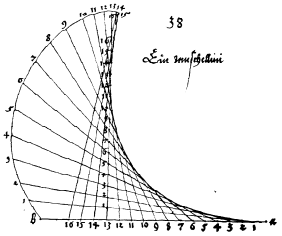
Abstracts of the

International Conference on

Multigrid and Multiscale Methods in Computational Sciences

Bruchsal Palace
Germany
December 6 - 9, 2016



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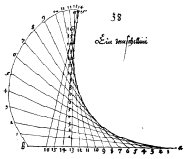
International Conference on

Multigrid and Multiscale Methods in Computational Sciences

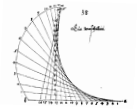
December 6 - 9, 2016

Organization

Alfio Grillo (Torino)
Rolf Krause (Lugano)
Babett Lemke (Frankfurt)
Zeyao Mo (Beijing)
Arne Nägel (Frankfurt)
Gillian Queisser (Philadelphia)
Volker Schulz (Trier)
Christian Wieners (Karlsruhe)
Gabriel Wittum (Frankfurt)
Jinchao Xu (University Park)



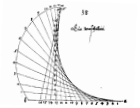
The conference provides a forum for researchers to present and discuss recent research in multigrid, multilevel and multiscale methods. Previous conferences known as European Multigrid Conference (EMG) were held in Cologne (1981, 1985), Bonn (1990), Amsterdam (1993), Stuttgart (1996), Gent (1999), Hohenwart (2002), Scheveningen (2005), Bad Herrenalb (2008), Ischia (2010), Schwetzingen (2012) and Leuven (2014).



International Conference on Multigrid and Multiscale Methods in Computational Sciences 2016

Tuesday, December 6, 2016

	Kammermusiksaal: Keynote Lectures		
9:00	R. Bank: Two Level Solver for hp Adaptive Subspaces		
9:45	M. Wheeler: Solvers for Conservative Flow and Transport Algorithms in Porous Media		
10:30	*Coffee Break*		
	Kammermusiksaal	**Styrumsaal**	**Huttensaal**
	MS1: Space-Time PDE Solvers (Part I) (U. Langer, C. Wieners)	MS2: Multilevel Algorithms and Theories (J. Xu)	MS3: PDE Constrained and Shape Optimization (V. Schulz, M. Siebenborn)
11:00	A. Reusken: Space-Time Trace FEM for PDEs on Evolving Surfaces		D. Gathungu: Multigrid Solution of an Elliptic Fredholm Partial Integro-Differential Equation with a Hilbert-Schmidt Integral Operator
11:25	S. Sauter: Adaptive Time Discretization for Retarded Potentials	U. Meier Yang: The Impact of Emerging Architectures on the Design of Algebraic Multigrid Methods	S. Schmidt: Generating Shape Derivatives and Repeated Differentiation Hessians Automatically
11:50	J. Ernesti: Weakly Conforming Least-Squares for First-Order Systems in Space-Time	R. Hiptmair: Multilevel Decomposition of Boundary Element Spaces and Applications	M. Siebenborn: High Performance Optimization Algorithms for Interface Identification Problems
12:15	M. Neumüller: Space-Time Multigrid Methods for Parabolic Problems	P. d'Ambra: Algebraic Multigrid Based on Maximum Weighted Matching in Matrix Graphs Exploiting an Auction Algorithm	V. Schulz: Efficient PDE Constrained Shape Optimization Based on Steklov-Poincare Type Metrics
12:40	*Lunch*		
	Kammermusiksaal: Keynote Lectures		
14:30	R. Kornhuber: Numerical Homogenisation and Multigrid		
15:15	R. Krause: Non-linear Multigrid and Domain Decomposition - A Survey		
16:00	*Coffee Break*		
	Kammermusiksaal	**Styrumsaal**	**Huttensaal**
	MS4: Applications of HPC in Fluid Dynamics (M. Resch)	MS5: Numerical Simulation Frameworks (Part I) (A. Nägel)	CP1: AMG
16:30	M. Resch: HPC as a Tool in Flow Simulation	D. Logashenko: Simulation of Free Surfaces in the Density-Driven Groundwater Flow	H. Zhang: A Unified Approach to the Construction of Coarse Spaces and Convergence Analysis in AMG
16:55	R. Schneider: Flow Simulations in Blood	S. Reiter: Mesh Generation for Thin Layered Domains and its Applicatios to Parallel Multigrid Simulation of Grourndwater Flow	K. Kahl: Optimal Interpolation in Algebraic Multigrid Methods
17:20	A. Ruopp: Flow Simulation in Water Power Plants	A. Vogel: Multigrid for an Adaptive Finite Volume Method Using Hanging Nodes	B. Metsch: Algebraic Multigrid for the Finite Pointset Method
17:45	J. Zhang: Flow Simulation in Nuclear Safety Applications	A. Nägel: Linear Implicit Extrapolation Methods for Density Driven Flow	A. Napov: An Efficient Algebraic Multigrid Method for Graph Laplacian Systems
18:10	*End*		



International Conference on Multigrid and Multiscale Methods in Computational Sciences 2016

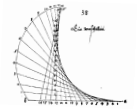
Wednesday, December 7, 2016

Kammermusiksaal: Keynote Lectures

9:00	P. Deuflhard: The Grand Four
9:45	J. Xu: A Unified Approach to the Construction of Coarse Spaces and Convergence Analysis in AMG
10:30	*Coffee Break*

	Kammermusiksaal MS6: Space-Time PDE Solvers (Part II) (U. Langer, C. Wieners)	Styrumsaal MS7: Computational Biosciences (Part I) (R. Krause, G. Queisser)	Huttensaal CP2: Special MG
11:00	R. Bank: Treating Time as Just Another Space Variable	M. Favino: VMS Methods for Reaction-Diffusion Problems: An Interesting Case with Multiple Residual Bubbles	S. Takacs: A Robust Multigrid Method for Isogeometric Analysis
11:25	M. Zank: A Space-Time Boundary Element Method for the Wave Equation	E. Babushkina: Adaptive Multilevel Monte Carlo Methods for Elliptic Problems with Uncertain Coefficients	T. Ludescher: A Multigrid Method for Unfitted Finite Element Methods
11:50	S. Findeisen: A Parallel and Adaptive Space-Time Method for Maxwell's Equations	M. Bolten: Usage of Block-Smoothers and Aggressive Coarsening to Improve Scalability of Multigrid	W. Zulehner: On the Analysis of Block Smoothers for Saddle Point Problems
12:15	U. Köcher: Space-Time Discretisation and Solver Technology for Biot's Model of Poroelasticity	R. Scott: Optimal Algortihms Using Optimal Meshes	M. Islahuddin: Algebraic Multigrid for a Pore Network Model of Moisture Transfer
12:40	*Lunch*		

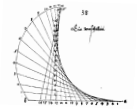
Social Event



International Conference on Multigrid and Multiscale Methods in Computational Sciences 2016

Thursday, December 8, 2016

	Kammermusiksaal: Keynote Lectures		
9:00	U. Langer: Fast Solvers for Large-Scale Systems of Galerkin IgA Equations		
9:45	Z. Mo: Automatically Parallelization and Highly Scalable Programming Frameworks for Numerical Simulation		
10:30	*Coffee Break*		
	Kammermusiksaal	Styrumsaal	Huttensaal
	MS8: Computational Biosciences (Part II) (R. Krause, G. Queisser)	MS9: Numerical Simulation Frameworks (SCHPC) (Part II) (Z. Mo)	MS10: Computational Models and Methods in Interdisciplinary Problems: Biomechanics, Electromagnetism, and Hydrogeology (Part I) (A. Grillo)
11:00	M. Stepniewski: Smooth Subdivision Geometric Multigrid Method with Application in (Neuro-)Biological Numerical Simulations	J. Cheng: JAUMIN: A Programming Framework for Unstructured Mesh Applications	S. Berrone: New Numerical Approaches for Large Scale Discrete Fracture Network Flow Simulations
11:25	M. Breit: Electro-Diffusion on Neuronal Micro-Domains - Dos and Don'ts	X. Xu: aSetup-AMG: An Adaptive Setup Based AMG Preconditioner for Solving Large-Scale Sparse Linear Systems in Multi-Physics Simulations	M. Carfagna: A Cahn-Hilliard Approach to Thermodiffusion in Porous Media
11:50	U. v. Rienen: Modeling and Simulation of Nerve-Electrode Interactions in Neuronal Implants	T. Cui: PHG: A Framework for Parallel Adaptive Finite Element Method	M. Icardi: Micro-Scale Simulation of Flow, Transport and Reaction in Porous Media
12:15	J. Hahne: Spiking Neurol Network Simulation Including Gap Junctions	G. Tan: Building an Autotuning and Composable AMG Solver for Exascale Computing	R. Penta: Can a Continuous Mineral Foam Explain the Stiffening of Aged Bone Tissue? A Micromechanical Approach to Mineral Fusion in Musculoskeletal Tissue
12:40	*Lunch*		
	Kammermusiksaal: Keynote Lectures		
14:30	G. Queisser: Optimized Multigrid for Life Science Applications		
15:15	C. Wieners: Parallel Inelastic Heterogeneous Multiscale Simulations		
16:00	*Coffee Break*		
	Kammermusiksaal	Styrumsaal	Huttensaal
	MS11: Computational Models and Methods in Interdisciplinary Problems: Biomechanics, Electromagnetism, and Hydrogeology (Part II) (A. Grillo)	MS12: Numerical Simulation Frameworks (SCHPC) (Part III) (Z. Mo)	CP3: Application
16:30	A. Schneider: Regional-Scale Modeling of Density-Driven Groundwater Flow	R. Xu: Mend-Centered Geometric Multi-Grid Algorithm for Solutions on Linear Problems in Computational Solid Mechanics	N. Kintscher: Geometric Multigrid for the Tight-Binding Hamiltonian of Graphene
16:55	K. Kröhn: 3D Flow and Solute Transport in Fractured Rock	H. An: Anderson Acceleration and Application to Three Temperature Energy Equations	K. Rafetseder: A Decomposition Result for Kirchhoff-Love Plate Bending Problems and Associated Discretization Approaches
17:20	M. Knodel: Application of Multigrid Solvers to Mathematical Models in Medicine and Biophysics at Realistic Geometries	A. Zhang: JASMIN: A High Performance Programming Framework for Numerical Simulation	P. Robbe: A Multi-Index Quasi-Monte Carlo Algorithm for Lognormal Diffusion Porblems
17:45	S. Falletta: A Mortar FEM-BEM Coupling for Wave Propagation Problems in Unbounded Domains		A. v. Barel: Robust Optimization with a Multilevel Monte Carlo Method
19:00	**Multigrid Award 2016 (Kammermusiksaal)**		



International Conference on Multigrid and Multiscale Methods in Computational Sciences 2016

Friday, December 9, 2016

	Kammermusiksaal: Keynote Lectures		
9:00	A. Grillo: A Poroplastic Approach to the Structural Reorganisation of Fibre-Reinforced Porous Media		
9:45	W. Hackbusch: The Hierarchical LU-Iteration - a Robust and Algebraic Method		
10:30	*Coffee Break*		
	Kammermusiksaal MS13: Modeling the Barrier Function of Human Skin (A. Nägel, G. Wittum)	Styrumsaal	Huttensaal
11:00	G. Wittum: Swelling of Corneocytes and Other Perspectives of Skin Modelling		
11:25	M. Heisig: Parameter Sensitivity Analysis of a Two-Dimensional Skin Diffusion Model		
11:50	A. Nägel: Mathematical Models for Skin Penetration		
12:15	R. Wittum: Three-Dimensionally Resolved Microscopic Model of Diffusion in Viable Epidermis		
12:40	*End of the Conference*		

Abstracts

Plenary Lectures

Randolph E. Bank

Two Level Solver for hp Adapive Subspaces

Department of Mathematics
University of California at San Diego, San Diego, USA

Higher order finite elements present certain challenges for multilevel methods. Such matrices have more nonzero elements and special block structure. In the case of hp adaptive methods, the block structure is more complicated. In this talk we present a simple two level solver for such systems, that exploits these special properties. The convergence rate is (empirically) multigrid-like, at least up to piecewise polynomials of degree nine. Numerical illustrations demonstrate its robustness on a wide variety of problems, including convection-diffusion and Helmholtz equations.

Peter Deuflhard

The Grand Four

ZIB, Berlin, Germany

Four affine invariance classes (affine covariance, affine contravariance, affine conjugacy, affine similarity) for stationary nonlinear problems lead to four different classes of adaptive Newton algorithms. Affine covariance applies to boundary value problems for differential equations (both ODEs and PDEs), affine contravariance applies to Fredholm integral equations, affine conjugacy leads to convex optimization, and, last but not least, affine similarity leads to pseudo-continuation methods for steady state problems in time dependent ODEs or PDEs. For the latter invariance class rather recent results are presented.

Alfio Grillo, Melania Carfagna, Salvatore Di Stefano, Markus Knodel

The Darcy-Forchheimer Law for Modelling Density-Driven Flow in Fractured Porous Media

Department of Mathematical Sciences (DISMA) "G. L. Lagrange"
Politecnico di Torino, Turino, Italy

In the course of their life, biological tissues rearrange their internal structure in order to adapt themselves to stimuli of various nature that act at different levels of observation. The structural evolution of a tissue may, or may not, be accompanied by overall changes of its shape as well as by growth and formation of patterns (see [1] for a review on the subject). In this contribution, we focus on the structural evolution alone, and we interpret it as an anelastic (plastic), dissipative process. Following the line of thought outlined in [2], such proccess is kept track of by introducing a kinematic description, which adds itself to the standard one, i.e., deformation, and represents the anelastic distortions driven by the tissue's structural evolution. As in [2] , the non-standard kinematic description is associated with its own balance law.

For our purposes, we summarise the poroplastic model of structural reorganisation presented in [3], which was formulated for isotropic biological tissues, and we generalise it to the transversely isotropic case. The anisotropy of the tissue is due to the presence of collagen fibres, whose directional orientation is assumed to be statistical. The model employed to describe the elastic behaviour of transversely isotropic, fibre-reinforced materials with statistical orientation of the fibres is taken from (see [4] and references therein).

Although rather customary in the theory of inelastic processes of elastoplastic type, we do not enforce here the Bilby-Kröner-Lee decomposition of the deformation gradient tensor $\mathbf{F}$. Rather, we follow the formulation introduce in [5], in which $\mathbf{F}$ is decomposed as $\mathbf{F}_e = \mathbf{F}\mathbf{K}$, with $\mathbf{K}$ being referred to as "transplant operator" [5]. Next, we deduce an evolution law for $\mathbf{K}$, in which an appropriate measure of the rate of inelastic distortions is related to its power-conjugate stress measure through fourth-order tensors depending on the fibre distribution. The model equations are solved numerically for some selected benchmark tests and the related relations are briefly commented. As a sample tissue, we consider articular cartilage, which we model by adopting histological data available in the literature [6].

References

[1] Cowin, S.C. How is a tissue built? J. Biomech. Eng. 122 (2000) 553–569
[2] DiCarlo, A., Quiligotti S. Growth and balance. Research Mechanics Communications 29 (2002) 449–456
[3] Grillo, A., Prohl, R., Wittum, G. A poroplastic model of structural reorganisation in porous media of biomechanical interest. Continuum Mechanics and Thermodynamics 28 (2016) 579–601
[4] Tomic, A., Grillo, A., Federico, S. Poroelastic materials reinforced by statistically oriented fibres—numerical implementation and application to articular cartilage. IMA Journal of Applied Mathematics 79 (2014) 1027–1059
[5] Epstein, M., Maugin, G.A. Thermomechanics of volumetric growth in uniform bodies. Internatio nal Journal of Plasticity 16 (2000) 951–978
[6] Aspden, R.M. Hukins, D.W.L. Collagen organization in articular cartilage, determined by X-ray diffraction, and its relationship to tissue function. Proc. R. Soc. B 212 (1981) 299–304

Wolgang Hackbusch

The Hierarchical LU-Iteration - A Robust and Algebraic Method

Kiel, Germany

First we define formally the property 'algebraic iteration'. A well-known example is the algebraic multigrid method. Next we recall the hierarchical LU decomposition. Under suitable conditions the overall computational cost and storage requirement is almost linear in the size of the (possibly fully populated) matrix. In the case of sparse matrices arising from boundary value problems, there is a variant using graph distances instead of geometric data. The arising variant leads to an algebraic iteration. We explain by this scheme is robust with respect to jumps in the coefficients of the pde.

Ralf Kornhuber

Numerical Homogenisation and Multigrid

Mathematics in Life Sciences
Freie Universität Berlin, Berlin, Germany

Joint work of Ralf Kornhuber, Daniel Peterseim and Harry Yserentant

Numerical homogenization tries to approximate the solutions of elliptic partial differential equations with strongly oscillating coefficients by functions from modified finite element spaces. Based on an iterative counterpart relying on two-level subspace decomosition, we present and analyze a class of new methods that is very closely related to the approach of Malqvist and Peterseim [Math. Comp. 83, 2014]. As in the approach of Malqvist and Peterseim, these new methods do not make explicit or implicit use of a scale separation. Their comparatively simple analysis is based on the theory of additive Schwarz or subspace decomposition methods.

Rolf Krause

Non-linear Multigrid and Domain Decomposition - A Survey

Institute of Computational Science
USI - Università della Svizzera italiana, Lugano, Switzerland

Domain decomposition and multigrid are by now well established methods for the solution of large scale linear systems. Their (quasi-)optimal complexity and their ability to run on massively parallel machines make these methods highly attractive, whenever large linear systems have to be solved. By now, their convergence theory has reached high maturity for the case of linear and symmetric positive definite problems.

In the context of non-linear problems, a straight-forward strategy is to use domain decomposition and multigrid methods as an "inner solver" for the linear problems occuring within a non-linear strategy such as, e.g., Newton's method or Trust-Region. In this, whatever non-linear strategy is used, will benefit from the fast solution of the linear sub-problems.

Ulrich Langer

Fast Solvers for Large-Scale Systems of Galerkin IgA Equations

Institute of Computational Mathematics
Johannes Kepler University, Linz, Austria

We consider multi-patch continuous and discontinuous Galerkin Isogeometric Analysis (IgA) techniques for discretizing elliptic boundary value problems. We admit segmentations crimes, i.e., incorrect domain decompositions containing undesirable gaps and / or overlaps between the subdomains (patches) [2, 3, 4]. Beside the generation of the system matrices, the solution of large-scale systems of IgA equations is the efficiency bottleneck in IgA, especially, in the case of the use of high-order spline or NURBS basis functions. These bottlenecks can be overcome by the use of domain decomposition techniques and their implementation on massively parallel computers.We propose and analyze exact and inexact Dual-Primal IsogEometric Tearing and Interconnecting (IETI-DP) methods for solving large-scale systems of IgA equations, see also [1]. In the single-patch case, p-robust multigrid methods have recently been proposed and analyzed in [6, 5]. These multigrid methods can nicely be used in inexact IETI-DP solvers for multi-patch IgA equations.

Finally, we look at parabolic initial-boundary value problems from an elliptic point of view. More precisely, we propose a stable space-time IgA variational scheme, the mesh-dependent bilinear form of which is uniformly elliptic and bounded on the IgA space with respect to special mesh-dependent norms. In contrast to implicit time-stepping methods, we have to solve only one huge system of linear algebraic equations. This can very efficiently be done by algebraic or special geometric multigrid methods on parallel computers [7].

The author would like to express his thanks to his IgA collaborators C. Hofer, S. Matculevich, S. Moore, M. Neumüller, S. Takacs and I. Toulopoulos as well as the Austrian Science Fund (FWF) for the financial support under the grants S 117-03 and W 1214-04.

References

[1] C. Hofer and U. Langer. Dual-Primal Isogeometric Tearing and Interconnecting solvers for multi-patch dG-IgA equations. Computer Methods in Applied Mechanics and Engineering, 2016, DOI 10.1016/j.cma.2016.03.031, in Press.

[2] C. Hofer, U. Langer and I. Toulopoulos. Discontinuous Galerkin Isogeometric Analysis of Elliptic Diffusion Problems on Segmentations with Gaps. SIAM Journal on Scientific Computing, 2016, accepted for publication.

[3] C. Hofer, U. Langer and I. Toulopoulos. Discontinuous Galerkin Isogeometric Analysis on non-matching segmentation: Error estimates and efficient solvers. RICAM Report 2016-23, Linz,2016,

[4] C. Hofer and I. Toulopoulos. Discontinuous Galerkin Isogeometric Analysis of Elliptic Problems on Segmentations with Non-Matching Interfaces. Computers & Mathematics with Applications, 2016, accepted for publication.

[5] C. Hofreither and S. Takacs. Robust multigrid for isogeometric analysis based on stable splittings of spline spaces. RICAM Report No. 2016-27, Linz, 2016.

[6] C. Hofreither, S. Takacs and W. Zulehner. A robust multigrid method for Isogeometric Analysis in two dimensions using boundary correction. Computer Methods in Applied Mechanics and Engineering, 2016, 10.1016/j.cma.2016.04.003, in Press.

[7] U. Langer, S. Moore and M. Neumueller. Space-time isogeometric analysis of parabolic evolution equations. Computer Methods in Applied Mechanics and Engineering, v. 306, 342-363, 2016.

Zeyao Mo

Automatically Parallelization and Highly Scalable Programming Frameworks for Numerical Simulation

Institute of Applied Physics and Computational Mathematics, Beijing, China

This talk reports on some theory and methods for the design of automatically parallelization and highly scalable programming frameworks for numerical simulation. Based on these frameworks, users only need to write serial codes for the development of parallel software efficiently running on supercomputers. This talk also shows the effectiveness by three frameworks such as JASMIN, JAUMIN and JCOGIN in China.

Gillian Queisser, M. Breit, M. Stepniewski

Molecular Organization of Skin Barrier Formation

Department of Mathematics
Temple University, Philadelphia, USA

In life sciences – and in particular neuroscience – interdisciplinary research has gained much traction over the last decades. Models and computational methods have been developed to describe biophysical processes, such as electrical and biochemical signals, in a variety of cell types and networks thereof. In this talk we will discuss options for advancement of spatial discretization and optimization of geometric multigrid methods for life science inspired problems, such as subdivision volume theory for optimized grid hierarchies, hybrid-dimensional discretization, and integration of reconstructed computational domains into detailed numerical simulations. Applications in computational neuroscience will be presented.

Mary Wheeler

Solvers for Conservative Flow and Transport Algorithms in Porous Media

Institute for Computational Engineering and Sciences
The University of Texas at Austin, Austin, USA

In this presentation we discuss solvers for two algorithms for modeling flow and transport. One algorithm currently represents the state-of-the-art for modeling an equation of state compositional flow for carbon sequestration and enhanced oil recovery techniques such as gas flooding, and other subsurface porous media applications. The multipoint flux mixed finite element (MFMFE) method is utilized for spatial discretization; it can handle complex reservoir geometries using general distorted hexahedral grid elements, as well as satisfy local mass conservation and compute accurate

phase fluxes. A parallel framework for the MFMFE is presented; here much of the non-linearity is due to the local flash and stability calculations associated with interphase mass transfer and phase behavior. Parallel multigrid linear solver libraries such as HYPRE are employed to solve the algebraic problems on each Newton step. We perform a variety of strong and weak parallel scaling studies up to 10 million elements and 1024 processors, and discuss possible load balancing issues.

The second algorithm, the enriched Galerkin (EG) method, was recently introduced for modeling miscible displacement and two phase flow. The EG is formulated by enriching the conforming continuous Galerkin finite element method (CG) with piecewise constant functions. This approach is shown to be locally and globally conservative while keeping fewer degrees of freedom in comparison with discontinuous Galerkin finite element methods (DG). Also, we present a fast and effective EG solver for flow simpler than DG and whose cost is roughly that of CG and can handle an arbitrary order of approximations. Dynamic mesh adaptivity using hanging nodes is applied to save computational cost for large-scale physical problems. Some numerical tests in two and three dimensions are presented to confirm our theoretical results as well as to demonstrate the advantages of EG.

Christian Wieners

Parallel Inelastic Heterogeneous Multiscale Simulations

Karlsruhe Institute of Technology, Karlsruhe, Germany

We recall the heterogeneous multiscale method for elasticity and its extension to inelasticity within a two-scale energetic approach, where the fine-scale material properties are evaluated in representative volume elements. These RVEs are located at Gauß points of a coarse finite element mesh. Within this FE^2 method the displacement is approximated on a coarse scale, and depending on the strain at the Gauß points in every RVE a periodic micro-fluctuation and the internal variables describing the material history in this RVE are computed. Together, this defines the global energy and the dissipation functional, both depending on coarse scale displacements as well as on fluctuations and internal variables on the fine-scale.

Here we introduce a parallel realization of this method which allows the computation of 3D micro structures with fine resolution. It is based on the parallel representation of the RVE with distributed internal variables associated to each Gauß points, and a parallel multigrid solution method in the nonlinear computation of the micro-fluctuations and for the up-scaling of the algorithmic tangent within the incremental loading steps of the macro-problem. The efficiency of the method is demonstrated for a simple damage model describing a PBT matrix material with glass fiber inclusions.

The presentation is joint work with Ramin Shirazi-Nejad in the BMBF project MuSiKo (in cooperation S.~Rjasanow, H. Andrä, R. Müller, and S. Diebels).

Jinchao Xu

A Unified Approach to the Construction of Coarse Spaces and Convergence Analysis in AMG

Center for Computational Mathematics and Applications
The Pennsylvania State University, University Park, USA

In this work, we present a general framework for the design and analysis of Algebraic or Abstract Multi-Grid (AMG) methods. Given a smoother, such as Gauss-Seidel or Jacobi, we provide a general approach to the construction of a quasi-optimal coarse space and we prove that under appropriate assumptions the resulting two-level AMG method for the underlying linear system converges uniformly with respect to the size of the problem, the coefficient variation, and the anisotropy. Our theory applies to most existing multigrid methods, including the standard geometric multigrid method, the classic AMG, energy-minimization AMG, unsmoothed and smoothed aggregation AMG, and spectral AMGe.

Minisymposia

MS 1: Space-Time PDE Solvers (Part I)

Organized by U. Langer and C. Wieners

Johannes Ernesti

Weakly Conforming Least-Squares for First-Order Systems in Space-Time

KIT, Institute of Applied and Numerical Mathematics, Karlsruhe, Germany

We introduce a novel substructuring discretization scheme for first order systems in space-time. It is based on a skeleton reduction procedure related to the recently introduced discontinuous Petrov-Galerkin (DPG) methods. While being applicable to a variety of problems, the substructuring approach is flexible with respect to the selection of trial and test spaces allowing for problem-specific nonconforming choices with desired approximation and conservation properties. The scheme yields a discrete equation that can be solved in two steps, where first a representation of the solution restricted to the skeleton is obtained by solving a symmetric positive definite linear system. In a second step the approximate solution on each cell is reconstructed from the skeleton values.
As a model problem, we consider the linear acoustic wave equation on a bounded interval in one dimension formulated as a first order system. We compare the performance of various discretization schemes, e.g., leap-frog finite differences, space-time LSFEM of different orders, to the new substructuring approach.

Martin Neumüller

Space-Time Multigrid Methods for Parabolic Problems

Johannes Kepler University Linz, Linz, Austria

In this talk we will consider for parabolic problems two different space-time multigrid techniques. We will show their advantages and disadvantages buy looking at the Fourier mode analysis. Moreover we will combine the two approaches to obtain a method which allows an efficient parallel implemention with respect to space and time.

Arnold Reusken

Space-Time Trace FEM for PDEs on Evolving Surfaces

Chair for Numerical Mathematics, RWTH-Aachen, Aachen, Germany

Joint work with J. Grande (Aachen), C. Lehrenfeld (Göttingen), M. Olshanskii (Houston).

We present a particular class of finite element methods for the solution of partial differential equations on (evolving) surfaces. The evolving hypersurface is characterized as the zero level of a level set function. The finite element method is based on a (discontinuous in time) space-time variational formulation of a class of diffusion problems on the space-time manifold. Based on this variational formulation a discontinuous Galerkin (DG) space-time finite element discretization is developed. This FEM employs traces of standard volumetric elements on the space-time manifold. This space-time method is explained and results of numerical experiments are presented that illustrate its properties. Results of a discretization error analysis are briefly addressed. An important diffculty related to this type of trace finite element techniques is the fact that the stiffness matrix can be extremely ill-conditioned depending on how the manifold intersects the underlying fixed outer triangulation. A new stabilization technique which results in a stiffness matrix with much better conditioning properties is treated. For the case of a stationary manifold an analysis of the effect of this stabilization method is presented.

Stefan Sauter

A Generalized Convolution Quadrature with Variable Time Stepping

Universität Zürich, Zürich, Switzerland

Work in collaboration with Maria Lopez-Fernandez and Martin Schanz.

We will present a generalized convolution quadrature for solving linear parabolic and hyperbolic evolution equations. The original convolution quadrature method by Lubich works very nicely for equidistant time steps while the generalization of the method and its analysis to non-uniform time stepping is by no means obvious. We will introduce the generalized convolution quadrature allowing for variable time steps and develop a theory for its error analysis. This method opens the door for further development towards adaptive time stepping for evolution equations. As the main application of our new theory we will consider the wave equation in exterior domains, which is formulated as a retarded boundary integral equation. Numerical results for a real-world application will illustrate the performance of the method.

MS 2: Multilevel Algorithms and Theories
Organized by J. Xu

P. D'Ambra[1], S. Filippone[2], and P. S. Vassilevski[3]

Algebraic Multigrid Based on Maximum Weighted Matching in Matrix Graphs Exploiting an Auction Algorithm

[1]Istituto per le Applicazioni del Calcolo
National Research Council of Italy, Naples, Italy

[2]Centre for Computational Engineering Sciences, School of Aerospace, Transport and Manufacturing
Cranfield University, Cranfield, UK

[3]Center of Applied Scientific Computing
Lawrence Livermore National Laboratory, Livermore, CA, USA

Recently, we proposed the use of maximum weighted matching on the adjacency graph of SPD matrices as a reliable and completely automated way to coarsen sparse matrices in Algebraic Multigrid Methods (AMG) [1, 2].

Our algorithm, named coarsening based on compatible weighted matching, exploits a maximum product matching in the original matrix graph to enhance matrix diagonal dominance, reecting the convergence properties of an appropriately defined compatible relaxation scheme.

The matched nodes are aggregated to form coarse index spaces and standard, piecewise constant or smoothed, interpolation operators are applied for the construction of a multigrid hierarchy, without referring to any a priori knowledge of matrix origin and/or any assumed strength of connection definition. Instead, information about the smooth error is generated and used to define edge weights assigned to the original matrix graph.

A key issue in this approach is to find an efficient yet accurate enough computation of a maximum product matching; this accounts for the largest part of the computational time needed to build the AMG solver. The most widely used algorithm for maximum weighted matching [3] generally exhibits a superlinear computational complexity; for our purposes, we needed a linear cost algorithm, thus we resorted to an approximate algorithm producing matchings whose weight is at least $1=2$ of the optimum [4].

In this work, we propose the use of an auction algorithm for solving the maximum product cardinality matching problem; we analyze performance results on linear systems stemming from PDE applications, both in terms of effectiveness of the coarsening scheme as well as of the overall execution time.

The auction algorithm, as implemented in the HSL-Spral package [5], has been demonstrated to compute high-quality matchings for scaling sparse matrices in Sparse Direct Linear Algebra Compu-

tations and it is also readily parallelizable. We show here that it can also improve the quality of the coarsening with respect to the previously studied half-approximate algorithm, giving results which are comparable to the ones obtained by using exact maximum product matching at a reasonable computational cost.

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R. Hiptmair

Multilevel Decompositions of Boundary Element Spaces and Applications

Seminar for Applied Mathematics
ETH Zürich, Zürich, Switzerland

On the triangulated surface of a Lipschitz polyhedron Ω we consider finite element subspaces of trace spaces, so-called boundary element spaces, of the energy spaces $H^1(\Omega)$, $\boldsymbol{H}(\mathrm{curl};\,)$, and $\boldsymbol{H}(\mathrm{div};\Omega)$ associated with secondorder boundary value problems. Taking for granted hierarchies of nested meshes, we investigate the stability of multilevel decompositions of boundary element space in natural trace norms. A key tool is a general theory due to P. Oswald that teaches, when such stability results can be inferred from corresponding stability results for related finite element spaces on Ω. Thus we obtain new insights, for instance, into multilevel splittings of surface edge elements.

Stability of multilevel decompositions has important consequences, of which we mention

- the asymptotic optimality of multilevel diagonal scaling (BPX-type) preconditioners for linear systems of equations arising from boundary element Galerkin discretisation of first-kind boundary integral equations [2]
- and the derivation of inverse estimates for the extension by zero in trace spaces [1].
  (joint work with S.-P. Mao, LSEC Beijing, PR China, and C. Jerez-Hanckes, PUC, Santiago, Chile)

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Ulrike Meier Yang

The Impact of Emerging Architectures on the Design of Algebraic Multigrid Methods

Computational Math Group Leader, Center for Applied Scientific Computing
Lawrence Livermore National Laboratory, Livermore, CA, USA

Computational science is facing several major challenges with future architectures: non-increasing clock speeds are being offset with added concurrency (more cores) and limited power resources are leading to reduced memory per core, and highly complex heterogeneous architectures. To meet these challenges and yield fast and efficient performance, solvers need to exhibit extreme levels of parallelism, and minimize data movement. While multilevel methods have shown excellent scalabity on many high performance computer, to achieve good performance on exascale computers requires careful design.

In this talk, we will summarize recent efforts to improve the performance of the linear solvers library hypre for exascale computers, including efforts to reduce communication, improve numerical and computational scalability and increase structure.

MS 3: PDE Constrained and Shape Optimization

Organized by V. Schulz and M. Siebenborn

D. Gathungu, and A. Borzì

Algebraic Multigrid Based on Maximum Weighted Matching in Matrix Graphs Exploiting an Auction Algorithm

Julius Maximilian University of Würzburg, Würzburg, Germany

An efficient multigrid finite-differences scheme for solving elliptic Fredholm partial integro-differential equations (PIDE) is discussed. This scheme com- bines a second-order accurate finite difference discretization of the PIDE prob- lem with a multigrid scheme that includes a fast multilevel integration of the Fredholm operator allowing the fast solution of the PIDE problem. Theoretical estimates of second-order accuracy and results of local Fourier analysis of con- vergence of the proposed multigrid scheme are presented. Results of numerical experiments validate these estimates and demonstrate optimal computational complexity of the proposed framework.

Stephan Schmidt

Generating Shape Derivatives and Repeated Differentiation Hessians Automatically

Julius Maximilian University of Würzburg, Würzburg, Germany

A fully automatic framework for generating weak and strong form shape derivatives is discussed. Repeated application of the generator leads to shape Hessians, preferably in a weak sense. To this end, the mathematical problem is formulated in the Uniform Form Language (UFL) and then processed by a semantic analysis, which automatically applies the formal differentiation rules of shape calculus.

Based on regularity assumptions of the problem provided by the user, the analysis step then, on its own, chooses or omits tangential calculus, such as the divergence theorem in tangent spaces, and generates the surface representation of the shape derivative if applicable. Otherwise, volume expressions can also be generated.

As the directional shape derivative is generated within the UFL language, the resulting UFL expression can next be seamlessly processed by the FEniCS or DUNE environment, thereby automatically generating the complete optimization loop, including the primal and dual solver.

The talk focuses on applications and inverse problems for wave phenomena and computational fluid dynamics.

Volker Schulz, Martin Siebenborn, and Kathrin Welker

Efficient PDE Constrained Shape Optimization Based on Steklov-Poincare Type Metrics

Trier University, Trier, Germany

Recent progress in PDE constrained optimization on shape manifolds is based on the Hadamard form of shape derivatives, i.e., in the form of integrals at the boundary of the shape under investigation, as well as on intrinsic shape metrics. From a numerical point of view, domain integral forms of shape derivatives seem promising, which rather require an outer metric on the domain surrounding the shape boundary. This paper tries to harmonize both points of view by employing a Steklov-Poincaré type intrinsic metric, which is derived from an outer metric. Based on this metric, efficient shape optimization algorithms are proposed, which also reduce the analytical labor, so far involved in the derivation of shape derivatives.

Martin Siebenborn

High Performance Optimization Algorithms for Interface Identification Problems

Department of Mathematics
Trier University, Trier, Germany

Joint work with: Arne Nägel, Volker Schulz and Kathrin Welker

In many applications, which are modeled by partial differential equations, there is a small number of spatially distributed materials or parameters distinguished by interfaces. The problem is then to optimize the shape of these interfaces such that given measurements are reflected by the model. Depending on the application the parameter distribution may form complex contours. Thus, high resolutions are required in the underlying finite element discretizations. The challenge here is to combine methods from PDE constraint shape optimization with HPC techniques and prepare algorithms for supercomputing.

In this talk we present an algorithm that utilizes multigrid strategies and limited memory BFGS updates in order to achieve scalability on very large shape optimization problems. We also show how this can be implemented into an augmented Lagrangian method such that geometric constraints on the shape can be incorporated additionally. In this context optimizing shapes automatically means to deform finite element meshes iteratively. This usually deteriorates the quality of the discretization and thus affects the performance of the solver. We therefore introduce novel shape metrics that show good performance in retaining aspect ratios of discretization elements.

The presented algorithm is shown to perform on two applications. A standard test case is to identify the shape that minimizes energy dissipation in a Stokes flow. Here we demonstrate that the proposed algorithm retains good mesh quality. Furthermore, it is shown how geo- metric constraints are incorporated. The second application is the identification of the shape of human skin cells. It is demonstrated how the distribution of permeability coefficients in a computational model for the human skin are fitted to measurements.

MS 4: Applications of HPC in Fluid Dynamics

Organized by M. Resch

M. Resch

HPC as a Tool in Flow Simulation

R. Schneider

Flow Simulations in Blood

A. Ruopp

Flow Simulation in Water Power Plants

J. Zhang

Flow Simulation in Nuclear Safety Applications

MS 5: Numerical Simulation Framework (Part I)

Organized by Arne Nägel

Dmitry Logashenko

Simulation of Free Surfaces in the Density-Driven Groundwater Flow

Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt, Germany

Dynamics of the free surface separating saturated and unsaturated parts of the domain is an important topic in the simulations of the groundwater flow. The position of the free boundary is influenced not only by the movement of the liquid phase, but also by the recharge (in particular, due to the precipitation) or sinks (for example, by rivers etc). And the configuration of the free surface determines the dynamics of the fluid phase in the domain. In our talk, we consider numerical methods for the simulation of the density-driven Darcy flow with a free surface. We present results of the numerical experiments in 3d, in particular, parallelized computations in a domain with thin geological layers.

Arne Nägel[1], Peter Deuflhard[2], Gabriel Wittum[1]

Linear Implicit Extrapolation Methods for Density Driven Flow

[1]Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt Germany
[2]Beijing Institute for Scientific and Engineering Computing (BISEC)
Beijing University of Technology , Beijing, China

Many problems in porous media science and geophysics comprise interactions of processes, and are typically formulated as a system of coupled PDEs. In most cases, these systems are transient and non-linear. Developing efficient solvers is a delicate task, since one needs to must combine suitable schemes for (i) time integration, (ii) linearization, and (iii) (geometric and/or algebraic) multilevel solvers, finally being employed in a (iv) parallel computing environment.

In this presentation we focus on the problem class of density-driven-flow of brine in a porous media. Previous studies, e.g. [1], investigated different non-linear solvers for this problem class. As the governing equations form a differential algebraic equation of index 1, linear implicit extrapolation methods [2, 3] are applicable. It is one striking feature of these methods, that inexact approximations of the Jacobian are admissible, when used as a so called W-method. In this presentation, we investigate different approximations and classify, which are the most favourable w.r.t. the computational effort. We present numerical experiments, report on results, and provide examples where these methods significantly improved efficiency, thus allowing to address new sets of problems.

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Sebastian Reiter

Mesh Generation for Thin Layered Domains and its Applications to Parallel Multigrid Simulations of Groundwater Flow

Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt Germany

A crucial step for simulations of groundwater flow in thin layered domains is the generation of the discrete computing grid. For the application of efficient geometric multigrid solvers the generated mesh has to be sufficiently coarse while still capturing all relevant details of the underlying domain. A fully automated, parametrized algorithm for the construction of such coarse grids from height data of individual layers of a given layered domain will be presented and applications to hierarchy construction, solver convergence, and parallelization will be explored.

Andreas Vogel, Sebastian Reiter, and Gabriel Wittum

Multigrid for an Adaptive Finite Volume Method Using Hanging Nodes

Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt Germany

Vertex-centered finite volume schemes are a common discretization method for partial differential equations based on conservation laws. In order to balance the discretization effort and the solution quality for spatially varying solutions and errors, we employ the vertex-centered finite volume scheme on adaptively refined computational grids with hanging nodes. Therefore, the arising linear system of equations is to be solved on such grids and we employ the multigrid method on the adaptively refined grid hierarchies for this task. Empirical studies for diffusion equations and problems in the context of density driven flow in porous media together with aspects of the implementation are presented.

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MS 6: Space-Time PDE Solvers (Part II)
Organized by U. Langer and C. Wieners

Randolph E. Bank

Treating Time as Just Another Space Variable

Department of Mathematics
University of California at San Diego, San Diego, USA

We explore the simple idea of treating time as a space variable, and not employing the usual time-stepping approach. While this increases the space dimension of a given PDE problem by one, it introduces a static convection term that can be treated by a variety of techniques. This approach can be especially beneficial in the setting of parallel adaptive finite element computations.

Stefan Findeisen

A Parallel and Adaptive Space-Time Method for Maxwell's Equations

Institute for Applied and Numerical Mathematics
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

We consider linear hyperbolic first-order systems

$$M\partial_t u + Au = f, \qquad t \in (0,T), \qquad u(0) = u_0,$$

for functions u: $(0, T) \to D(A)$, defined on the domain $D(A) \subset L_2(\Omega)^J$, $J \in \mathbb{N}$, of the operator A on $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$. Two typical examples are investigated: The first one is the linear advection equation with $M = 1$ and $A(u)=(\boldsymbol{q}\cdot\nabla u)$ for a given vector field $\boldsymbol{q} \in W^{\{1,\infty\}}(\Omega)^D$. The second case with $M(\boldsymbol{H}, \boldsymbol{E}) = (\mu\,\boldsymbol{H}, \varepsilon, \boldsymbol{E})$ and $A(\boldsymbol{H}, \boldsymbol{E}) = (-\nabla\cdot\boldsymbol{H}, \nabla\cdot\boldsymbol{E})$ leads to the linear Maxwell system for electromagnetic waves. Here μ and ε are given material parameters and $\boldsymbol{H}$ and $\boldsymbol{E}$ describe the magnetic and electric field, respectively. We present a fully implicit parallel space-time approach in $Q = \Omega \times (0, T)$ as an alternative to established time stepping methods.

We use a tensor product ansatz with a discontinuous Galerkin finite element method for the spatial discretization and a Petrov-Galerkin discretization in time. The upwind flux is used to approximate continuity across cell faces. The computational domain Q is decomposed into space-time cells $R = K \times (t_-, t_+) \in \mathcal{R}$ such that $\overline{Q} = \bigcup_{R\in\mathcal{R}} \overline{R}$, where $K \subset \Omega$ and $(t_-, t_+) \subset (0, T)$. Hence they can be distributed among different processes, to solve the complete problem in parallel in space and time. Hence we get a continuous ansatz space and discontinuous test space in time, whereas ansatz and test space are both dis-

continuous in space. For local polynomial ansatz and test spaces $V_{h,R}$, $W_{h,R}$ our ansatz and test spaces V_h and W_h are defined as

$$V_h = \Big\{ v_h \in \mathrm{H}^1(0,T;L_2(\Omega)^J) \colon v_h(x,0) = 0 \text{ for a.a. } x \in \Omega \text{ and } v_{h,R} = v_h|$$

$$W_h = \Big\{ w_h \in L_2(0,T;L_2(\Omega)^J) \colon w_{h,R} = w_h|_R \in W_{h,R} \Big\}.$$

Since the discretization is implicit in time, no CFL limitation applies. The full space-time linear system is solved by using a parallel multilevel preconditioner.
Our method is *p*-adaptive with different polynomial degrees in space and time. A dual weighted error estimator (goal-oriented) is realized for the adaptive selection of polynomial degrees on every space-time cell. Hence we are able to reduce the error towards a given error functional (e.g. energy error functional) in a space-time region of interest during several adaptive iterations.
The linear advection equation is used as a test case for a transport problem to show the reliability of the method and the error estimator. First results in 2+1 dimensions for Maxwell's equations with more than 100 million space-time degrees of freedom on 1000 processors illustrate the parallel efficiency of the method.
Reference:
Willy Dörfler, Stefan Findeisen, and Christian Wieners: Space-time discontinuous galerkin discretizations for linear first-order hyperbolic evolution systems. *Comput. Methods Appl. Math.* 16(3):409-428, 2016.

Uwe Köcher

Space-time Discretisation and Solver Technology for Biot's Model of Poroelasticity

Department of Mechanical Engineering, Numerical Mathematics
Helmut-Schmidt-University, University of the German Federal Armed Forces Hamburg, Germany

(joint work with Markus Bause)

In this contribution a high-order variational space-time discretisation and linear system solver technology including preconditioning for the multi-physics problem of coupled flow and deformation of a fluid-saturated porous media described by Biot's model of poroelasticity is presented.

For the discretisation in time a discontinuous Galerkin method is applied. For the discretisation in space a mixed finite element method is applied. The quasi-static elasticity problem is discretised with a standard conforming method in space. The flow problem is discretised with a Raviart-Thomas finite element method for the flux and a discontinuous Galerkin method for the pressure in space.

The arising coupled linear block systems are solved with different iterative and operator splitting approaches. The solver technology and preconditioning strategy is under strong development and the latest results are presented.

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Marco Zank

A Space-Time Boundary Element Method for the Wave Equation

Institute of Computational Mathematics
Graz University of Technology, Graz, Austria

For the discretisation of the wave equation by boundary element methods the starting point is the so-called Kirchhoff's formula, which is a representation formula by means of boundary potentials. In this talk different approaches to derive weak formulations of related boundary integral equations are considered. First, weak formulations based on the Laplace transform and second, space-time energetic formulations are introduced. In both cases coercivity is shown in appropriate Sobolev spaces. To derive an adaptive scheme an a posteriori error estimator based on the representation formula is used.

Finally, numerical examples for a one-dimensional spatial domain are presented and discussed.

MS 7: Computational Biosciences (Part I)

Organized by R. Krause and G. Queisser

Evgenia Babushkina, Ralf Kornhuber

Adaptive Multilevel Monte Carlo Methods for Elliptic Problems with Uncertain Coefficients

Freie Universität Berlin, Berlin, Germany

While multilevel Monte Carlo (MLMC) methods for the numerical approximation of partial differential equations with uncertain coefficients enjoy great popularity, combinations with spatial adaptivity seem to be rare. We present an adaptive MLMC finite element approach based on deterministic adaptive mesh re nfinement for the arising "pathwise" problems and outline a convergence theory in terms of desired accuracy and required computational work. Our theoretical and heuristic reasoning together with the efficiency of our new approach are confi rmed by numerical experiments.

Matthias Bolten

Usage of Block-Smoothers and Aggressive Coarsening to Improve Scalability of Multigrid

Universität Kassel, Kassel, Germany

Multigrid methods are widely used to solve large-scale problems in science and engineering due to their excellent scaling behavior. This behavior is only limited by the amount of work that has to be carried out on the coarser levels. The limitation has no visible effect when small to mid-size parallel computers are used, it becomes apparent on large machines, only, so it is relevant for exascale machines. To reduce the effect and move the limit to larger core numbers aggressive coarsening can be used. Decreasing the size of the coarse space by aggressive coarsening automatically leads to worse convergence rates. The original convergence rate can be restored by using more efficient smoothing, e.g., more smoothing steps. We propose to use block-smoothers to improve the convergence rate, as they can be implemented at very low cost on modern computer architectures. To allow for analysis of these block smoothers we extended the local Fourier analysis (LFA) framework to deal with blocks, as well. In this talk the idea and the analysis as well as numerical examples will be presented.

M. Favino, R. Krause

VMS Methods for Reaction-Diffusion Problems: An Interesting Case with Multiple Residual Bubbles

Center for Computational Medicine in Cardiology, Institute of Computational Science
Università della Svizzera italiana, Lugano, Switzerland

Standard Finite Element Methods (FEM) are not a robust approach for problems exhibiting multiscale phenomena, such as Convection-Diffusion Problems (CDPs) or poroelasticity. For this models, stabilised FEM have been developed ensuring an improved stability of the method but often affecting the accuracy [1, 2].

Variational Multiscale methods (VMS), developed by Hughes, provide a mathematical framework for considering sub-grid phenomena in FEMs [3]. They are enhanced Galerkin methods in which the solution is written as a sum of a coarse and a fine scale component. The first one is solved with FEM while the second is determined analytically. Methods based on Residual Free Bubbles (RFBs) are a particular case of VMS in which the subgrid scale is defined locally on each element by solving exactly or approximately the analytical problem [4]. RFBs have been mostly applied to CDPs characterised by only one residual bubble function for each element. For this method super convergence in the one-dimensional case and stabilising effects in the multi-dimensonal cases were proven.

In this work, we will focus on the application of RFB to reaction-diffusion problems. The study of them is interesting both on the theoretical and practical point of view. Differently from CDM, they present multiple residual bubbles. Hence, the static condensation of them requires the solution of a small linear system on each element. We will show that

(1) eliminating the additional degrees of freedom associated to the sub grid scale defines a novel stabilised discretisation characterised by a higher accuracy without increasing the dimension of the stiffness matrix;
(2) the resulting stiffness matrix is an M-matrix, ensuring hence the convergence of algebraic MG solvers.
(3) monotonicity of the solution is ensured.

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L. Ridgway Scott

Optimal algorithms using optimal meshes

University of Chicago, Chicago, USA

We discuss two issues regarding adaptive meshes. The first relates to non-nested multigrid in two and three dimensions. We review what is known theoretically and describe some recent work related to optimal implementation. The second relates to error estimators for problems with singularities.

MS 8: Computational Biosciences (Part II)

Organized by R. Krause and G. Queisser

Markus Breit

Electro-Diffusion on Neuronal Micro-Domains - Dos and Don'ts

Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt, Germany

Dendritic spines, the posterior part of a synapse connecting two neurons, are commonly believed to play a significant role in learning and memory storage processes. In order to gain a quantitative understanding of the influence of the spine's micro- and nanoscale-scale architecture on the electro-chemical signals transferred to dendrites, we are developing a numerical framework to solve the Poisson-Nernst-Planck (PNP) equations describing an electro-diffusion model for the involved ions. Computational complexity is addressed by introducing a novel hybrid-dimensional approach based on a Finite Volumes discretization and geometric multi-grid solvers. Several problems arising from the presence of static charges on the sub-cellular structure are discussed and propositions for their treatment by specialized numerical methods are given.

Jan Hahne

Spiking Neural Network Simulation Including Gap Junctions

Bergische Universität Wuppertal, Wuppertal, Germany

Contemporary simulation technology for neuronal networks enables the simulation of brain-scale networks using neuron models with a single or a few compartments. However, distributed simulations with correct cell densities are still lacking the electrical coupling between cells via so called gap junctions. This is due to the absence of efficient algorithms to simulate gap junctions on large parallel computers. The reason is that current simulation codes for spiking neurons like the NEST simulator rely on delayed communication, whereas gap junctions require an instantaneous interaction between the coupled neurons. Here, we present our recently published novel approach based on a waveform relaxation technique that has been incorporated into NEST with version 2.10.0. The framework is on the one hand compatible with the communication strategy of current spiking simulators and on the other hand provides a high accuarcy for the simulation of gap junctions.

Martin Stepniewski

Smooth Subdivision Geometric Multigrid Method with Application in (Neuro-)Biological Numerical Simulations

Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt, Germany

A major endeavor of scientific computing in the field of life sciences lies in the detailed mathematical modeling and numerical simulation of time- and space-dependent physical, chemical and biological processes. Well-established models comprise non-linear instationary partial differential equations with corresponding initial value and boundary conditions defined on a time interval $T := [t_{start}; t_{end}] \subset R$ and a bounded physical problem domain $\Omega \subset R^n$, $n \in \{1; 2; 3\}$. The computation of such models with the help of the computer for running in-silico experiments necessarily requires the underlying systems of (coupled) PDEs, together with the corresponding time interval and problem domain, to be discretized. Preprocessing non-linearities with the Newton Method where applicable, Geometric Multigrid Methods, since their introduction in the early second half of the 20th century [1], have proven to be a highly effcient way to solve the emerging and in practice vast systems of linear equations $Ax = b$ in each Newton and time step.

However, building grid hierarchies by applying classical linear grid refinement strategies to complex morphologies that appear in common biological applications (cell morphologies, organelle morphologies or combinations of both) can produce numerically unfavorable grids (e.g. irregular element shapes) and increase the number of iterations needed for convergence. Also, classical linear grid refinement strategies are limited in their ability to approximate the boundary of the computational domain, unless using a fine base grid level at the expense of increased computational cost.

In this talk we present a novel approach to use Subdivision Schemes, which since the ground-laying work by Catmull and Clark [2] in 1978 have become efficient and popular algorithms in computer graphics to describe smooth curves, surfaces [3] and also more recently volumes [4], to overcome these shortcomings and construct a hierarchy of very regular grids with provably good boundary approximation that can be used in a multigrid setting. We demonstrate the beneficial effects of this new technique in terms of improved convergence rates (and thereby reduced number of iterations and decreased computation time) as well as tackling unphysical behavior of the numerical solution inherent to limitations in domain approximation in a numerical simulation series of test problems and (neuro-)biological applications from current research.

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Ursula van Rienen

Modeling and Simulation of Nerve-Electrode Interactions in Neuronal Implants

IEF, Institut für Allgemeine Elektrotechnik
Rostock University, Rostock, Germany

In this talk, we present the challenges in modeling of nerve-electrode interactions in the context of Neurochips, Cochlear Implants and Deep Brain Stimulation (DBS). We highlight on the biological processes that need consideration in modeling the extracellular phenomena and their interaction with the electrodes. We emphasize on the importance of mathematical models in abstracting the biological phenomena of nerves. We also show how a multi-physical approach is needed in these mathematical models to improve the functionality of the neuronal implants. We present some of the features that may influence the nerve electrode interaction in Cochlea implants and DBS.

MS 9: Numerical Simulation Frameworks (SCHPC) (Part II)

Organized by Z. Mo

With the installation of 100 PFlops supercomputers and the planning of Exascale systems, how to realize effective and efficient extreme-scale simulations, however, remains a grand challenge. Acting as a bridging middleware between supercomputers and application domains, frameworks provide domain experts the parallel computing capabilities without the complexity of architecture and runtime details. Thus, high performance numerical simulations can be achieved with minimal efforts.

This minisymposium will focus on aspects of high performance numerical simulation frameworks developed in China, including the domain-specific frameworks, solvers, and Autotuning tools. Major topics include programming models, data structures, fast algorithms, performance optimization techniques, software design and application developments. The current efforts and challenges toward the Exascale computing will also be discussed at this minisymposium.

Jie Cheng[1], Qingkai Liu[2], Weibo Zhao[2]

JAUMIN: A Programming Framework for Unstructured Mesh Applications

[1]CAEP Software Center for High Performance Numerical Simulations, Beijing, China.
[2]Institute of Applied Physics and Computational Mathematics, Beijing, China

The goal of JAUMIN is to boost the development of unstructured mesh applications that run on large scale parallel computers. JAUMIN achieves this goal by providing patch-centric programming model, where users only have to provide serial programs, including patch programs to implement numerical schemes on a “patch (subdomain)”, and a driver program to assemble the computation flow. Various data communication patterns are encapsulated into components that are ready for the

users to call in their driver programs. In this talk we will give an overview of JAUMIN's design, some implementation issues, and the progress and performance evaluation of some applications.

Tao Cui, Wei Leng, and Linbo Zhang

PHG: A Framework for Parallel Adaptive Finite Element Method

State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences

PHG (Parallel Hierarchical Grid) is a general framework for developing parallel adaptive finite element method applications. The key feature of PHG includes: bisection based conforming adaptive tetrahedral meshes, various finite element bases support and hp adaptivity, finite element code automatic generation, etc. We also introduce a few applications of PHG performed on Tianhe-2 and Sunway Tiahu Light, including earthquake simulation, calculation of electronic structure of materials, parasitic extraction simulation of large scale interconnects.

Guangmin Tan

Building an Autotuning and Composable AMG Solver for Exascale Computing

Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China

In order to tackle the complexity of computer architectures and algorithmic variants, we propose a methodology to build an autotuning and composable sparse numerical solvers for exascale computing. We defines a set of programming interfaces who act as who hierarchical layers of performance and algorithm. The performance layer is composed of sparse matrices operations which are commonly used in various sparse solvers. They are implemented as an autotuning library. The algorithm layer is composed of high-level algorithmic primitives which is customized by users. We demonstrate the usability of the programming interfaces with the case study of AMG solver.

Xiaowen Xu, Zeyao Mo, and Hengbin An

αSetup-AMG: An Adaptive Setup Based AMG Preconditioner for Solving Large-Scale Sparse Linear Systems in Multi-Physics Simulations

Institute of Applied Physics and Computational Mathematics, Beijing, China

AMG is one of the most popular preconditioners in real applications, however, it will lead to poor parallel scalability due to its coarse-level construction and visiting. In our presented adaptive setup strategy called αSetup-AMG, coarsening is performed based on the smoothing behavior on each level, instead of constructing via an independent setup phase in traditional procedure. As a results, αSetup-AMG performs relaxations on finer-levels as much as possible, while the required coarse level numbers are as less as possible. The results for a realistic radiation hydrodynamics simulations on $O(10^4)$ cores show the efficiency and improvement of the adaptive strategy.

MS 10: Computational Models and Methods in Interdisciplinary Problems: Biomechanics, Electromagnetism, and Hydrogeoloy (Part I)

Organized by A. Grillo

Stefano Berrone, Andrea Borio, Sandra Pieraccini, Stefano Scialò, Fabio Vicini

New Numerical Approaches for Large Scale Discrete Fracture Network Flow Simulations

Dipartimento di Scienze Matematiche
Politecnico di Torino, Torino, Italy

A Discrete Fracture Network model describes a fractured geological reservoir as a system of intersecting planar polygons representing the network of fractures in the underground. Fracture intersections are called traces.

Standard finite element methods or mixed finite elements are widely used for obtaining a numerical solution also in this context, but they require mesh elements to conform with the traces. This poses a severe limitation, since realistic fracture networks are typically very intricate, with fractures inter secting each other with arbitrary orientation, position, density and dimension. A conforming meshing process may result infeasible, or might generate a poor quality mesh.

In [1, 2, 3, 4] the authors propose a PDE-constrained optimization approach to simulations on arbitrary DFNs, in which neither fracture/fracture nor fracture/trace mesh conformity is required. The method is based on the minimization of a quadratic functional constrained by the state equations describing the ow on the fractures. The approach totally circumvents the problem of mesh generation, without any need of geometrical modification. By using a gradient based method for the minimization of the functional, the solution of the flow equations on each fracture of the network is carried on independently of the solution on the other fractures. This in turn, together with the meshing process independently performed on each fracture, allows in a natural way for parallel implementation of the overall method. This is of paramount importance both for addressing computations on huge networks, and for performing massive simulations for uncertainty quantification [5] in stochastically generated networks. The approach can be exended to more complex models, as for example the simulation of unsteady transport of a passive scalar within the DFN.

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Melania Carfagna, Alfio Grillo

A Cahn-Hilliard Approach to Thermodiffusion in Porous Media

DISMA "G. L. Lagrange"
Politecnico di Torino, Torino, Italy

For a given physical system, we observe a cross-effect [1], when the flux of an extensive quantity (for instance, heat or mass) can be related not only to the gradient of the state variable that is directly linked to it (i.e., temperature and chemical potential, respectively), but also to the gradients of the other state variables of the model. Thus, if the Onsager-Casimir relations are exploited, the flux of the considered extensive quantity depends linearly on the gradients of all the other state vabiables [1].

In this contribution, the cross-effect giving rise to thermodiffusion, also known as Soret effect, will be discussed in the framework of density and temperature driven flows in porous media. In a mixture exposed to a non- uniform thermal field, this phenomenon occurs when the thermal gradient is capable of inducing the mass flux of the species of the mixture.

In a thermogravitational cell, due to the presence of concurrent buoyancy and thermal forces, an initially uniform mixture separates. We present numerical results of such experiment, retrieved by means of the standard thermodiffusion model, and compare them with experimental evidences, and previous results available in the literature [2, 3, 4]. Finally, we discuss the practical and theoretical consequences of choosing, in the framework described so far, a Helmholtz free energy density of the Cahn-Hilliard type [5].

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Matteo Icardi[1], Gianluca Boccardo[2], Eleonora Crevacore[3]

Micro-Scale Simulation of Flow, Transport and Reaction in Porous Media

[1]Warwick Mathematics Institute
[2]Tel Aviv University
[3]Politecnico di Torino

Classical continuum models to describe transport phenomena in porous media, based on Darcy's and Advection Diffusion Equations, are often limited by a poor knowledge of the actual parameters and the validity itself of the model. This is why, in the recent years, many computational studies have been done directly at the pore-scale, i.e., by solving the free fluid flow equations and associated transport equations. In this work, we summarise our recent computational advances in the simulation of Navier-Stokes and reactive scalar transport in complex three-dimensional pore geometries. One of the main difficulties here is to identify a representative pore structure and appropriate computational setup for a meaningful upscaling. When dealing with random media, for example, effective transport parameters can show significant variations. Here, a multilevel Monte Carlo sampling algorithm is proposed to estimate macroscopic parameters, such as diffusivity and permeability, in random geometries. In other cases, the definition of the effective parameters is itself controversial. When solutes undergo infinitely fast reactions on the grains surface (e.g.: deposition, modelled as homogeneous Dirichlet boundary conditions), no rigorous upscaling is possible and different effective reaction rate (or deposition efficiency) can be defined. Here we analyse the different choices and we propose a novel computational setup to consistently estimate the effective linear reaction rate in periodic media with a self-similar solution.

Computational details regarding CAD, meshing and finite volume discretisation of the pore-space will also be presented.

Raimondo Penta

Can a Continuous Mineral Foam Explain the Stiffening of Aged Bone Tissue? A Micromechanical Approach to Mineral Fusion in Musculoskeletal Tissues

Departamento de Mecanica de los Medios Continuos y T. Estructuras,
E.T.S. de caminos, canales y puertos,
Universidad Politecnica de Madrid, Madrid, Spain

Recent experimental data revealed a stiffening of aged cortical bone tissue, which could not be explained by common multiscale elastic material models.We explain this data by incorporating the role of mineral fusion via a new hierarchical modeling approach exploiting the asymptotic (periodic) homogenization (AH) technique for three-dimensional linear elastic composites. We quantify for the first time the stiffening that is obtained by considering a fused mineral structure in a softer matrix in comparison with a composite having non-fused cubic mineral inclusions. We integrate the AH approach in the Eshelby-based hierarchical mineralized turkey leg tendon model (Tiburtius et al

2014 Biomech. Model. Mechanobiol. 13 1003–23), which can be considered as a base for musculoskeletal mineralized tissue modeling. We model the finest scale compartments, i.e. the extrafibrillar space and the mineralized collagen fibril, by replacing the self-consistent scheme with our AH approach. This way, we perform a parametric analysis at increasing mineral volume fraction, by varying the amount of mineral that is fusing in the axial and transverse tissue directions in both compartments. Our effective stiffness results are in good agreement with those reported for aged human radius and support the argument that the axial stiffening in aged bone tissue is caused by the formation of a continuous mineral foam. Moreover, the proposed theoretical and computational approach supports the design of biomimetic materials which require an overall composite stiffening without increasing the amount of the reinforcing material

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MS 11: Computational Models and Methods in Interdisciplinary Problems: Biomechanics, Electromagnetism, and Hydrogeoloy (Part II)

Organized by A. Grillo

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[1]Silvia Bertoluzza, [2]**Silvia Falletta**, and [2]Giovanni Monegato

A Mortar FEM-BEM Coupling for Wave Propagation Problems in Unbounded Domains

[1]IMATI-CNR, Pavia, Italy

[2]Politecnico di Torino, Torino, Italy

We consider the scattering of a wave by an obstacle of $\mathbf{R}^2$, having a sufficiently smooth boundary Γ. In particular, we solve the time-dependent wave equation in the finite computational domain Ω, bounded internally by Γ and externally by an artificial boundary B where we impose an exact Non Reecting (transparent) Boundary Condition (NRBC) (see [1]).

The NRBC is defined through a space-time Boundary Integral Equation (BIE), which defines a relationship between the solution of the differential problem and its normal derivative on the artificial boundary B. We discretize the BIE on B by combining a second order (in time) BDF convolution quadrature and a Galerkin (or a collocation) method in space. Such a discretization is then coupled with an unconditionally stable ODE time integrator and a FEM in space.

In previous works, we have tested the robustness of the proposed NRBC discretization, and its higher accuracy with respect to that of the associated FEM. Such properties justify a decoupling of the NRBC grid from that of the FEM. In particular, the discretization of the transparent condition can be constructed on a grid defined on B which is coarser than the one inherited by the triangulation of Ω. In this context, we propose a non conforming coupling of the FEM-BEM scheme, by using a mortar technique. The method consists in decomposing the FEM-BEM interface into two disjoint sides and in replacing the strong point-wise continuity condition of the traces of the solution on B by a weak one, by imposing that the jump of the traces is orthogonal to a suitable multiplier space.

Such an approach allows to reduce the computational cost of the NRBC and to couple discretizations of different type. We will present numerical results obtained for problems of waves scattered by fixed and rotating obstacles, non trivial data, and sources far away from the computational domain Ω.

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Markus M. Knodel[1], A. Nägel[2], S. Reiter[2], A. Vogel[2], G. Wittum[2]

Application of Multigrid Solvers to Mathematical Models in Medicine and Biophysics at Realistic Geometries

[1]Dipartimento di Scienze Matematiche
Politecnico di Torino, Torino, Italy
[2]Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt, Germany

A recent review from medicines [1] described the present state of mathematical oncology in the following way: "Although the clinical use of spatial mathematical models is far from being actually effective, they have many short and medium term future prospects in the clinical assessment in surgery or interventional radiology by determine tumor margins". This alarming statement holds true for all biomedical fields.

We will give insight into the numerical aspects of the evaluation of our mathematical models within computational virology and continuum mechanics. The latter one is a very important brick in the computational evaluation of advanced models which represent the complexity of cancer progression. Our workow splits into three steps: (1) Reconstruction of realistic geometries with the aid of NeuRA2 and the application of UG4 for (2) the FV/FE discretization of the models and (3) the solution of the subsequent linear equation systems with massively parallel multigrid solvers at supercomputers like the HLRS Hazel Hen. We used reaction-diffusion equation models which are applied to reconstructions of complex realistic intracellular geometries which allowed us for the estimation of the diffusion constant of a viral protein of the Hepatitis C virus. Our multiscale mathematical modelling of growth and structural adaptation of soft biological tissues and tumour masses reflects a synergetic approach encompassing electro-chemo-mechanical phenomena, based at the first step especially upon continuum mechanic models of strain dynamics of elastic and plastic deformations [2], incorporating recently also anisotropic effects. We discuss the work in progress of the evaluation of isotropic and anisotropic models of soft tissue deformation. Based upon the FE discretization of a Gateau-linearization of the virtual powers and the ow rule combined with a nested two Newton steps method, we evaluate the technical challanges of the combination of FE discretization, numerical and analytical differentiations of the basic equations to which we apply massively parallel multigrid solvers. Whereas in a first step, the strain mechanics computations are performed on sim-ple geometries for a better understanding of the properties of the models and to be able to compare our results with those of commercial programs, we intend to apply the models soon to already reconstructed realistic geometries derived from human CT data.

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Klaus-Peter Kröhn

3D flow and solute transport in fractured rock

GRS gGmbH, Braunschweig, Germany

In-situ experiments in the only potential host rock for nuclear waste repositories in Swe-den, that is crystalline rock, are performed at the Hard Rock Laboratory (HRL) at Äspö. In the framework of the Tracer Retention Understanding Experiments (TRUE) the TRUE Block Scale Project at the HRL /WIN 02/ formed the basis for setting up the "TRUE Block Scale hydrostructural model" which comprises a cubic volume with a side length of 200 m /DER 03/.

Of the 22 deterministic fractures with an extension larger than 50 m known to exist within this volume only 11 appeared to be suitable for the model. Gaps in the actual field data were therefore filled by geostatistical means leading to a semi-synthetic geostatistical model that included the remaining 11 deterministic and 19 additionally generated syn-thetic 100-m scale fractures /DER 03/. Smaller fractures, called background features, could only be described in terms of statistics from the very start. A total of 5660 synthetic background features was also generated and added to the model. The matrix, however, was not considered.

In the framework of the TRUE Block Scale project also the tracer test "C2" was per-formed /AND 02/. A solution containing four tracers with different sorption coefficients was injected in a certain fracture and extracted from a different but hydraulically con-nected fracture. Breakthrough curves at the extraction point were measured.

Modelling of fracture flow at other locations of the HRL has indicated that the hydraulic influence of the background fractures on the flow can be represented by an increase of permeability of the continuous matrix /KRÖ 15/. The conceptual model considered here consists therefore of large-scale deterministic fractures and the matrix which represents also the whole set of background fractures by an accordingly increased permeability.

The modelling reported here was performed with the code d3f++ /SCN 12/, /SCN 16/ and concerns the resulting flow field and the pathway of the conservative tracer. The related calculated breakthrough curve at the extraction point matches the measurements satisfy-ingly well.

Acknowledgements
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Anke Schneider[1], Kristopher L. Kuhlman[2], D. Logashenko[3], S. Reiter[3], A. Vogel[3]

Regional-Scale Modeling of Density-Driven Groundwater Flow

[1]GRS gGmbH, Braunschweig, Germany

[1]Sandia National Laboratories, Albuquerque, USA

[3]Goethe-Center for Scientific Computing
Goethe University Frankfurt, Frankfurt, Germany

The code d^{3}f++ /SCH 12/, /SCH 16/, based on UG4 /VOG 14/, is a powerful tool for modeling density-driven groundwater flow and nuclide transport, that has been developed since 1995 in the framework of several joint projects. The progress of an application of d^{3}f++ to a regional 3d basin model is presented here.

The Waste Isolation Pilot Plant (WIPP) is a repository for transuranic waste situated in a semi-arid region east of the City of Carlsbad, New Mexico, USA, in a thick, Permian-age deposit of bedded salt. This host rock formation is covered by flat bedded Permian halite, dolomite, anhydrite and clastic hydrogeological units as well as Triassic and Quaternary sandstone. Various modeling studies to examine groundwater flow in the rocks overlying the WIPP repository were performed in the past by Sandia National Laboratories, from 2d modeling up to a 3d basin-model covering an area of about 6,000 km. /DAV 89/, /COR 00/.

Were previous models of GRS considering density effects restricted to 2d or small scale domains, the present model covers the whole overburden in the entire basin. The model domain has a depth of about 700 m and consists of 10 flat bedded layers with contrasts in their permeabilities up to seven orders of magnitude, where the two main aquifers have a mean thickness of only 3 m. These characteristics combined with the large horizontal extension of the model domain evoke high numerical anisotropies. A second challenge is the large free groundwater surface with extremely low groundwater recharge rates as an upper boundary condition.

The objective of the current modeling is to enhance the understanding of the groundwater flow dynamics in the basin in a time frame of tens of thousands of years and forecasting the impact of density effects. This includes varying recharge rates while checking the position of the water table and the groundwater flow patterns. Finally, a comparison of the d^3f++ results with PFLOTRAN-simulations /LIC 14/ is planned.

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MS 12: Numerical Simulation Frameworks (SCHPC) (Part III)

Organized by Z. Mo

With the installation of 100 PFlops supercomputers and the planning of Exascale systems, how to realize effective and efficient extreme-scale simulations, however, remains a grand challenge. Acting as a bridging middleware between supercomputers and application domains, frameworks provide domain experts the parallel computing capabilities without the complexity of architecture and runtime details. Thus, high performance numerical simulations can be achieved with minimal efforts.

This minisymposium will focus on aspects of high performance numerical simulation frameworks developed in China, including the domain-specific frameworks, solvers, and Autotuning tools. Major topics include programming models, data structures, fast algorithms, performance optimization techniques, software design and application developments. The current efforts and challenges toward the Exascale computing will also be discussed at this minisymposium.

Hengbin An

Anderson Acceleration and Application to Three Temperature Energy Equations

Institute of Applied Physics and Computational Mathematics

Anderson acceleration method is an algorithm for accelerating the convergence of general fixed point iteration or Picard iteration. The method was first proposed in 1965 to accelerate the convergence of self-consistent field iteration in electronic structure computation, and it has being used successfully in that area ever since. However, until recently, Anderson acceleration method began to attract attention from the community of numerical analysis and algorithm development and some other application areas. Compared with Newton-like method, one advantage of Anderson accelerati on method is that there is no need to form the Jacobian matrix. Therefore, the method is easy to be implemented. In this paper, Anderson accelerated Picard method is employed to solve a kind of strong nonlinear radiation diffusion equation, three temperature energy equations. To improve the robustness of Anderson acceleration method, two strategies are incorporated into Anderson acceleration method. One strategy is used so that the iteration satisfying physical constraint. Another strategy is about monitoring matrix condition number for the least squares problem in the implementation of Anderson acceleration so that numerical stability is guaranteed. Numerical results show that Anderson accelerated Picard method can solve three temperature energy equation effectively. Compared to Picard method without accelerating, at least half iteration numbers can be saved by using Anderson acceleration method. Comparison for Jacobian-free Newton-Krylov method to Picard method and Anderson acceleration method is given.

key words: Anderson Acceleration, Picard method, fixed point iteration, JFNK, iteration acceleration, three temperature energy equation

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This is joint work with Homer F. Walker. This project was supported by National Natural Science Foundation of China (No. 11671051, No. 11171039, No. 61370066). Some of the work is implemented on the Turing machine in WPI while the author visiting WPI.

Ran Xu [*†‡], Hanlin Ding [‡], Jie Cheng [*†] Weibo Zhao [*†] and Bin Liu [‡]

Mend-centered Geometric Multi-Grid Algorithm for Solution of Linear Problem in Computational Solid Mechanics

* Institute of Applied Physics and Computational Mathematics, Beijing, 100088, China
† CAEP Software Centre for High Performance Numerical Simulation, Beijing, 100088, China
‡ AML, Department of Engineering Mechanics, Tsinghua University, Beijing, 100084, China

A mend-centered geometric multi-grid algorithm is proposed for the solution of linear problem from implicit FEA works. Contrasting to the widely-used Algebraic multi-grid method, geometric version is more efficient, especially for structural problem, but hard to build the nested-coarse-grid and infrequency in FEA. In this proposed algorithm, we use the temporary outcome of discretization to build the geometric-grid-system for the V- or W-cycle smoothening, in which the overcome can be negligible for the modern meshing methods and packages always execute a step-by-step refining strategy to reach the aimed characteristic size. Because of the existing of curved planes, the grid-system is always not nesting, which means that the nodes in coarser grid level can not be found in the finer grid level. Therefore, a new interpolation is developed to settle the non-nesting fact. More, a mend-centered idea is putted forward to supervise coarser grid dicretization, which means that we can mend the hole, flat the curved plane and ignore other locally geometric character to make the middle meshing procedure notably easily. The reason of mending or flatting is that the locally geometric characters play as a high frequency residual corresponding to the Saint-Venant principle in solid mechanics, which should be smoothened in the finer grid. The effect of the proposed method is tested by two numerical experiments of symmetric and non-symmetric geometry, and the algorithm can be easily parallel implemented on cluster for the extraordinary studies for the strongpoint received from all multi-grid theory.

Key words: *Computational Solid Mechanics, Finite element method, Linear Equations, Geometric Multi-grid Method, Mend*

Aiqing Zhang, Zeyao Mo, and Hengbin An

JASMIN: A High Performance Programming Framework for Numerical Simulation

Institute of Applied Physics and Computational Mathematics, Beijing, China

This talk reports on the progress of JASMIN as a high performance programming framework for numerical simulation on structured mesh. This framework aims to isolate the design and implementation of parallel algorithm from application software and to make the application experts develop their software in the style of "Think Parallel, Write Sequential". The main software components and architectures are introduced. Some parallel applications are also given for the verification of their success in the field of numerical simulation.

MS 13: Modeling the Barrier Function of Human Skin

Organized by A. Nägel and G. Wittum

M. Heisig, A. Nägel, G. Wittum

Parameter Sensitivity Analysis of a Two-Dimensional Skin Diffusion Model

Goethe-Center for Scientific Computing (G-CSC)
Goethe University Frankfurt, Frankfurt, Germany

Diffusion and partition coefficients are important input parameters for diffusion models of skin absorption. To provide new insights into the impact of changes in different diffusion and partition coefficients on transient transdermal drug penetration after finite dosing, a sensitivity analysis with our two-dimensional mathematical diffusion model (Naegel et al. 2011, Selzer et al. 2013) has been accomplished. The sensitivity analysis provides a quantitative evaluation of the effect the input parameters (i.e. diffusion and partition coefficients) have on transient mass profiles in different skin compartments (donor, stratum corneum (SC), deeper skin layers (DSL), i.e. viable epidermis and dermis, acceptor) for the lipophilic flufenamic acid (FFA) and the hydrophilic caffeine (CAF).

The sensitivity of the input parameters was calculated using the sensitivity index (SI) proposed by Hoffman and Gardner (Hoffman and Gardner, 1983): $SI = (D_{max} - D_{min})/D_{max}$, where D_{max} is the output result when the parameter in question is set at its maximum value and D_{min} is the output result for the minimum parameter value.

A sensitivity ranking list was created for the input parameters to estimate their influence on the model output.

In case of FFA the donor diffusion coefficient has the lowest sensitivity on mass profiles over time. The diffusion coefficient of the deeper skin layers shows a low sensitivity to the outcomes, but is more sensitive than the deeper skin layers-lipid partition coefficient. The lipid diffusion coefficient reveals a high sensitivity to the outcomes. The lipid-donor partition coefficient has a very high sensitivity to the outcomes which is more sensitive than the corneocyte diffusion coefficient. The sensitivity of the corneocyte diffusion coefficient exceeds that of the corneocyte-lipid partition coefficient. The parameter sensitivities of CAF show a similar behaviour, with the exception that the diffusion coefficient of the deeper skin layers is less sensitive than the deeper skin layers-lipid partition coefficient and the corneocyte diffusion coefficient is less sensitive than the corneocyte-lipid partition coefficient.

In a further study the influence of skin thickness on transient skin penetration of two model substances has been analysed.

In conclusion, the sensitivity analysis helps to identify the key parameters for predicting transient skin penetration for a broad range of non-volatile substances after finite dosing in an aqueous vehicle system using a two-dimensional mathematical diffusion model.

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Arne Nägel

Mathematical Models for Skin Penetration

Goethe-Center for Scientific Computing (G-CSC)
Goethe University Frankfurt, Frankfurt, Germany

The skin is an organ with an ordered, highly differentiated structure, providing vitally important barrier properties for the organism. In particular the stratified epithelial layer of the epidermis includes various sources of heterogeneities both with respect to morphology as well as to function. Complementing the experiment, mathematical modelling and corresponding simulations are attractive tools for improving our understanding the skin and its barrier properties, e.g., by

identifying rate-limiting steps, providing predictions and guiding the experimental design.

In this spirit, the focus of this presentation will be on a mechanistic bottom-up description. The corresponding model is based on first principles from physics, thermodynamic considerations, and comprises microscopic sub-structures. This yields a multi-scale model in which structural effects spanning a variety length and time scales need to be included. We present examples of on-going research in the field, provide application-oriented results and also comment on the underlying mathematical tools and numerical algorithms.

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Gabriel Wittum

Swelling of Corneocytes and Other Perspectives of Skin Modelling

G-CSC, Universität Frankfurt and ECRC, KAUST

Skin is the largest organ of our body. In particular, it is the barrier protecting the body from the uncontrolled penetration of alien substances. Originating in pharmacy, quantitative understanding of the barrier function of human skin more and more becomes crucial for a several aspects of medicine. In this context, mathematical models including detailed cellular and subcellular structures are devleoped. To treat problems of this complexity, novel mathematical models, methods and software tools are necessary. In recent years, such models, numerical methods and tools have been developed, allowing to attack these problems. In the talk, we present such models, discuss some of the major challenges of the problem and show the impact of the simulation results on the understanding w.r.t. penetration of xenobiotics through human skin.

Rebecca Wittum

Three-Dimensionally Resolved Microscopic Model of Diffusion in Viable Epidermis

KIT, Karlsruhe, Germany

In-silico models of solute transport through skin using sub-cellular resolution allow more accurate identification of rate limiting factors as well as improving our understanding of diffusion in cellular membranes.

Typically these microscopic models solve diffusion problems on idealized geometries allowing systematic investigation of geometry-transport interaction. A state of the art model formulated in three spatial dimensions exists for the stratum corneum using tetrakaidecahedra as cell templates [1] as well as for the viable epidermis using hexagonal prisms and several structural simplifications [2].

In our study, we adapted the epidermal model from [2] for complex geometries and investigated the effect of using more realistic cell representations on the effective diffusion coefficient. Using this model with more realistic morphology, we found a significant lowering of permeability for multiple

cell layers compared to small changes in case of prismatic cells and demonstrated further possibilities of the extended model by introducing copermeation and simple coupling.

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Contributed Paper

CP 1: AMG

Karsten Kahl

Optimal interpolation in algebraic multigrid methods

Bergische Universität Wuppertal, Wuppertal, Germany

In this talk we derive, based on the exact two-grid theory, an optimal interpolation operator for two-grid algebraic multigrid methods. We show that it matches the exact convergence rate of the theory and is in agreement with the limiting cases of the theory, namely when the two-grid method becomes an exact solve. As a side-product we can obtain a relation between the convergence rate of the optimal two-grid method and the dimension of the coarse-grid space which can be used to optimize the dimension of the coarse grid space by using a suitable model for the operation complexity. Equipped with the information on its dimension, we develop a method that locates representatives of the coarse-grid degrees of freedom that allow for a sparse approximation of the optimal interpolation operator. This analysis thus indicates if a practical method, which prescribes the sparsity of interpolation can achieve a near-optimal convergence rate.

While the optimal interpolation is an interesting theoretical tool, which reveals a lot of information about the problem and the constituents of the two-grid method, its direct practical use is limited. Thus we finish the talk by presenting ideas on how to integrate the concept of optimal interpolation into the Bootstrap algebraic multigrid framework and present numerical results for a variety of applications.

Bram Metsch

Algebraic Multigrid for the Finite Pointset Method

Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI
Schloss Birlinghoven, Sankt Augustin, Germany

The Finite Pointset Method (FPM) is a grid-free approach for the simulation of fluid dynamics and continuum mechanics problems. The underlying partial differential equations are discretized at a point cloud using generalized finite differences, which are computed automatically by a least-squares method.

The structure of the linear systems evolving from this method. differs in several aspects from more conventional discretizations. As the discretization stencils are computed independently for each point, each matrix row the resulting matrices are non-symmetric. Furthermore, the least-squares method produces large stencils (∼40) to reach the desired discretization accuracy, generates off-di agonal entries with both positive and negative sign, and employs per-row scalings that might hide the underlying physics.

Depending on its settings, FPM requires the solution of scalar systems, coupled velocity systems or pressure-velocity Stokes-like systems. In this talk we present our strategies to solve these systems using the SAMG solver. We illustrate the effective operation of our methods on several examples from science and engineering.

(This is joint work with the Grid-free methods group at Fraunhofer ITWM.)

A. Napov, Y. Notay

An Effcient Algebraic Multigrid Method for Graph Laplacian Systems

Service de Métrologie Nucléaire
Université Libre de Bruxelles, Belgium

We present an aggregation-based algebraic multigrid method for sparse linear systems whose matrices are Laplacians of undirected graphs. Such systems are challenging for any algebraic solver because of the diversity of the connectivity patterns that they exhibit, ranging from structured grids to scale-free graphs. The proposed approach combines static elimination of degree-one vertices with the degree-aware rooted aggregation. The resulting combination performs well compared to the state-of-the art solver, but sometimes lacks of robustness [1]. It is therefore supplemented with the quality control for the resulting aggregates [2]. Since large aggregates (over a thousand of unknowns) are not uncommon, the quality check is performed in a cost-effective way. The approach with quality control is shown to be robust, whereas it execution time is shown comparable to the one without quality control.

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Hongxuan Zhang

A unified approach to the construction of coarse spaces and convergence analysis in AMG

The Pennsylvania State University, University Park, USA

In this work, we present a general framework for the design and analysis of two-level AMG methods. The approach is to find a basis for locally-the-best coarse space, such as the space of constant

vectors for standard discretizations of scalar elliptic partial differential equations. The locally defined basis elements are glued together using carefully designed linear extension maps to form a global coarse space. Such coarse spaces, constructed locally, satisfy global approximation property and by estimating the local Poincar{\' e} constants, we obtain sharp bounds on the convergence rate of the resulting two-level methods. To illustrate the use of the theoretical framework in practice, we prove the uniform convergence of the classical two level AMG method for finite element discretization of a jump coefficient problem and anisotropic problems on a shape regular mesh.

CP 2: Special MG

M. Islahuddin[1], S. Vandewalle[2], and H. Janssen[1]

Algebraic Multigrid for a Pore Network Model of Moisture Transfer

[1]Department of Civil Engineering, Building Physics Section
KU Leuven, Leuven, Belgium
[2]Department of Computer Science, Numerical Analysis and Applied
KU Leuven, Leuven, Belgium

A promising approach to model moisture transfer in porous building materials is pore network modelling, wherein pore-scale physics are applied on a network of pores and throats. The pore network represents the material's void space and is highly irregular and anisotropic, inherited from the actual pore structure extracted from a micro-CT image. Moreover, porous building materials commonly have a wide pore radius range, from nano- to millimeter, which results in large networks with millions of pores and highly varying coefficients.

A direct solver rapidly becomes prohibitively expensive for solving the resulting system of linear equations. To speed up the process we therefore applied various algebraic multigrid (AMG) solvers. In this work, we apply various coarsening methods, smoothers, and cycle types to networks of different size and compare the approaches with respect to CPU time, memory and convergence.

AMG performs well in water- and air-saturated conditions, where the matrix of the linear system is symmetric and weakly diagonally dominant. In the dry state, the Ruge-Stüben AMG solver performs better than both a smoothed aggregation and a root-node aggregation technique. In the wet state, root-node aggregation slightly outperforms the other approaches. These observations are mainly related to the homogeneous spatial distribution of the moisture conductivities.

The AMG solvers do however not converge as stand-alone methods in the dry-wet transition range. This range is indicated by the early construction of a spanning water cluster connecting in- and outlet. The standard homogeneous coarsening methods fail to adequately represent the dominant localised flow through that continuous water cluster. Using AMG as a preconditioner for GMRES does however significantly enhance the convergence speed.

To further increase the computation time, the coarsening methods, interpolations, and smoothers will be adjusted. Alternatively, implementing existing parallel AMG codes in super computer will provide more acceleration.

Thomas Ludescher[1], Sven Groß[1], Hardik Kothari[2], Rolf Krause[2], Arnold Reusken[1]

A Multigrid Method for Unfitted Finite Element Methods

[1]Chair of Numerical Mathematics, RWTH Aachen University, Germany
[2]Institute of Computational Science, USI Lugano, Switzerland

For the numerical treatment of interface problems, such as the fluid dynamics in twophase flows or crack propagation in solid mechanics, it is important to capture the discontinuous behavior of the solution at the interface in order to obtain a good approximation quality and optimal convergence rates. Discretizations of such interface problems with standard finite element methods on a mesh that is not fitted to the interface do not yield satisfactory results. In unfitted FEM (also called XFEM or CutFem) the solution space is enriched by a set of cut standard basis functions close to the interface, which then allows an accurate representation of discontinuities. Typically, the arising linear systems are very ill-conditioned when the interface is close to an elemend node and hence the design of an efficient linear solver becomes a challenging task.
In this talk we present a multigrid solver for the efficient solution of this type of unfitted finite element discretizations. One important component of multigrid methods is transfer of information between different grid levels. For that purpose suitable prolongation and restriction operators need to be designed. Unfortunately, standard techniques cannot be applied for unfitted finite element discretizations.
A general method for constructing appropriate prolongation and restriction operators is presented which is based on a pseudo-$\mathbf{L}^2$-projection and has been developed for information transfer in the context of mortar methods [1]. The method will be explained and results of several numerical experiments, e.g. for a Poisson interface problem using a Nitsche discretization [2], will be presented.

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Clemens Hofreither, **Stefan Takacs**, Walter Zulehner

A Robust Multigrid Method for Isogeometric Analysis

Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria

Isogeometric analysis was proposed in the year 2005 by T. Hughes for a better connection between CAD modeling and FEM simulation. The idea is to use (tensor-product) B-splines or non-uniform rational B-splines (NURBS) as ansatz functions and a global geometry transformation. This approach has many nice features, however the condition number of the resulting stiffness matrix for the Poisson problem grows exponentially in the polynomial degree p and the usual way, i.e., like h^{-2} in the grid size.

The setup of a multigrid method being robust only in the grid size is standard. Numerical evidence shows that such standard approaches do not work well if the polynomial degree p is increased. In this talk, we will discuss how to set up a p-robust multigrid method for a model problem being discretized with B-splines. The main focus is set on the construction of smoothers such that the convergence properties of the multigrid solver do not deteriorate if the polynomial degree p is increased.

This is done based on the recent paper on a robust approximation error estimate for B-splines, where a p-robust approximation error estimate and a p-robust inverse inequality are proven for a subspace of the whole spline spaces. In one dimension, this subspace is the space of all splines, whose odd derivatives vanish on the boundary. So, for typical problems, that space is almost as large as the whole spline space. Based on that result, it is possible to set up a stable splitting of spline space, where for each of the subspaces its own smoother is applied. In the talk both convergence analysis and numerical experiments are presented. They confirm that the proposed method behaves optimal in both the grid size h and the polynomial degree p.

Walter Zulehner[1], Lorenz John[2], Ulrich Rüde[3], Barbara Wohlmuth[2]

On the Analysis of Block Smoothers for Saddle Point Problems

[1]Institute of Computational Mathematics
Johannes Kepler University Linz, Linz, Austria
[2]Institute for Numerical Mathematics
Technische Universität München, Garching b. München, Germany
[3]Institute of Systemsimulation
University of Erlangen-Nuremberg, Erlangen, Germany

In this talk, we discuss several classes of Uzawa smoothers for the application in multigrid methods in the context of saddle point problems. Beside commonly used variants, such as the inexact and an approximate block factorization version, we also introduce a new symmetric method, belonging to the class of Uzawa smoothers. For these variants we present a unified analysis of the smoothing property, which is an important part in the multigrid convergence theory. As an example, these methods are applied to the Stokes problem, where several numerical experiments illustrate the obtained theoretical results.

CP 3: Application

Nils Kintscher, Karsten Kahl

Geometric Multigrid for the Tight-Binding Hamiltonian of Graphene

Bergische Universität Wuppertal, Wuppertal, Germany

Since the Nobel prize has been awarded in 2010 for the isolation of graphene, research on this miraculous 2-dimensional material has flourished. In order to calculate the electronic properties of graphene structures a tight-binding approach can be used. The tight-binding formulation leads to linear systems of equations which are maximally indefinite and can be seen both as a discretization of a system of PDEs or a staggered discretization. This poster presents a geometric multigrid method for this problem and the results of the two-level convergence analysis obtained by local Fourier analysis. Numerical tests show the scalability of the multigrid method with respect to various geometric parameters.

Katharina Rafetseder and Walter Zulehner

A Decomposition Result for Kirchhoff-Love Plate Bending Problems and Associated Discretization Approaches

Johannes Kepler University Linz, Linz, Austria

In this talk, we introduce a new mixed variational formulation for a Kirchhoff-Love plate bending problem. The plate is considered to be clamped, simply supported and free on different parts of the boundary.

The new mixed formulation uses for the deection the standard Sobolevfspace $\mathbf{H}^1$ (with appropriate boundary conditions), but involves a nonstandard Sobolev space for the auxiliary variable, the bending moments, which are related to the Hessian of the deection. The new formulation satisfies Brezzi's conditions and is equivalent to the original problem. Based on a Helmholtz-like decomposition of this nonstandard Sobolev space, a decomposition of the fourth-order problem into three (consecutively to solve) second-order elliptic problems in standard Sobolev spaces is achieved.

Based on this decomposition result, we can derive in a natural way families of finite elements for triangular and quadrilateral meshes and also isogeometric discretizations. Note, this method is only based on standard components for second-order problems regarding both the discretization and the solver of the discrete problem. Moreover, we present numerical experiments.

Possible extensions to more general fourth-order problems, e.g., Kirchhoff-Love shells, will also be shortly discussed.

Pieterjan Robbe

A Multi-Index Quasi-Monte Carlo Algorithm for Lognormal Diffusion Problems

KU Leuven, Leuven, Belgium

We present a Multi-Index Quasi-Monte Carlo method for the solution of elliptic partial differential equations with random coefficients and inputs. By combining the multi-index sampling idea with randomly shifted rank-1 lattice rules, the algorithm constructs an estimator for the expected value of some functional of the solution. The efficiency of this new method is illustrated on a three-dimensional subsurface flow problem with lognormal diffusion coefficient with underlying Mat\'ern covariance function. This example is particularly challenging because of the small correlation length considered, and thus the large number of uncertainties that must be included. We show strong numerical evidence that it is possible to achieve a cost inversely proportional to the requested tolerance on the root-mean-square error.

Andreas Van Barel, Pieterjan Robbe, Vyacheslav Kungurtsev, Stefan Vandewalle

Robust Optimization with a Multilevel Monte Carlo Method

KU Leuven, Leuven, Belgium

We consider PDE-constrained optimization problems, where the partial differential equation has uncertain coefficients modelled by means of random variables or random fields. The goal of the optimization is to determine an optimum that is satisfactory in a broad parameter range, and as insensitive as possible to parameter uncertainties. First, an overview is given of different deterministic goal functions which achieve the above aim with a varying degree of robustness. Next, a multilevel (Quasi-) Monte Carlo method is presented which allows the efficient calculation of the gradient and the Hessian arising in the optimization method. The convergence behaviour for different gradient and Hessian based methods is then illustrated for a model elliptic diffusion problem with lognormal diffusion coefficient. We demonstrate the efficiency of the algorithm, in particular for a large number of optimization variables and a large number of uncertainties.

List of Participants Bruchsal Palace, December 5 - 9, 2016

Aizinger	Vadym	Friedrich-Alexander-Universität Erlangen-Nürmberg
An	Hangbin	Institute of Applied Physics and Computational Mathematics, CAS
Babushkina	Evgenia	Freie Universität Berlin
Bank	Randy	University of California
Bastian	Peter	IWR, Universität Heidelberg
Berrone	Stefano	Dipartimento di Scienze Matematiche Politecnico di Torino
Birken	Klaus	itemis AG
Bolten	Matthias	Universität Kassel
Börm	Steffen	Christian-Albrechts-Universität
Braess	Dietrich	
Breit	Markus	Goethe-Universität Frankfurt
Cheng	Jie	Institute of Applied Physics and Computational Mathematics
Claus	Lisa	University of Kassel
Cui	Tao	Chinese Academy of Sciences, Beijing
D'Ambra	Pasqua	Instituto per le Applicazioni del Calcolo of the National Research Council of Italy (IAC-CNR)
Deuflhard	Peter	ZIB
Di Stefano	Salvatore	Politecnico di Torino
Ernesti	Johannes	Karlsruher Institut für Technologie, KIT
Falletta	Silvia	Dipartimento di Scienze Matemaiche Politecnico di Torino
Favino	Marco	Universitá della Svizzera Italiana
Feuchter	Dirk	Karlsruher Institut für Technologie
Findeisen	Stefan	Karlsruher Institut für Technologie, KIT
Gathungu	Duncan	Julius Maximilian University of Wuerzburg
Grasedyck	Lars	RWTH Aachen
Grillo	Alfio	Politecnico di Torino
Hackbusch	Wolfgang	Max-Planck-Institut Mathematik in den Naturwissenschaften
Hahne	Jan	Bergische Universität Wuppertal
Hansford	Victoria	ECRC, KAUST

Heisig	Michael	Goethe-Universität Frankfurt
Hiptmair	Ralf	ETH Zürich
Hittler	Jochen	
Hoffer	Michael	Goethe-Universität Frankfurt
Hoffmann	Wolfgang	Sico-Solutions
Holland	Jan	Springer-Verlag
Höllbacher	Susanne	Goethe-Universität Frankfurt
Huurdeman	Bernhard	
Huymaier	Myra	Goethe-Universität Frankfurt
Icardi	Matteo	University of Warwick
Islahuddin	Muhammed	KU Leuven
Jungblut	Daniel	Goethe-Universität Frankfurt
Kahl	Karsten	Bergische Universität Wuppertal
Khoromskij	Boris	Max-Planck-Institute for Mathematics in the Sciences
Kintscher	Nils	Bergische Universität Wuppertal
Knodel	Markus	Dipartimento di Scienze Matematiche Politecnico di Torino
Köcher	Uwe	Helmut-Schmidt-University
Kornhuber	Ralf	Freie Universität Berlin
Krause	Rolf	Università della Svizzera italiana
Kröhn	Klaus-Peter	Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH
Kurz	Stefan	TU Darmstadt
Lampe	Michael	Goethe-Universität Frankfurt
Langer	Ulrich	Johannes Kepler University Linz
Larisch	Lukas	Goethe-Universität Frankfurt
Le Borne	Sabine	Hamburg University of Technology
Lemke	Babett	Goethe-Universität Frankfurt
Logashenko	Dmitrij	Goethe-Universität Frankfurt
Lohrengel	Maxi	Goethe-Universität Frankfurt
Ludescher	Thomas	RWTH Aachen
Lund-Nguyen	Kathryn	Bergische Universität Wuppertal
Maar	Bernd	
Meier Yang	Ulrike	Lawrence Livermore National Laboratory

Metsch	Bram	Fraunhofer SCAI
Mo	Zeyao	Institute of Applied Physics and Computational Mathematics, CAS
Nägel	Arne	Goethe-Universität Frankfurt
Napov	Artem	Université Libre de Bruxelles
Neumüller	Martin	Johannes Kepler Universtiy Linz
Nikolov	Teodor	University of Wuppertal
Penta	Raimondo	Universidad Politecnica de Madrid
Pieper	Joanna	Goethe-Universität Frankfurt
Queisser	Gillian	Temple University
Rafetseder	Katharina	Johannes Kepler University Linz
Reichenberger	Volker	ESb Business School Reutlingen University
Reinhardt	Lukas	Goethe-Universität Frankfurt
Reiter	Sebastian	Goethe-Universität Frankfurt
Rentz-Reichert	Henik	PROTOS Software GmbH
Resch	Michael	HLRS Stuttgart
Reusken	Arnold	RWTH Aachen
Robbe	Pieterjan	KU Leuven
Sauter	Stefan	University Zürich
Schmidt	Stephan	University of Würburg
Schneider	Anke	Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH
Schneider	Johannes	Goethe-Universität Frankfurt
Schulz	Volker	University of Trier
Scott	Ridgway	University of Chicago
Shanks	James D.	AWE plc Aldermaston
Siebenborn	Martin	Universtität Trier
Soler	Johnny Ramc	Universtiät Stuttgart
Stepniewski	Martin	Goethe-Universität Frankfurt
Takacs	Stefan	Johann Radon Institute for Computational and Applied Mathematics (RICAM)
Tan	Guangming	Institute of Computing Technology Chinese Academy of Sciences
Van Barel	Andreas	KU Leuven

van Rienen	Ursula	Rostock University
Vogel	Andreas	Goethe-Universität Frankfurt
Wagner	Christian	The Boston Consulting Group GmbH
Wan	Justin	University of Waterloo
Wheeler	Mary	The University of Texas at Austin
Wieners	Christian	Karlsruhe Institute of Technology KIT
Wittum	Gabriel	Goethe-Universität Frankfurt ECRC, KAUST
Xu	Jinchao	The Pennsylvania State University
Xu	Xiaowen	Institute of Applied Physics and Computational Mathematics, CAS
Xu	Ran	Institute of Applied Physics and Computational Mathematics, CAS
Xylouris	Kosta	Goethe-Universität Frankfurt
Yserentant	Harry	Technische Universität Berlin
Zank	Marco	TU Graz
Zhang	Hongxuan	Penn State University
Zhang	Aiqing	Institute of Applied Physics and Computational Mathematics, CAS
Zulehner	Walter	Johannes Kepler University Linz