the stiffness matrices corresponding to FEM and BEM problems. The algorithms rely on recursion and two fundamental algebraic operations: the simultaneous multiplication of an $\mathcal{H}^2$-matrix by k vectors and the update of an $\mathcal{H}^2$-matrix by a matrix of rank k. Both operations can be performed in linear complexity and give rise to higher-level algorithms of complexity $\mathcal{O}(nk^2 \log n)$.

In particular, we can construct efficient preconditioners for FEM and BEM problems in $\mathcal{O}(n \log n)$ operations requiring $\mathcal{O}(n)$ units of storage, and we can perform a step of the "slicing the spectrum" method for approximating arbitrary eigenvalues of PDEs in $\mathcal{O}(n \log n)$ operations.

A new level-dependent coarse grid correction scheme for indefinite Helmholtz problems

Siegfried Cools
Mathematics and Computer Science
University of Antwerp
joint work with Bram Reps and Wim Vanroose

Fast and efficient numerical solvers for indefinite Helmholtz problems are of great interest in many scientific domains that study acoustic, seismic or electromagnetic wave scattering. Applications such as engine design, oil exploration, medical imaging, but even quantum mechanical problems describing particle interaction [1], are governed by underlying Helmholtz equations of the form

$$Hu(\mathbf{x}) = (-\Delta - k(\mathbf{x})^2)u(\mathbf{x}) = f(\mathbf{x}), \qquad \text{with } \mathbf{x} \in \mathbb{R}. \tag{1}$$

Pushed by the rising interest in high resolution requirements and high-dimensional applications, the diffusion term in the Laplacian equation drives the condition number of the associated discretized operator to undesirable sizes for standard iterative methods to converge rapidly. In addition, for realistic values of the wavenumber $k(\mathbf{x})$ in (1), the Helmholtz operator H becomes indefinite, destroying the convergence behaviour of much preferred sparse linear system solvers such as e.g. Krylov subspace methods and classical geometric multigrid.

When the negative shifting term $-k(\mathbf{x})^2$ in the Helmholtz operator in (1) is replaced by a complex valued shift $-(\beta_1 + \imath\beta_2)k(\mathbf{x})^2$ the resulting operator is still closely related to the original, yet can efficiently be inverted with e.g. standard multigrid methods. This idea defined a well-known and successful Helmholtz preconditioning technique called complex shifted Laplacian [2]. The choice of the optimal value of the scaling parameter $\beta_1 + \imath\beta_2$ is a trade-off between a good preconditioner on the one hand and a computationally cheap inversion of that preconditioner on the other hand.

Inspired by the complex shifted Laplacian, we present the construction and analysis of a modified multigrid method that is capable of solving the original indefinite Helmholtz equation (1) on the finest grid using a series of multigrid cycles with a level-dependent complex shift, i.e. gradually perturbing the original Helmholtz operator throughout the hierarchy, leading to a stable correction scheme on all levels.

It is rigorously shown that the adaptation of the complex shift throughout the multigrid cycle maintains the functionality of the two-grid correction scheme, as no smooth modes are amplified in or added to the error. Complementary, a sufficiently smoothing relaxation scheme should be applied to ensure damping of the oscillatory error components. Contrary to classical multigrid preconditioning techniques like shifted Laplacian, the proposed level-dependent multigrid scheme is capable of directly solving the Helmholtz system (1) instead of being used as a preconditioner.

Numerical experiments on various physically relevant benchmark problems show the level-dependent multigrid solver to be competitive with or even outperform contemporary multigrid-preconditioned Krylov methods that use the classical level-fixed complex shift preconditioner.

References

[1] W. Vanroose, F. Martin, T.N. Rescigno and C.W. McCurdy, *Complete photo-induced breakup of the H2 molecule as a probe of molecular electron correlation*, Science, **310**(5755), pp. 1787–1789, 2005.

[2] Y.A. Erlangga, C.W. Oosterlee and C. Vuik, *A novel multigrid based preconditioner for heterogeneous Helmholtz problems*, SIAM Journal on Scientific Computing, **27**(4), pp. 1471–1492, 2006.

[3] S. Cools, B. Reps and W. Vanroose, *A new level-dependent coarse grid correction scheme for indefinite Helmholtz problems*, Numerical Linear Algebra with Applications, doi:10.1002/nla.1895, 2013.

BootCMatch: an alpha-AMG solver based on Compatible Weighted Matching

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In [2] we introduced a new adaptive Algebraic Multigrid (αAMG) method to solve symmetric positive definite (s.p.d.) systems of linear equations without exploiting any a-priori knowledge or assumptions on characteristics of the algebraic smoothness (or near null components of the system). Our method relies on a bootstrap strategy aimed to compute a sequence of AMG hierarchies composed in a multiplicative way. The goal is to obtain a composite solver with a desired convergence rate. Starting from a general (random) given vector, at each step of the bootstrap procedure, a new algebraically smooth vector related to the current composite solver is computed. Each successive hierarchy is built by using pairwise aggregation of unknowns driven by a weighted matching algorithm with weights depending on the most recently computed algebraically smooth vector utilizing a notion of the compatible relaxation [1]. Matching algorithms in a matrix graph were successfully exploited in reordering schemes designed to enhance matrix diagonal dominance in sparse direct methods [3]; we apply linear-time complexity approximate weighted matching in a graph [4] to form aggregates of unknowns and build the coarse-vector space by simple piecewise constant interpolation of the current algebraically smooth vector. This coarsening process, which we referred to as *compatible weighted matching*, is completely automatic and algebraic, and it replaces the commonly used characterization of strength of connections in both the coarse space selection and in the interpolation scheme.

In the present work, we describe an extension of the method, including aggressive coarsening obtained by combining multiple sweeps of the pairwise aggregation procedure, as well as utilizing more accurate interpolation operators obtained by weighted-Jacobi smoothing of the piecewise constant interpolation operators. This leads to smoothed aggregation type adaptive AMG (or SA-αAMG) method, which exhibits improved convergence properties and reduced building setup cost.

We present some main features of the *BootCMatch: αAMG based on Bootstrap Compatible Matching*, a C-language implementation of the method, and discuss performance results on a suite of symmetric positive-definite linear systems arising from discretization of elliptic PDEs as well as on problems from the University of Florida Sparse Matrix Collection.

References

[1] A. Brandt, *General Highly Accurate Algebraic Coarsening*, Electronic Transactions on Numerical Analysis, Vol. 10, pp. 1-20, 2000.

[2] P. D'Ambra, P. S. Vassilevski, *Adaptive AMG with Coarsening based on Compatible Weighted Matching* , to appear in Computing and Visualization in Science.

[3] I. S. Duff, J. Koster, *On Algorithms for Permuting Large Entries to the Diagonal of a Sparse Matrix*, SIAM J. on Matrix Analysis and Applications, Vol. 22, pp. 973-996, 2001.

[4] R. Preis, *Linear Time 1/2-Approximation Algorithm for Maximum Weighted Matching in General Graphs*, in STACS'99, LNCS, Springer-Verlag, Vol. 1563, pp. 259-269, 1999.

Challenges in multigrid for mixed elliptic/hyperbolic problems in radiation transport

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The Boltzmann transport equation is a linear PDE which governs the transport of neutral particles (i.e., neutrons, photons) in radiation transport problems. The steady-state, monoenergetic version of this PDE has 3 spatial dimensions (which we discretise with the FEM on unstructured grids) and 2 angular dimensions (of which there are several common discretisations), which results in a very large linear system, which forces the use of matrix-free methods. Furthermore, given different physical materials, the PDE can behave in both an elliptic or hyperbolic fashion in a single domain.

This makes designing effective multigrid schemes challenging, as directional information in hyperbolic regions is encapsulated within angular variables. Traditional AMG approaches also perform poorly on this system. An approach based on coarsening algorithms from AMGe and simple interpolation will be presented that performs well in diffuse regions, but suffers from difficulties in strongly hyperbolic regions.

A Fast Method for Modeling Water Infiltration in Porous Media

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joint work with Mookwon Se, Derrick Cerwinsky, and Han Yu

Water infilitration from the surface to the groundwater level is usually simulated using a model based on either Richards equation or a reservoir model. In this talk we present a model derived from Darcy's law known as the Talbot-Ogden (T-O) model. Instead of one of the usual 3D models, we have a depth versus water content based on a water content domain. We investigate three ways of implementing the T-O model and evaluate each in terms of computational complexity, parallelism potential, and accuracy based on lab and field experiments and data.

Optimal-order multigrid preconditioners for linear systems arising in the semi-smooth Newton solution of certain PDE-constrained optimization problems

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We present a new technique for constructing multigrid preconditioners arising in the semi-smooth Newton solution process of optimization problems of the form

$$\min_{u\in L^2(\Omega)} \frac{1}{2}\|\mathcal{K}u - b\|^2 + \frac{\beta}{2}\|u\|^2 \ , \quad \underline{u} \le u \le \overline{u} \ , \tag{2}$$

where $\mathcal{K} : L^2(\Omega) \to \mathcal{Y}$ is a bounded linear operator, with the embedding $\mathcal{Y} \hookrightarrow L^2(\Omega)$ being compact, and $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, is bounded domain. Problem (1) can be regarded as the reduced form of

a PDE-constrained optimization problem with $\mathcal{K}$ being the solution operator of a PDE (for example, $\mathcal{K} = (-\Delta)^{-1} : L^2(\Omega) \to H_0^1(\Omega)$).

For a piecewise constant discretization of the discrete control space V_h, each semi-smooth Newton (outer) iteration requires the solution of a linear system whose matrix is a principal submatrix of $G_h = K_h^T K_h + \beta I$, where K_h is the matrix representing the discretization of $\mathcal{K}$, and h is the mesh size. In a large-scale context these (inner) linear systems are solved using preconditioned conjugate gradient. An earlier technique [1] produced a multigrid preconditioner M_h for G_h that satisfies, under reasonable conditions

$$1 - C\frac{h^{\frac{1}{2}}}{\beta} \leq \frac{\langle M_h u, u\rangle}{\langle G_h u, u\rangle} \leq 1 + C\frac{h^{\frac{1}{2}}}{\beta}, \quad \forall u \in V_h \setminus \{0\} \ . \tag{3}$$

As a result of (2), the number of inner linear iterations needed to solve the system at each outer iteration decreases with $h \downarrow 0$. While this result is interesting from a theoretical point of view (and qualitatively consistent with the behavior of the preconditioner for the full system), its practicality is limited by the suboptimal factor $h^{1/2}$ in (2).

The new technique, relying on constructing larger and non-conforming coarse spaces, produces multigrid preconditioners M_h that are able to capture the character of the operator G_h in an optimal way, namely we have

$$1 - C\frac{h}{\beta} \leq \frac{\langle M_h u, u\rangle}{\langle G_h u, u\rangle} \leq 1 + C\frac{h}{\beta}, \quad \forall u \in V_h \setminus \{0\} \ .$$

References

[1] Andrei Drăgănescu, *Multigrid Preconditioning of Linear Systems for Semismooth Newton Methods Applied to Optimization Problems Constrained by Smoothing Operators*, Optimization Methods and Software (DOI:10.1080/10556788.2013.854356), 2013.

Algebraic Multigrid Methods for Velocity Pressure Coupling in CFD

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In standard commercial Computational Fluid Dynamics (CFD) programs the Navier-Stokes equations are solved using the SIMPLE algorithm, which is a segregated approach that solves only for one single physical unknown at a time (velocity, pressure).
Here a coupled approach is investigated where velocity and pressure equation are solved simultaneously, which leads to a block matrix system. For both segregated and coupled approach we use Algebraic Multigrid Methods as preconditioner. We compare the two approaches regarding convergence and robustness with respect to mesh size and quality. Further we investigate the application of block preconditioners for the matrix which arises from the coupled approach.
The velocity pressure coupling is implemented in the framework of the CFD software AVL FIRE®. We illustrate our results by industrial benchmark examples.

Parallel time integration with multigrid for parabolic problems

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joint work with Robert Falgout, Tzanio Kolev, Scott MacLachlan, and Jacob Schroder

With current trends in computer architectures leading towards systems with more, but not faster, processors, faster time-to-solution must come from greater parallelism. These trends particularly impact the numerical solution of the linear systems arising from the discretization of partial differential equations (PDEs) with evolutionary behavior, such as parabolic (space-time) problems. The classic view of applying multigrid to this class of problems is based on a time-marching approach: discretization of the PDE leads to a discrete elliptic problem at each time step when an implicit scheme is used. Multigrid is then used as an iterative solver for these elliptic equations. Parallelization in this approach is limited to parallelization in the elliptic (spatial) solver, since the time-stepping procedure is sequential.

While two-level methodologies, such as parareal, are well-established for parallel-in-time integration, true multilevel approaches remain uncommon. In this talk, we present one such technique, derived based on multigrid reduction principles. The resulting multigrid-reduction-in-time (MGRIT) algorithm is a non-intrusive approach, which only uses an existing time propagator and, thus, easily allows one to exploit substantially more computational resources than standard sequential time stepping. We discuss progress to date in applying MGRIT to parabolic (space-time) problems. In particular, we demonstrate that MGRIT offers excellent strong and weak parallel scaling up to thousands of processors for solving diffusion equations in two and three space dimensions.

Condition number estimates for higher order NURBS discretizations

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joint work with Satyendra Tomar and Craig Douglas

The discretization matrix A gets denser by increasing the polynomial degree p. Therefore, the cost for solving large problems becomes prohibitively expensive. The most practical way to solve them is to resort to a iterative method. Since the convergence rate of such methods ,e.g. multigrid methods, is strongly affected by the condition number of the system matrix A, it is important to assess this quantity as a function of the mesh size h for the h-refinement, or as a function of the degree p for the p-refinement.

In this talk, we will derive bounds for the minimum and maximum eigenvalues and the spectral condition number of matrices for higher order NURBS discretizations of elliptic partial differential equations in an open, bounded, simply connected Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$. We consider refinements based on mesh size h and polynomial degree p with maximum regularity of spline basis functions. For the h-refinement, the condition number of the stiffness matrix is bounded above by a constant times h^{-2} and the condition number of the mass matrix is uniformly bounded. For the p-refinement, the condition number grows exponentially and is bounded above by $p^{2d+2}4^{pd}$ and $p^{2d}4^{pd}$ for the stiffness and mass matrices, respectively. Rigorous theoretical proofs of these estimates will be provided and supporting numerical results.

MGOPT Methods for Optimization Problems Arising in Non-Newtonian Fluids Simulation

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This work is concerned with the application of multigrid methods to the numerical solution of the following class of optimization problems: find $y \in W_0^{1,\nu}(\Omega)$ such that

$$\min_{y \in W_0^{1,\nu}} J(y) := \frac{1}{\nu} \int_\Omega |\nabla y|^\nu \, dx + g \int_\Omega |\nabla y| \, dx - \int_\Omega f y \, dx,$$

where $g > 0$ and $f \in W^{-1,\nu'}(\Omega)$ is a given function. This kind of problems arise in the modelization of non-Newtonian fluids e.g. the Herschel-Bulkley model . We propose a Huber regularization of the non-differentiable term in the functional J. Well posedness of the regularized problems is proved, and convergence of the regularized solutions to the solution of the original problem is verified. Further, we discuss the finite element discretization of the problem. Our main interest is to develop a multigrid algorithm to solve these kind of problems at big scale. Therefore, we propose a multigrid for optimization method (MGOPT) for the numerical solution of the discretized problem. This method is based on the well known full approximation storage (FAS) scheme. As an important feature of this work, we propose to use a preconditioned descent method combined with an innovative linesearch method as the smoothing process. Finally, several numerical experiments are carried out to show the efficiency of the approach. Particularly, we discuss the application of our algorithm to simulate the flow of non-Newtonian fluids.

References

[1] J.C. De los Reyes and S. González Andrade, *Numerical simulation of two-dimensional Bingham fluid flow by semismooth Newton methods*, Journal of Computational and Applied Mathematics, 235 (2010) 11-32.

[2] R.R. Huilgol and Z. You, *Applications of the augmented Lagrangian method to steady pipe flows of Bingham, Casson and Herschel-Bulkley fluids*, Journal of Non-Newtonian Fluid Mechanics, 128 (2005) 126-143.

[3] S.G. Nash,*A multigrid approach to discretized optimization problems*, Optim. Methods Soft., 14 (2000) 99-116.

[4] M. Vallejos and A. Borzì,Multigrid optimization methods for linear and bilinear elliptic control problems, Computing, 82 (2008) 31-52.

Truncated Nonsmooth Newton multigrid methods for vector valued minimization problems

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joint work with Oliver Sander

The extension of the classical Gauß–Seidel method to scalar problems with separable nonsmooth terms is straight forward. In contrast to this vector valued block separable problems demand for smoothers with local solvers tailored to the structure on the nonsmooth terms. Similarly the construction of coarse grid corrections has to take care on this structure.

We will present truncated nonsmooth Newton multigrid (TNNMG) methods that rely on nonlinear inexact block Gauß–Seidel smoothers and linear coarse grid corrections derived using ideas from nonsmooth analysis. While the performance and efficiency of TNNMG is comparable to linear multigrid it is more flexible and easier to implement than other schemes. Numerical examples from applications in material science, continuum mechanics, and glacier modeling show the flexibility, efficiency, and robustness of this approach.

Comparison of different AMG implementations for non-symmetric problems in CFD

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In our approach to multiphase flow simulations, we encounter the well-known convection-diffusion equation and a weighted sum of diffusion operators, with one diffusion term per phase. In our finite volume discretization, both (scalar) equations result in non-symmetric linear systems.

We applied the AMG implementations BoomerAMG, ML, GAMG and AGMG as well as our finite volume based aggregation scheme to a number of test cases. The presentation contains the obvious convergence comparisons in terms of number of iterations, sequential wall-clock times and memory consumption, and also some remarks on usability from a user's point of view.

Parallel Hierarchical Hybrid Multigrid Solver for Variable Viscosity

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joint work with B. Gmeiner, U. Rüde, C. Waluga, B. Wohlmuth

The hierachical hybrid grid (HHG) framework is designed to close the gap between the flexibility of finite elements and the performance of geometric multigrid by employing semi-structured meshes. It provides excellent scalability up to a million parallel threads and can solve in excess of 10^{12} unknowns in less than 2 minutes compute time on state of-the-art supercomputers. The framework has recently been extended to solve the Stokes system as a building block for geophysical flow simulations. In this presentation we will concentrate on the analyzing the multigrid convergence in case of variable viscosity. In the cases of interest, close to optimal multigrid convergence can be maintained by combining suitable smoothers and Krylov space acceleration.

A Multilevel Bilinear Programming Algorithm for the Vertex Separator Problem

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joint work with William Hager and Ilya Safro

Given a simple undirected graph G, the vertex separator problem (VSP) is to find the smallest collection of vertices whose removal separates G into two disconnected sets of approximately the same size. Applications include VLSI design, sparse matrix factorizations, and hypergraph partitioning. In this talk, we present a multilevel algorithm for solving large-scale instances of this VSP. A key feature of our algorithm is in the refinement phase. While most modern multilevel graph partitioners carry out refinements using node-swapping heuristics such as the Fiduccia Mattheyses algorithm, our algorithm refines solutions by solving a recently discovered continuous bilinear programming formulation of the VSP. Numerical results are given comparing our algorithm with the VSP solver METIS, which employs traditional node-swapping heuristics.

A Hybrid Multigrid Algorithm for Elliptic Problems using Adaptive Higher-Order Cut Cells

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joint work with D. Graves, P. Devendran

We propose a hybrid geometric-algebraic multigrid approach for solving elliptic equations on domains with complex geometries. The discretization uses a novel higher-order ($p = 2, 4, 6$) *finite volume, cell average* cut cell representation to discretize the variable coefficient elliptic operator on a Cartesian mesh. The benefit of this is a regular stencil in most of the domain, thereby avoiding difficulties associated with algebraic coarsening of a global mesh. However, the challenge introduced with cut cells is two-fold: the resulting operators are typically not symmetric, and small cut cells can generate very large negative eigenvalues in the finite volume formulation. In addition, traditional geometric coarsening introduces very different representations of the cut cell operator on coarser meshes, and can produce topological constraints on the coarsest mesh, where we can apply an algebraic solver more effectively. We find that the hybrid approach realizes many of the benefits of geometric coarsening while retaining the robustness of algebraic multigrid. We demonstrate this approach for a number of examples of complex geometries in an adaptive mesh hierarchy implemented in the *Chombo* parallel framework. Our results show that we obtain both higher-order accuracy and near-optimal multigrid convergence rates, without being constrained by traditional aggregation methods or adjoint operators for restriction and prolongation.

Structure Preserving Algebraic Multigrid

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joint work with James Brannick

We develop an algebraic multigrid method for solving linear systems of equation with non-Hermitian matrices that possess a simple symmetrizing operator, e.g., Saddle-point problems, Hamiltonian matrices. In particular we develop a method for the Wilson discretization of the 2-dimensional Dirac equation. The

proposed approach uses a bootstrap setup algorithm based on a multigrid eigensolver. It computes test vectors which define the least squares interpolation operators by working mainly on coarse grids, leading to an efficient and integrated self learning process for defining algebraic multigrid interpolation.

The algorithm is motivated by the γ_5-symmetry of the Dirac equation, which carries over to the Wilson discretization. This discrete γ_5-symmetry is used to reduce a general Petrov Galerkin bootstrap setup algorithm to a Galerkin method for the Hermitian and indefinite formulation of the Wilson matrix. Kaczmarz relaxation is used as the multigrid smoothing scheme in both the setup and solve phases of the resulting Galerkin algorithm. Extensive numerical results are presented to motivate the design and demonstrate the effectiveness of the proposed approach.

Multigrid method on Intel Xeon Phi (MIC)

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The multigrid method is a well-known, fast and efficient algorithm to solve many classes of problems. In general, the ratio of the communication costs to computation costs increases on the coarser level, i.e., the communication costs are high on the coarser levels in comparison to the computation costs. So, reducing the costs of the communication is a major issue in implementation of the parallel multigrid method. Using a hybrid programming model which uses OpenMP for parallelization inside node and MPI for message passing between nodes and can reduce the number of MPI tasks, we have better scaling properties on a massively parallel computer.

Modern computer architectures have highly hierarchical system design, i.e., multi-socket multi-core shared-memory computer nodes which are connected via high-speed interconnects, and now accelerators such as Intel Xeon Phi (MIC) coprocessors or GPUs (Graphics Processing Units) are emerged. The OpenMP 4 standard supports to use these accelerators. In this talk, we present the performance results of the parallel multigrid method with hibridization implementation on a MIC partition of the Helios machine which is dedicated machine for Europe and Japan Fusion community.

GPU Multigrid Solver for the Navier-Stokes Equations

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joint work with Petr Bauer and Tomas Oberhuber

This contribution present a GPU implementation of a multigrid method for the problem of 2D air flow over a simplified urban canopy governed by the incompressible Navier-Stokes equations. In the first part we present this problem which is discretized by means of the mixed finite element method with semi-implicit time stepping and then the arising linear saddle-point problem which is solved by the geometric multigrid method with the Vanka type smoother.

In the second part the GPU implementation itself and issues that had to be resolved are described. Finally the obtained speed-ups will be shown. We have achieved the speed-up of 5 compared to the parallel code based on OpenMP and 26 compared to the sequential code.

Mechanistic dynamics of Hepatitis C virus replication in single liver cells

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joint work with A. Nägel, S. Reiter, M. Rupp, P. Targett-Adams, E. Herrmann, G. Wittum

Infection with hepatitis C virus (HCV) causes chronic liver diseases. HCV-related liver damage is the main reason for liver transplantations in the western world. Spatial resolution is an aspect that has not yet been appreciated in current modeling simulations despite strong biological evidence that suggests intracellular spatial dependence is a crucial factor in the process the virus uses to replicate its RNA genome. HCV replication is believed to occur in specialized compartments within virus-infected cells, termed replication complexes, which are derived from altered regions (called the membranous web) of the endoplasmic reticulum (ER - the ER is a central structure of each cell). Trafficking of both replication complexes, and their components, is likely a dynamic process occurring in three dimensions that is both difficult to capture experimentally and conceptually visualize. Therefore, we are developing a spatially-resolved biophysical model of HCV replication dynamics in single liver cells. We used data derived from 3D confocal microscopy of HCV-infected human hepatoma cells labeled for the ER membrane in order to reconstruct 3D geometries of single hepatocytes using NeuRA2. On top of these geometries, we developed a model using (surface) partial differential equation of viral RNA replication dynamics with particular emphasis upon RNA movement, viral protein production, cleavage and movement, and viral RNA replication within the membranous web. The arising (s)pde s on the ER surface are solved using the simulation platform UG4 within a Finite Volume framework combined with multigrid techniques. Our approach is based on two columns which are intended to grow together in the middle run: On the one hand side, we are doing parameter estimations of single components of viral replication based on the Gauss-Newton algorithm in order for extracting e.g. the diffusion constant of basic viral proteins on the surface of the ER using experimental FRAP time series. On the other hand side, we are developing the model which mimics the interplay of all important component of virus replication, e.g. viral RNA and various states of viral proteins. The estimated parameters are entering the model step by step. Therefore, the presented work is a practical application of the powerful tool UG4 and its multigrid techiques for the case of a huge number of DoFs (about 10^6) already at base level and demonstrates the excellent usability (and scalability) of UG4 in the context of modern biophysical research.

References

[HLN13] Heppner I., Lampe M., Nägel A., Reiter S., Rupp M., Vogel A., Wittum G.: Software Framework ug4: Parallel Multigrid on the Hermit Supercomputer. In: Nagel W., Kröner D., Resch M. (eds) High Performance Computing in Science and Engineering '12. Springer (2013)

[VRR13] Vogel A., Reiter S., Rupp M., Nägel A., Wittum G.: UG4—a novel flexible software system for simulating PDE based models on high performance computers. Comp. Vis. Sci., in press (2013)

[JW11] Jungblut D, Queisser G, and Wittum G (2011). Inertia Based Filtering of High Resolution Images Using a GPU Cluster. Comp. Vis. Sci., 14:181-186.

[MPR07] Nature Reviews Microbiology 5, 453-463 (2007) Replication of hepatitis C virus. Darius Moradpour, François Penin & Charles M. Rice

[MLTA07] Mobility analysis of an NS5A-GFP fusion protein in cells actively replicating hepatitis C virus subgenomic RNA. Jones DM, Gretton SN, McLauchlan J, Targett-Adams P. J Gen Virol. 2007 Feb;88(Pt 2):470-5.

[TAML08] J Virol. 2008 Mar;82(5):2182-95. Epub 2007 Dec 19. Visualization of double-stranded RNA in cells supporting hepatitis C virus RNA replication. Targett-Adams P1, Boulant S, McLauchlan J.

[TAW11] Small molecules targeting hepatitis C virus-encoded NS5A cause subcellular redistribution of their target: insights into compound modes of action. Targett-Adams P, Graham EJ, Middleton J, Palmer A, Shaw

SM, Lavender H, Brain P, Tran TD, Jones LH, Wakenhut F, Stammen B, Pryde D, Pickford C, Westby M. J Virol. 2011 Jul;85(13):6353-68.

[RBB13] Three-dimensional architecture and biogenesis of membrane structures associated with hepatitis C virus replication. Romero-Brey I, Merz A, Chiramel A, Lee JY, Chlanda P, Haselman U, Santarella-Mellwig R, Habermann A, Hoppe S, Kallis S, Walther P, Antony C, Krijnse-Locker J, Bartenschlager R. PLoS Pathog. 2012;8(12):e1003056. doi: 10.1371/journal.ppat.1003056. Epub 2012 Dec 6.

[BSK13] Replication vesicles are load- and choke-points in the hepatitis C virus lifecycle. Binder M, Sulaimanov N, Clausznitzer D, Schulze M, Hüber CM, Lenz SM, Schlöder JP, Trippler M, Bartenschlager R, Lohmann V, Kaderali L. PLoS Pathog. 2013;9(8):e1003561. doi: 10.1371/journal.ppat.1003561. Epub 2013 Aug 22.

Block H-LU preconditioners for higher-order FEM

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The finite element discretization of partial differential equations requires the selection of suitable finite element spaces. While higher order finite elements lead to solutions of higher accuracy, their associated discrete linear systems of equations are often more difficult to solve than those of lower order elements.

Here, we present efficient preconditioners for these types of linear systems of equations. More specifically, we will use hierarchical ($\mathcal{H}$-) matrices to build block $\mathcal{H}$-LU preconditioners. $\mathcal{H}$-matrices provide a powerful technique to compute and store approximations to dense matrices in a data-sparse format. The basic idea is the approximation of matrix data in hierarchically structured subblocks by low rank representations. The preconditioners will be of a "hybrid blackbox" nature: The setup of the preconditioner will occur in a "blackbox" fashion, i.e., only the stiffness matrix is needed as input. However, the "hybrid" part implies that certain knowledge of the origin of the system is available and will possibly be exploited. Such knowledge could include a certain sparsity structure (e.g. produced through particular types of finite elements) or even a certain block structure (e.g. in mixed finite elements). We conclude with numerical results.

A simulation technique for density-driven flow in porous media with complicated fracture networks

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joint work with A. Grillo, S. Reiter, S. Stichel and G. Wittum

In the talk, we present a discretization and numerical solvers for a model of density driven flow in a fractured porous medium. The flow is described by the Darcy law, in particular with the Forchheimer correction. The fractures are considered to be filled with an essentially more permeable porous medium as the bulk medium. These fractures are represented by low-dimensional manifolds with their own functions for the solution. The solution in the bulk medium may have jumps over the fractures. For the discretization, the manifolds are resolved by the grid and filled with degenerated grid elements. This enables to place several degrees of freedom at every geometric point and therefore to represent the jumps. This technique allows to consider all possible configurations of intersecting fracture in 2 and 3 dimensions. The coupled system of the discretized equations for the bulk medium and the fractures is solved using multigrid methods.

Multigrid Method for Systems of Nonlinear Equations arising from Poroelasticity Problem

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joint work with F.J.Gaspar and C.W.Oosterlee

Shale gas is natural gas which is formed by being trapped within shale layer formations. Shale layers have typically very low permeability which dramatically reduces the mobility of this so-called unconventional gas. Hydraulic fracturing has been regarded as one of key methods of extracting these gas resources. It is a process in which the energy from the injection of a highly pressurized fluid creates fractures within the rock.

The coupled seepage and stress process in saturated geological media can be interpreted by means of Biot's theory of consolidation. It describes the time-dependent interaction between the deformation of porous material and the fluid flow pressure inside of it. Our 2D problem can be formulated as a system of partial differential equations for the unknowns displacements u,v and pore pressure of the fluid p. The governing equations are given by:

$$\begin{cases} -(\lambda+2\mu)u_{xx} - \mu u_{yy} - (\lambda+\mu)v_{xy} + \alpha p_x = f_1, \\ -(\lambda+\mu)u_{xy} - \mu v_{xx} - (\lambda+2\mu)v_{yy} + \alpha p_y = f_2, \\ \frac{1}{Q}p_t + (u_x+v_y)_t - k(\sigma,p)(p_{xx}+p_{yy}) = f_3 \end{cases}$$

Here λ and μ are Lame coefficients. k is the coefficient of permeability which depends on the stress and fluid pressure, resulting in a nonlinear set of equation.

Numerical approximation is necessary to solve this problem. As it is a nonlinear system of equations, we would like to use a nonlinear multigrid method, such as FAS and Newton-multigrid, as an iterative solution method for the discretized partial differential equations. It is the challenge to determine suitable multigrid components. We would like to discrete equations on collocated grids. However, such discretization may be unstable, because some oscillations may appear in the first time steps of numerical solution. After this phase, the solution becomes smoother and these oscillations tend to disappear. We need to take some special care in order to construct a stable discretization for the whole process. This can be achieved by adding an artificial elliptic pressure term to the seepage equation. The artificial term is $\varepsilon\frac{\partial\triangle p}{\partial t}$, with $\varepsilon = \frac{h^2}{4(\lambda+2\mu)}$. When the grid size $h \to 0$, the artificial pressure term tends to 0. Since this term is proportional to h^2, second order accuracy can also be maintained. With respect to the smoother, we choose the so-called box relaxation which solves the discrete equations locally cell by cell. In practice, this means that five unknowns centered around a pressure point are relaxed simultaneously. So in one smoothing iteration all displacement unknowns are updated twice, whereas pressure unknowns are updated once. Numerical experiments will show the good convergence of multigrid and also the simulation of crack formation.

A robust structured incomplete Cholesky preconditioner

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We consider a new algebraic factorization preconditioner for the iterative solution of large sparse symmetric positive definite linear systems. The preconditioner is based on a sparse variant of Cholesky factorization in which the off-diagonal part of the block rows of the factor is approximated by low-rank matrices. We use low-rank approximations that satisfy a specific orthogonality condition: the approximation is orthogonal to the corresponding approximation error. The resulting factorization is

then shown breakdown-free, and further, the corresponding condition number is bounded as a function of the accuracy of individual approximations.

On the practical side, the preconditioner exploits, in an algebraic manner, the low rank structure available in PDE applications. This is achieved through the reordering of unknowns which is based on the sparsity pattern of the system matrix, and which preserves the sparsity patter of the resulting factor. A preliminary implementation of the method is presented and compared with similar Cholesky and incomplete Cholesky factorizations based on dropping of individual entries.

A parallel space-time multigrid solver for the Navier-Stokes equations

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For evolution equations we present a space-time method based on Discontinuous Galerkin finite elements. Space-time methods have advantages if we have to deal with moving domains and if we need to do local refinement in the space-time domain. For this method we present a multigrid approach based on space-time slabs. This method allows the use of parallel solution algorithms. In particular it is possible to solve parallel in time and space. Furthermore this multigrid approach leads to a robust method with respect to the polynomial degree which is used for the DG time stepping scheme. Numerical examples for the Stokes and Navier-Stokes equations will be given which show the performance of this space-time multigrid approach.

Robust preconditioners for PDE-constrained optimization with limited observations

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joint work with Kent-André Mardal, Bjørn Fredrik Nielsen

Regularization-robust preconditioners for PDE-constrained optimization problems have been successfully developed. These methods, however, typically assume that observation data is available throughout the entire domain of the state equation. For many inverse problems, this is an unrealistic assumption. We propose and analyze preconditioners for PDE-constrained optimization problems with limited observation data, e.g. when observations are only available at the boundary of the computational domain. Our methods are robust with respect to both the regularization parameter and the mesh size. That is, the number of required MINRES iterations is bounded uniformly, regardless of the size of the two parameters. The theoretical findings are illuminated by several numerical results.

A new multigrid strategy for Stokes problems

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Standard discretizations of Stokes problems lead to linear systems of equations in saddle point form:

$$\begin{pmatrix} A & B^T \\ B & -C \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{0} \end{pmatrix},$$

where the matrix block C is either zero in case of a stable discretization, or a small stabilization term. Due to this possible zero block, the direct application of algebraic multigrid methods is notoriously difficult.

In this talk, we propose a new approach to overcome this difficulty. It consist in first transforming the above system by pre- and post-multiplication with simple (and algebraic) sparse block triangular matrices; doing thus a form of pre-conditioning in the literal sense, designed to make sure that the transformed matrix is "well adapted" to multigrid.

More precisely, after transformation, all the diagonal blocks are symmetric positive definite, and resemble or correspond to a discrete Laplace operator. The idea is then to associate to each block a prolongation that works well for it, and to combine these to obtain a global prolongation. Observe that this can be achieved with virtually any algebraic or even geometric multigrid method.

Finally, nothing more is needed: for damped Jacobi-smoothing, uniform two-grid convergence can be guaranteed for the global system under the sole assumption that the two-grid schemes for the different diagonal blocks are themselves uniformly convergent – a requirement easy to meet given that these blocks are discrete Laplace-like matrices.

The approach will be illustrated by a few examples, showing further that time-dependent problems and variable viscosity can be handled in a natural way, without requiring a particular treatment.

A Multilevel Proximal Algorithm for Large Scale Composite Convex Optimization

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Composite convex optimization models consist of the minimization of the sum of a smooth convex function and a non-smooth convex function. Such models arise in many applications where, in addition to the composite nature of the objective function, a hierarchy of models is readily available. It is common to take advantage of this hierarchy of models by first solving a low fidelity model and then using the solution as a starting point to a high fidelity model. We adopt an optimization point of view and show how to take advantage of the availability of a hierarchy of models in a consistent manner. We do not use the low fidelity model just for the computation of promising starting points but also for the computation of search directions. We establish the convergence and convergence rate of the proposed algorithm and compare our algorithm with two widely used algorithms for this class of models (ISTA and FISTA). Our numerical experiments on large scale image restoration problems suggest that, for certain classes of problems, the proposed algorithm is significantly faster than both ISTA and FISTA.

Local Fourier analysis for ILU smoothers on triangular grids

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joint work with Carmen Rodrigo and Francisco José Gaspar

This work is focused on the design of efficient multigrid methods for discretizations on triangular grids. For this purpose, a local Fourier analysis is developed. An ILU smoother for the discretization of diffusion problems by linear finite elements on such grids is analyzed. A two-grid Fourier analysis is performed to analyze the behavior of the multigrid method. Numerical test calculations validate the theoretical predictions.

A Multiscale Model of Synaptic Contacts between Brain Cells

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joint work with Stephan Grein

Biological processes are typically active on multiple, coupled scales. An example are the chemical contacts between brain cells. We present a multiscale model of chemical synapses, that couples the molecular dynamics of cell-adhesion Cadherin molecules interacting with calcium ions and the continuum scale model representing synaptic function. For this purpose we developed a tetrahedral volume grid representation of a synapse used in a Finite Volume discretization of the synaptic model (described by a system of PDEs). On the molecular scale we use molecular dynamics (MD) simulations and couple these to the discrete function space of the PDE-problem, using transfer operators that map between the cartesian space and function space. The three-dimensional non-linear diffusion-reaction system with non-linear interface conditions is solved using parallel multi-grid methods and time-parallel methods. Simulation results demonstrate the methods applied to the model of intercellular coupling between nerve cells and the necessity to employ a multiscale model solved with multi-level solvers.

A FE based Multigrid scheme for elliptic Nash-equilibrium optimal control problems

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joint work with Alfio Borzi

A finite-element based multigrid scheme for elliptic Nash-equilibrium multiobjective optimal control problems with control constraints will be presented. The multigrid computational framework implements a nonlinear multigrid strategy and collective smoothing for solving the multiobjective optimality system discretized with finite elements. Error estimates for the optimal solution and two-grid local Fourier analysis of the multigrid scheme are also discussed. Results of numerical experiments are presented to demonstrate the effectiveness of the proposed framework.

On a highly scalable infrastructure for massively parallel multigrid solvers

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joint work with Andreas Vogel and Gabriel Wittum

Application of parallel geometric multigrid solvers on adaptively refined grids requires a careful design of the involved load-balancing and load-migration routines as well as fast communication between copies of distributed objects. In error-estimation based refinement strategies, multiple rebalancing steps may be required to provide a uniform element distribution between all processors in all steps. In order to perform such operations efficiently on supercomputers with millions of cores, one has to extend existing load balancing and communication schemes.

We outline the parallel infrastructure for distributed multigrid hierarchies in the simulation framework UG4 and present experimental scaling studies for our geometric multigrid solver on adaptive and non-adaptive grid hierarchies on up to 262144 processes. We focus on an efficient hierarchical organization of the involved processes, on efficient horizontal and vertical communication schemes as well as on the parallel refinement and load-balancing strategies used.

A high arithmetic intensity multigrid preconditioner based on matrix polynomials

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joint work with Wim Vanroose

One of the current tendencies in the development of new computer hardware is the increasing number of processors per chip. This naturally brings along the challenge of larger communication costs, relative to the speed of computation. The number of useful floating point operations per data-read from slow memory, i.e. the arithmetic intensity, plays a determining role in the efficiency of a numerical algorithm. Indeed, communication is avoided if more computations can be done with the data that is already in cache. In addition, algorithms require a minimal arithmetic intensity to benefit from vectorization inside a processor. In this presentation we discuss the efficiency of a multigrid method to solve the sparse linear system

$$Ax = b,$$

given by a stencil for matrix A, taking into account the arithmetic intensity.

A single Chebyshev smoothing step, $x_{i+1} = x_i + p_m(A)r_i$, relies on m successive matrix vector multiplications $w = Av$. The arithmetic intensity of the smoother can therefore be raised with a stencil compiler that rearranges the nested loops over the vector elements for optimized temporal data-locality and vectorization. As a consequence, the average time of one multigrid cycle drops with an increasing degree m of the Chebyshev polynomial. And thus, although the effect on the error reduction per multigrid cycle might be minor, the time to solution on multi- or many-core hardware can reduce if m increases.

Chebyshev polynomials are also used to improve the convergence rate in preconditioned Krylov subspace methods. The polynomial q_m of degree $m-1$ is chosen such that the condition number of the preconditioned system,

$$q_{m-1}(A)Ax = q_{m-1}(A)b \Leftrightarrow p_m(A)x = \hat{b}, \tag{4}$$

is optimally reduced. The method then requires less iterations to converge, yet in each iteration the matrix vector multiplication $w = Av$ is now replaced by $w = p_m(A)v$ at a higher computational cost. However, the latter operation can be computed with a higher arithmetic intensity, based on a stencil compiler.

Finally we choose a Krylov subspace method with a suboptimal polynomial p_m that only reduces the high frequency eigenmodes of A. Our multigrid method is then used as a complementary preconditioner for system (1), built upon the same computational kernel $w = p_m(A)v$ with high arithmetic intensity in the smoother.

Local Fourier Analysis of Pattern Structured Operators

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joint work with K. Kahl and M. Bolten

Multigrid methods [5] are used to compute the solution u of the system of equations

$$Lu = f\,,$$

where L is typically a discretization of a partial different equations (PDE) and f a corresponding, given right hand side. Local Fourier Analysis (LFA) [2, 5, 6] is well known to provide quantitative estimates for the speed of convergence of multigrid methods, by analyzing the involved operators in the frequency domain.

For the initial formulation of LFA [1] it was crucial to assume that all involved operators have constant coefficients. For many PDE operators the coefficients vary continuously in space. Thus if the grid is fine enough the discrete operator L will only vary slightly between neighboring grid points and hence can be well approximated by an operator with *locally* constant coefficients. Thus constant coefficient are often reasonable assumption.

However, when analyzing more complex problems or even the multigrid method as a whole this assumption is too restrictive. Interpolation and restriction operators typically act differently on variables that have a coarse grid representative and those who do not have one. Another example are patter relaxation schemes like the Red-Black Gauß-Seidel method where red points of the grid are treated differently from the black ones.

It is possible to analyze these cases [3, 4] when allowing for interaction of certain frequencies (see also [5, 6]). Even more, it turns out that when we allow for more frequencies to interact we can analyze operators given by increasingly complex patterns. In our talk we will illustrate a general framework for analyzing pattern structured operators, i.e., operators whose action is invariant under certain shifts of the input function. Furthermore, we discuss different applications.

References

[1] A. Brandt. Multi-level adaptive solutions to boundary-value problems. *Math. Comput.*, 31(138):333–390, 1977.

[2] A. Brandt. Rigorous quantitative analysis of multigrid, I: Constant coefficients two-level cycle with L_2-norm. *SIAM J. Numer. Anal.*, 31(6):1695–1730, 1994.

[3] K. Stüben and U. Trottenberg. Multigrid methods: fundamental algorithms, model problem analysis and applications. In *Multigrid methods (Cologne, 1981)*, volume 960 of *Lecture Notes in Math.*, pages 1–176. Springer, Berlin-New York, 1982.

[4] C.-A. Thole and U. Trottenberg. Basic smoothing procedures for the multigrid treatment of elliptic 3D operators. *Appl. Math. Comput.*, 19(1-4):333–345, 1986.

[5] U. Trottenberg, C. W. Oosterlee, and A. Schüller. *Multigrid.* Academic Press, 2001.

[6] R. Wienands and W. Joppich. *Practical Fourier Analysis For Multigrid Methods.* Chapman Hall/CRC Press, 2005.

A multigrid based iterative solver for the frequency domain elastic wave equation

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joint work with Wim Mulder

A preconditioned Krylov subspace method is presented for the solution of the elastic isotropic wave equation in the frequency domain. We exploit an idea successfully employed for the acoustic wave equation by a number of authors: the preconditioner is based on the damped elastic differential operator and an approximation to its inverse is obtained by a multigrid cycle.

Local mode analysis highlights that the various multigrid components must be adapted to the elastic case. Different P- and S-wave propagation velocities produce grid anisotropy that should be accounted for by effective smoothing. Clearly, the direction of strong coupling varies with respect to the different components of the wave-field. Numerical results confirm the prediction of the smoothing analysis.

Finite element multigrid framework for mimetic finite difference discretizations

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joint work with Francisco José Gaspar, Xiaozhe Hu and Ludmil Zikatanov

We are interested in the efficient multigrid solution of the algebraic systems of equations resulting from the mimetic finite difference (MFD) schemes for elliptic partial differential equations. Such discretizations work on general unstructured and irregular grids not necessarily aligned with coordinate axes. Moreover, the mimetic finite differences result in discrete grid operators which satisfy the compatibility conditions (exact sequence properties) connecting grad, div and curl operators on the continuous level.
We show how such MFD schemes can be derived using standard finite element spaces in H(curl). In this way, using the finite element framework, we are able to analyze the convergence of the MFD discretizations and design multigrid methods for the solution of the resulting linear systems. We propose, and, via the local Fourier analysis (LFA) framework we also analyze geometric multigrid algorithms for such problems. Finally, we present several numerical tests which demonstrate the efficiency of the proposed multigrid methods and the sharpness of the LFA estimates of the convergence rate.

Parallel Filtering Algebraic Multigrid for Linear Elasticity Problems

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joint work with Arne Nägel, Gabriel Wittum

We present improvements of the Filtering Algebraic Multigrid (FAMG) method applied to Linear Elasticity problems. The FAMG method ([1, 2]) is an AMG method based on minimization of the two-grid correction operator

$$\|(I - PA_H^{-1}P^TA)S\| \leq C \underbrace{\|D^{1/2}(I - PR^{\text{inj}})SD^{-1/2}\|}_{\text{minimize}} \underbrace{\max_{e\neq 0} \frac{\|D^{1/2}A^{-1/2}e\|}{\|e\|}}_{\text{filter}}$$

The construction of the interpolation P is done by performing a minimization over

$$\min_P \|D^{1/2}(I - PR^{\text{inj}})SD^{-1/2}\|_F,$$

incorporating the smoother S, while requiring a filtering condition for all testvectors t_k with $\|Dt_k\| \gg \|At_k\|$ (algebraic smooth vectors):

$$(1 - PR^{\text{inj}})t_k = 0$$

The choice of the testvectors t_k is crucial. For simple diffusion problems, the testvectors only consist of the constant vector, while for linear elasticity, the rigid body modes need to be used. We present parallel results on choosing the appropriate testvector set and coarsening schemes, and a new way of generating local testvectors which combines techniques from [3] and [4].

References

[1] Wagner C.: *On the algebraic construction of multilevel transfer operators.* Computing, Vol. 65, No. 1, pp. 73–95, 2000.

[2] Nägel A., Falgout R.D., Wittum G.: *Filtering algebraic multigrid and adaptive strategies.* Computing and Visualization in Science, Vol. 11, No. 3, pp. 159–167, 2008.

[3] Brandt, A., Brannick, J., Kahl, K., Livshits, I: *Bootstrap AMG.* SIAM J. Sci. Comput., Vol. 33 Issue 2, April 2011, pp. 612–632, 2008..

[4] Henson, Van E. and Vassilevski, Panayot S.: Element-Free AMGe: General Algorithms for Computing Interpolation Weights in AMG. SIAM J. Sci. Comput., Vol. 23 (February 2001), pp. 629-650.

Multigrid algorithms for high-order Discontinuous Galerkin discretizations

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joint work with Paola F. Antonietti, Marco Verani

We present W-cycle multigrid algorithms for the solution of the linear system of equations arising from a wide class of *hp*-version discontinuous Galerkin discretizations of elliptic problems. Starting from a classical framework in multigrid analysis, we define a smoothing and an approximation property, which are used to prove the uniform convergence of the W-cycle scheme with respect to the granularity of the grid and the number of levels. The dependence of the convergence rate on the polynomial approximation degree p is also tracked, showing that the contraction factor of the scheme deteriorates with increasing p. A discussion on the effects of employing inherited or non-inherited sublevel solvers is also presented. Numerical experiments confirm the theoretical results.

A Non-Linear OC Multigrid Topology Optimization Scheme

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joint work with Mohammad Tanvir Rahman, Alfio Borzi

Multigrid techniques for topology optimization are often limited to the process of solving the linear elasticity state equation. Within the context of optimization, rather than simulation, multigrid methods are usually also used in a linear fashion when solving the KKT-system arising from the necessary optimality conditions.

A very popular method to solve topology optimization problems is the non-linear optimality criteria method (OC), which is not directly based on the KKT-system and therefore usually not in the scope of classical multigrid methods in the context.

We present a novel approach to multigrid techniques within topology optimization which are based on the non-linear OC-scheme and can therefore be used nicely to accelerate a given topology optimization solver without the need to change the whole optimization scheme to a classical KKT-based method.

Coarse-grid-correction preconditioner for the Helmholtz Equation

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joint work with Domenico Lahaye, Kees Vuik

Many wave phenomena are well described by the wave equation. When the considered wave has a fixed frequency the wave equation is mostly re-written in the frequency domain which results in the Helmholtz equation

$$-\Delta u(\mathbf{x}) - k^2(\mathbf{x}) = g(\mathbf{x}). \tag{5}$$

It is also possible to approximate the time domain solution with a summation of solutions for several frequencies. Applications consist of the propagation of sound, sonar, seismic, and many more. We emphasize on the seismic imaging used for searching oil and gas in the subsoil. In order to have a good image of the under ground, often high frequencies are chosen for high resolution. The discrete analogue of the Helmholtz Equation (1) is a combination of a symmetric positive definite matrix (Poisson) and the mass matrix i.e.

$$L + iC - M = g \tag{6}$$

where C represents the boundary conditions.
The discretized linear System (2) has two characteristic properties :

- the product of the wave number and the step size should be smaller than a given constant,
- if the wavenumber increases the operator has more and more negative eigenvalues.

Solving the discretized Helmholtz equation have been a challenging problem. Krylov methods with classical preconditioners and Multigrid methods tend to break down due to high indefiniteness for high wavenumber problems. During the year 2005, the idea of using complex shifted Laplacian as preconditioner (CSLP) [1] gave rise to fast and robust Krylov solvers for Helmholtz. It appears that the amount of work increases linearly with the wavenumber. This happens as the near kernel components tend to appear more frequently as the wavenumber increases.

The combination of the complex shifted Laplacian with a multigrid deflation technique was first proposed in [2] and later analyzed in [3]. In these works the shifted Laplacian is attributed the role of

Frequency	Solve Time	Solve Time	Iterations	Iterations
	SLP-F	**ADEF1-F**	**SLP-F**	**ADEF1-F**
$f = 1$	1.23	5.08	13	7
$f = 10$	40.01	21.83	106	8
$f = 20$	280.08	131.30	177	12
$f = 40$	20232.6	3997.7	340	21

Table 1: SLP and ADEF1 performance comparison for Marmousi problem.

a multigrid smoother. Where as the coarse grid correction (CGC) is performed as Preconditioner to the outer Krylov iterations. We investigate several CGC techniques that differ in the choice of the coarse grid operator. A rigorous Fourier mode analysis for the one-dimensional problem with Dirichlet boundary conditions is performed to distinguish these different techniques based on different coarse grid operator. This creates opportunity to optimize the coarse grid correction preconditioner. The CGC technique combined with CSLP has been implemented in multilevel fashion, similar to that of multigrid in Petsc. We refer this combination of CSLP and CGC techniques as ADEF1 preconditioner. Numerical results for two-dimensional and three-dimensional problems show significant speed up in comparison with CSLP and other preconditioners. The iteration count remains constant for medium wavenumbers and increases mildly for high wavenumber at the application cost of CGC. However one can notice that the proposed deflation preconditioner pays off and which is illustrated by a gain in solve time for industrial problems. Such evidence is presented in Table (1), where a brief comparison of iteration and solve time is presented in Table for CSLP and ADEF1 preconditioners.

References

[1] Y.A. Erlangga and C.W. Oosterlee and C. Vuik A Novel Multigrid Based Preconditioner For Heterogeneous Helmholtz Problems SIAM J. Sci. Comput.,27, pp. 1471-1492, 2006

[2] Y. A. Erlangga and R. Nabben, On a Multilevel Krylov Method for the Helmholtz Equation Preconditioned by Shifted Laplacian, ETNA, pp. 403-424, 31, 2008.

[3] A.H. Sheikh and D. Lahaye and C. Vuik On the convergence of shifted Laplace preconditioner combined with multilevel deflation Numerical Linear Algebra with Applications, 20, pp. 645-662, 2013 `http://ta.twi.tudelft.nl/nw/users/vuik/papers/She13LV.pdf`

Time-parallelism using inexact PFASST

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joint work with M. Bolten, M. Emmett, M. Minion, and D. Ruprecht

The "parallel full approximation scheme in space and time" (PFASST) introduced by Emmett and Minion in 2012 is an iterative, multilevel strategy for the temporal parallelization of ODEs and discretized PDEs. As the name suggests, PFASST is similar in spirit to a space-time FAS multigrid method performed over multiple timesteps in parallel. In benchmarks runs on 448K cores, the space-time parallel combination of PFASST with a parallel multigrid solver (PMG) already showed significantly better strong scaling than the space-parallel code alone.

The key for optimal parallel efficiency in PFASST is a suitable choice of coarsening strategies in space and time. Besides straightforward approaches like reducing the number of degrees-of-freedom and/or integration nodes, recent works focussed on the reduction of the spatial discretization order as well as inexact solves of systems arising in implicit steps on the coarse levels. This last concept can be extended to form an "inexact" PFASST algorithm (IPFASST), in which also on the finer levels only a limited number

of multigrid cycles is performed. The iterative nature of IPFASST provides continuously improving initial guesses in each iteration, so that full solves can be replaced by inexact approximations of the solutions of the implicit systems on all levels, leading to significantly improved runtimes.

In this talk we present optimality and scalability results for a 3D heat equation benchmark. Along the building blocks of IPFASST, i.e. inexact single- and multi-level spectral deferred corrections, we demonstrate the impact of inexact solves and different coarsening strategies. In addition, we describe the extension of the code for the 3D viscous Burgers equation and show first results.

Symbol-based multigrid methods for isogeometric analysis

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joint work with M. Donatelli, C. Garoni, C. Manni and S. Serra-Capizzano

We consider the stiffness matrices coming from the Galerkin B-spline Isogeometric Analysis approximation of classical elliptic problems. By exploiting specific spectral properties compactly described by a symbol, we design efficient multigrid methods for the fast solution of the related linear systems. Despite the theoretical optimality, the convergence rate of the two-grid methods with classical stationary smoothers worsens exponentially when the spline degree increases. With the aid of the symbol we provide a theoretical interpretation of this exponential worsening. Moreover, by a proper factorization of the symbol we provide a preconditioned conjugate gradient "smoother", in the spirit of the multi-iterative strategy, that allows us to obtain a good convergence rate independent both of the matrix size and of the spline degree. A numerical experimentation confirms the effectiveness of our proposal and the numerical optimality with a uniformly high convergence rate, also for the V-cycle multigrid method and large spline degrees.

Subdivision surfaces refinement for generating multigrid hierarchies with application in neuroscientific numerical simulations

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joint work with Gillian Queisser

An important goal in neuroscience is understanding how networks of neurons are processing information. Chemical synapses define interfaces where signals are exchanged between neurons and other (neural) cells and thus play an essential role in this context. To pursue this goal we are developing detailed mathematical models of synaptic processes. Amongst others the models comprise the description of three-dimensional reaction-diffusion dynamics with non-linear (inner) boundary conditions. This leads to systems of coupled partial differential equations, which have to be discretized in space and time. Multigrid methods are a highly efficient way of finally solving the resulting and in practice vast systems of linear equations.

However, realistic neurobiological applications of numerical simulation occur on arbitrarily complex domains including neuron networks, single neurons, cell structures like axons, dendrites, dendritic spines or cell organelles facing the challenge of unstructured computational grids with severe anisotropies, invaginations, nestings and branches. To meet this challenge accurate and robust refinement techniques are essential.

We present a modified multigrid method with a new refinement strategy based on grid hierarchies which are generated by using Loop's smooth subdivision surface refinement [1] of the boundary and ordninary linear refinement of the inner grid in combination with a Laplacian smoothing [2]. Starting with

a triangulated surface geometry, which approximates the boundary of the corresponding neurobiological domain, Loop's refinement scheme defines a smooth subdivision surface as limit of successive refinements and vertex repositionings by distinct position masks. The vertices of the initial surface geometry are first projected onto their position on the subdivision surface and then a constrained Delaunay tetrahedrization [3] is generated as coarse grid. The multigrid hierarchy is now created by linear refinement operations projecting the boundary vertices of each refinement level onto their final position on the subdivision surface resulting in a particularly smooth approximation of the computational domain. To prevent degenerate volume elements to emerge especially in the vincinity of the boundary an optimization-based Laplacian smoothing is used to reposition inner vertices of each refinement level.

References

[1] C. Loop. *Smooth Subdivision Surfaces Based on Triangles.* Master's thesis, University of Utah, Department of Mathematics, 1987.

[2] L. R. Hermann. *Laplacian-Isoparametric Grid Generation Scheme.* Journal of the Engineering Mechanics Division 102 (5): 749-756, 1976.

[3] J. R. Shewchuk. *Constrained Delaunay Tetrahedralizations and Provably Good Boundary Recovery.* Eleventh International Meshing Roundtable (Ithaca, New York), Sandia National Laboratories, September 2002, 193-204.

Adaptive fracture approximation

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joint work with D. Logashenko, A. Grillo, G. Wittum

Numerical simulations of flow in fractured porous media follow two main approaches. The fractures are either represented by low-dimensional manifolds motivated by the anisotropic geometry or as three-dimensional objects resolving all physical phenomena taking place in the fractures. Results of the two approaches are compared for some benchmark problems and it can be observed that only for sufficiently small fracture widths the cheaper low-dimensional approach gives acceptable results. In this work a criterion based on fracture characteristics and flow parameters is introduced to indicate the validity of the low-dimensional approach. A dimension-adaptive method is presented that can represent the fractures either full- or low-dimensional depending on the value of this criterion. Using this approach the full resolution with corresponding cost is only used if necessary.

A hybrid multigrid-domain decomposition method for the Helmholtz equation

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Fast Helmholtz solvers are of interest in forward and inverse modelling problems, like for example those from exploration seismology. In such computations often the same equation is solved for many right hand sides. Recently the author and others have developed double sweep domain decomposition methods that lead to a (near-) linear cost per solve. So far those methods appear quite memory intensive. In this talk we will address this using a second recent innovation, the dispersion optimised multigrid method. In

this method the number of grid points in the coarse grid is reduced to a number close to the Nyquist limit for the oscillatory solutions, while retaining small iteration numbers for convergence to the solution. The combined method, the double-sweep multigrid method, leads to a substantial reduction of the memory use and the computational cost compared to the individual methods.

Theoretical Advances in non-Galerkin Algebraic Multigrid

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joint work with Jacob B. Schroder, Rob Falgout and Irad Yavneh

Algebraic multigrid (AMG) is a popular and effective solver for systems of linear equations that arise from discretized partial differential equations. While AMG has been effectively implemented on large scale parallel machines, challenges remain, especially when moving to exascale. In particular, stencil sizes (the number of nonzeros in a row) tend to increase further down in the coarse grid hierarchy and this growth leads to more communication. Thus, as problem size increases and the number of levels in the hierarchy grows, the overall efficiency of the parallel AMG method decreases, sometimes dramatically. This growth in stencil size is due to the standard Galerkin coarse grid operator, P^TAP, where P is the prolongation (i.e., interpolation) operator. For example, the coarse grid stencil size for a simple 3D 7-point finite differences approximation to diffusion can increase into the thousands on present day machines, causing an associated increase in communication costs. Previous work by the authors has successfully truncated coarse grid stencils in an algebraic fashion. First, the sparsity pattern of the non-Galerkin coarse grid is determined by employing a heuristic minimal "safe" pattern together with strength-of-connection ideas. Second, the nonzero entries are determined by collapsing the stencils in the Galerkin operator. The purpose of this talk is to provide some theoretical foundation for the method. In particular if the original two-grid Galerkin method is optimal, then the two-grid non-Galerkin method is shown to also be optimal. The impact of the theory on the algorithm, together with supporting serial and parallel results will also be given.

Multigrid for parametric PDEs with application to fuzzy partial differential equations

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Uncertain parameters in mathematical models are often described by means of random variables. This approach is very effective if the stochastic characteristics of the uncertain parameters are accurately known. When that is not the case, however, an uncertainty representation using alternative models, such as intervals or fuzzy numbers, may be more appropriate. In this talk we consider partial differential equations with interval and fuzzy parameters.

First, we will recall the concept of fuzzy numbers and fuzzy arithmetics, and provide a mathematical definition of a fuzzy differential equation and its solution. Next, we will elaborate on one particularly efficient solution approach, based on a polynomial response surface technique. This method leads to a large and coupled algebraic system of equations thatcan be solved efficiently by means of a multigrid method. Finally, we will demonstrate the approach by means of two numerical examples: a diffusion problem and an elasticity problem.

A Parallel Geometric Multigrid Solver for Density Driven Flow

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Multigrid methods for the solution of large sparse matrices arising from grid-based discretizations of partial differential equations are well known for their optimal complexity, i.e., the computation effort only increases linearly with the problem size. This makes them a promising algorithm when focusing on the weak scaling properties of such a matrix solver. However, while reducing the problem size within a multigrid algorithm on coarser grid levels is its strength, this gives rise to a potential performance bottleneck when parallelization is taken into account. Indeed, on coarser grid levels the inner to boundary ratio of the grid parts assigned to a process become unpleasant and a parallel smoother on those coarse levels will suffer from the fact that mostly communication at the boundary takes place and only little computation on the inner part is performed. In order to overcome this bottleneck we present an algorithm that avoids this situation by gathering coarser levels to fewer processors leaving the remaining processors idle. To this end we introduce vertical interface connections that allow this gathering process and adapt the transfer operators of the multigrid algorithm to respect these interfaces. Arriving at a single process on the coarsest level a serial base solver, e.g., LU factorization, can be used. We show that this approach leads to nice weak scaling behavior for an exemplary application: Discretizing a pde system for density driven flow using a vertex-centered finite volume scheme and implicit Euler time stepping we analyze the efficiency of the geometric multigrid solver in the first Newton linearization of the first time step. It turns out that up to 130,000 processors the weak scaling efficiency is still above 80%.

Multigrid Method for Solving Elliptic Monge-Ampere Equation Arising from Image Registration

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The Monge-Ampère equation is a nonlinear second order partial differential equation, which arises in differential geometry and other applications. In image registration, the problem is to transform one image to align with another image. One approach is based on the Monge-Kantorovich mass transfer problem. The goal is to find the optimal mapping M which minimizes the Kantorovich-Wasserstein distance. The optimal mapping can be written as $M = \nabla\psi$, where ψ satisfies the following Monge-Ampère equation

$$det(D^2\psi(x)) = \frac{I_1(x)}{I_2(\nabla\psi)},$$

where I_1 and I_2 are the given images. Here $det(D^2\psi(x))$ denotes the determinant of the Hessian of ψ. In this talk, we will present a multigrid method for solving the Monge-Ampère equation. Our approach is to reformulate the Monge-Ampère equation as a Hamilton-Jacobi-Bellman (HJB) equation. We will develop a monotone discretization scheme such that it will converge to a viscosity solution. We will then present a relaxation scheme which is a very slowly convergent method as a standalone solver but it is very effective for reducing high frequency errors. We will adopt it as a smoother for multigrid and demonstrate its smoothing properties. Finally, numerical results will be presented to illustrate the effectiveness of the method.

HYMLS: A Multilevel ILU approach for coupled fluid and transport equations

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Many flow problems deal with transport of matter and/or heat. This constitutes a challenging multiphysics problem if the transported entity also influences the flow. From a computing efficiency view point, it is best to treat the associated equations in a coupled manner [5]. If one employs a domain decomposition approach, all the unknowns related to one domain should be in the memory of the node which treats that part. Moreover, communication should be avoided as much as possible during the construction of the right-hand side, the construction of the Jacobian matrix and the solution process. Along this line we developed a finite volume package FVM and a solver HYMLS, both based on elements of the EPETRA-package (available within Trilinos (see http://trilinos.sandia.gov/)).

HYMLS is a linear system solver for steady state incompressible Navier-Stokes equations coupled to transport equations in 2 and 3D [1,2,3]. Recently, we constructed a multilevel variant of it, which makes it possible to solve 3D problems of over 10 million unknowns quickly on a parallel computer. The behavior of the method is very much like that of multigrid methods. The solver is very robust. For the problem described in [4], it allowed a quick increase in the Reynolds number to get into the interesting region around Re=2000. Here we will show the performance of the method on the Rayleigh-Bénard convection in a cube, with six no-slip walls [6].

To study the stability of the solutions we determine the eigenvalues using the ANASAZI-package, which contains a generalized version of the Arnoldi method. Also here we employ HYMLS to solve the linear systems that result from a Cayley transform of the generalized eigenvalue problem. In the talk we will give a more detailed explanation of the used algorithms and their performance.

References

[1] A.C. de Niet and F.W. Wubs. Numerically stable LDL^T factorization of F-type saddle point matrices. *IMA Journal of Numerical Analysis*, **29**(1), 208-234, 2009.

[2] F.W. Wubs and J. Thies, A robust two-level incomplete factorization for (Navier-) Stokes saddle point matrices, *SIAM J. Matrix Anal. Appl.*, **32**, 1475 - 1499, 2011.

[3] Jonas Thies and Fred Wubs, Design of a Parallel Hybrid Direct/Iterative Solver for CFD Problems. *Proceedings 2011 Seventh IEEE International Conference on eScience*, 5-8 December 2011, Stockholm, Sweden, pp 387 -394, 2011.

[4] Yuri Feldman and Alexander Yu. Gelfgat, Oscillatory instability of a three-dimensional lid-driven flow in a cube, *Phys. Fluids*, **22**, 2010.

[5] David E. Keyes et al., Multiphysics simulations: Challenges and opportunities, *International Journal of High Performance Computing Applications*, **27**(1), 4-83, 2013.

[6] Alexander Yu. Gelfgat, Different Modes of Rayleigh-Benard Instability in Two- and Three-Dimensional Rectangular Enclosures, *J. Comput. Phys.*, **156**, 300-324, 1999.

A Multilevel Approach for l-1 Regularized Convex Optimization with Application to Covariance Selection

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joint work with Eran Treister, Aviva Herman

We present an iterative multilevel framework for solving l-1 regularized convex optimization problems, which are common in the fields of computational biology, signal processing and machine learning. Such l-1 regularization is utilized to find sparse minimizers of convex functions, and is mostly known for its use in the LASSO problem, where the l-1 norm is applied to regularize a quadratic function. Taking advantage of the (typical) sparseness of the solution, we create a multilevel hierarchy of similar problems, which are traversed back and forth in order to accelerate the optimization process. This framework is applied for solving the Covariance Selection Problem, where the inverse of an unknown covariance matrix of a multivariate normal distribution is estimated, assuming that it is sparse. To this end, an l-1 regularized log-determinant optimization problem needs to be solved. This task is challenging for large-scale data sets because of time and memory limitations. Our numerical experiments demonstrate the efficiency of the multilevel framework for solving both medium and large scale instances of this problem.

A multigrid preconditioner for the Hellan-Herrmann-Johnson mixed method for biharmonic problems

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joint work with Wolfgang Krendl

In this talk we consider the biharmonic Dirichlet problem

$$\Delta^2 y = f \quad \text{in } \Omega, \qquad u = \frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega$$

on a polygonal two-dimensional domain Ω with boundary $\partial\Omega$. The Hellan-Herrmann-Johnson mixed method uses the Hessian $\mathbf{u} = \Delta^2 y$ as auxiliary variable. The well-posedness of the associated continuous mixed variational problem for $(\mathbf{u}, y)$ is shown in a nonstandard Sobolev space. Motivated by this analysis of the continuous problem a similar result is derived for the discretized problem. The resulting preconditioner is of optimal efficiency and is solely based on standard multigrid methods for second-order elliptic problems.

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