The International Multigrid Conference

IMG 2019

Aug 11–16, 2019 in Kunming, China

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http://www.multigrid.org/img2019/

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August 11-16, 2019, Kunming, China

Howard Johnson City of Flower Hotel Kunming

Topics

1. Multigrid Methods
2. Algebraic Multigrid Methods
3. Multilevel and Multigraph Methods
4. Multiscale Methods
5. Domain Decomposition Methods
6. Parallel and High-Performance Computing
7. Deep Neural Networks, Machine Learning
8. Computing Software and Tools

Invited Speakers

Randolph E. Bank, La Jolla
Zhiming Chen, Beijing
Martin Gander, Geneva
Lars Grasedyck, Aachen
Andreas Vogel, Bochum
Xiaowen Xu, Beijing
Harry Yserentant, Tübingen
Ludmil Zikatanov, University Park

Scientific Committee

Alfio Grillo, Torino
Rolf Krause, Lugano
Zeyao Mo, Beijing
Arne Nägel, Frankfurt
Gillian Queisser, Philadelphia
Arnold Reusken, Aachen
Volker Schulz, Trier
Gabriel Wittum, KAUST (Chair)
Jinchao Xu, University Park
Ulrike Meier Yang, Livermore

Organizing Committee

Hengbin An, Beijing
Long Chen, Irvine
Jun Hu, Beijing
Zeyao Mo, Beijing (Chair)
Lei Shi, Kunming
Hanquan Wang, Kunming
Gabriel Wittum, KAUST
Jinchao Xu, University Park
Chensong Zhang, Beijing (Co-Chair)

Sponsors

Yunnan University of Finance and Economics
Institute of Computational Physics and Applied Mathematics
School of Mathematical Sciences, Peking University
State Key Laboratory of Scientific and Engineering Computing

Local Organizer

Co-Innovation Research Center for
Scientific Computing and Data Mining in Yunan

Contacts

Email: img@multigrid.org

Contents

About

Welcome to the International Multigrid Conference (IMG), August 11-16, 2019 in Kunming, China. The IMG 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), Leuven (2014), and Bruchsal (2016).

Topics

1. Multigrid and Algebraic Multigrid Methods
2. Multilevel and Multigraph Methods
3. Multiscale Methods
4. Domain Decomposition Methods
5. Parallel and High-Performance Computing
6. Deep Neural Networks, Machine Learning
7. Computing Software and Tools

Scientific Committee

Alfio Grillo	Torino
Rolf Krause	Lugano
Zeyao Mo	Beijing
Arne Nägel	Frankfurt
Gillian Queisser	Philadelphia
Arnold Reusken	Aachen
Volker Schulz	Trier
Gabriel Wittum	KAUST (Chair)
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Organizing Committee

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Long Chen	Irvine
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Lei Shi	Kunming
Hanquan Wang	Kunming
Gabriel Wittum	KAUST
Jinchao Xu	University Park
Chensong Zhang	Beijing (Co-Chair)
Weifeng Zhang	Kunming

Timetable

Program At A Glance

Aug 11–12 Check-in and on-site registration

Aug 11–12 Short courses on *Multigrid and Deep Neural Network*

Aug 12 Conference reception

Aug 12–15 Plenary talks, MS sessions and contributed talks

Aug 15 Conference banquet

Aug 16 Embedded Workshop: Solver2019

Aug 17 Conference adjourn

8.11	8.12	8.13	8.14	8.15	8.16
Registration	Jinchao Xu	**Ludmil Zikatanov**	**Harry Yserentant**	**Martin Gander**	Embedded Workshop
Ludmil Zikatanov		**Andreas Vogel**	**Xiaowen Xu**	**Lars Grasedyck**	
		MS09 MS06	MS18 MS10	MS19 MS14	
		MS07 MS16	MS01 MS16	MS05 MS20	
Lunch Break					
Zhanxing Zhu	Opening	MS09 MS08	MS18 MS04	MS19 MS14	Social Event
	Zhiming Chen	MS02 MS21	MS01 MS03	MS13 MS11	
	MS17 MS06	MS09 CT MS08	MS18 MS04	MS14 MS13 MS11	
	MS15 MS12	MS02 MS21	MS05 MS03	**Randolph Bank**	
	Reception			Banquet	

PT Plenary Talk

SC Short Course

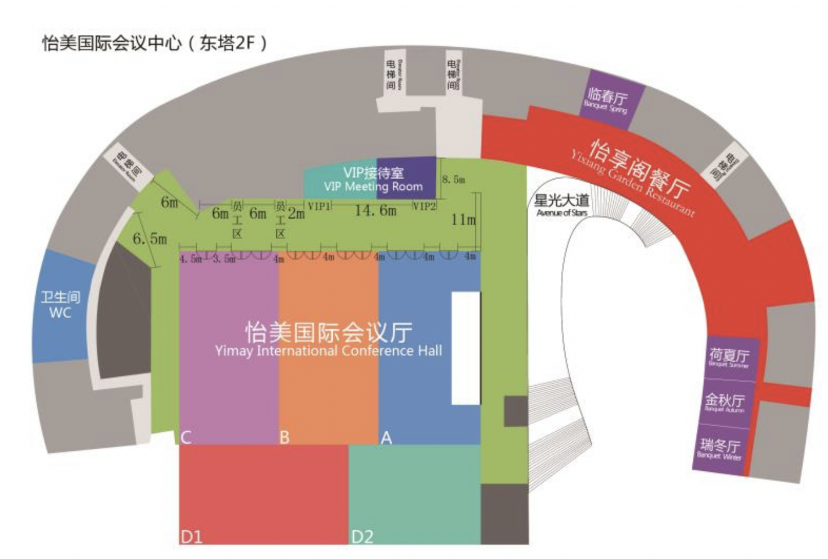
EM Embedded Workshop

MS Minisymposium

CT Contributed Talk

List of Minisymposium

Conference Rooms



RM1 Conference Hall C (2nd Floor)

RM2 Xiuxian Meeting Room (3rd Floor)

RM3 Zhihui Meeting Room (3rd Floor)

RM4 Yongjue Meeting Room (3rd Floor)

Please see directions at the conference venue.

11 of August, Sunday

8:00–9:30	**Registration (open all day)**			
9:30–10:30	SC	**Zikatanov, Ludmil** Penn State Univ, USA	An Introduction to GMG and AMG, Lecture 1	RM2
10:30–11:00	**Coffee Break, 3rd Floor**			
11:00–12:00	SC	**Zikatanov, Ludmil** Penn State Univ, USA	An Introduction to GMG and AMG, Lecture 2	RM2
12:00–14:00	**Lunch Break**			
14:00–15:30	SC	**Zhu, Zhanxing** Peking Univ, China	Introduction to Convolutional Neural Networks, Lecture 1	RM2
15:30–16:00	**Coffee Break**			
16:00–17:30	SC	**Zhu, Zhanxing** Peking Univ, China	Introduction to Convolutional Neural Networks, Lecture 2	RM2

12 of August, Monday

8:00–8:30	**Registration (open all day)**			
8:30–10:00	SC	**Xu, Jinchao** Penn State Univ, USA	An Integrated Introduction to Multigrid and Deep Learning, Lecture 1	RM2
10:00–10:30	**Coffee Break, 3rd Floor**			
10:30–12:00	SC	**Xu, Jinchao** Penn State Univ, USA	An Integrated Introduction to Multigrid and Deep Learning, Lecture 2	RM2
12:00–14:00	**Lunch Break**			
14:00–14:20	**Opening Remarks, Chair: Jinchao Xu**			
Plenary Talk	**Chair: Jinchao Xu**			
14:20–15:10	PT	**Chen, Zhiming** AMSS, Beijing, China	An adaptive high-order unfitted finite element method for elliptic interface problems	RM1
15:10–15:45	**Coffee Break, 2nd Floor**			
MS17	**Chair: Xiaozhe Hu**			
15:45–16:10	MS	**Mardal, Kent-Andre** University of Oslo, Norway	Preconditioners for multi-physics and multi-scale problems	RM1
16:10–16:35	MS	**Zhang, Shuo** LSEC & NCMIS, AMSS, CAS	Multigrid method for fourth order eigenvalue problem	RM1
16:35–17:00	MS	**Huang, Xuehai** Shanghai University of Finance and Economics	Multigrid Methods for Hellan-Herrmann-Johnson Mixed Method of Kirchhoff Plate Bending Problems	RM1
17:00–17:25	MS	**Wei, Huayi** Xiangtan University	Recovery-type a posteriori error estimation for adaptive virtual element method	RM1
17:25–17:50	MS	**He, Juncai** Peking University and Penn State	Finite Elements and ReLU Deep Neural Networks (DNNs)	RM1
MS06, Part 1	**Chair: Xiaoying Dai**			
15:45–16:10	MS	**Wu, Xinming** Fudan University	A Multilevel Correction Method for Interior Transmission Eigenvalue Problem	RM2

16:10–16:35	MS	**Xu, Fei** Beijing Institute for Scientific and Engineering Computing, Beijing University of Technology	A Type of Parallel Augmented Subspace Method for Eigenvalue Problems	RM2
16:35–17:00	MS	**Bi, Hai** School of Mathematical Sciences, Guizhou Normal University	Local and parallel finite element algorithms for fourth-order differential operator eigenvalue problems	RM2
17:00–17:25	MS	**Liu, Fang** Central University of Finance and Economics, China	Two-scale finite element approximations for semilinear parabolic equations	RM2
MS15		**Chair: Hanquan Wang**		
15:45–16:10	MS	**Wang, Hanquan** Yunnan University of Finance and Economics	An adaptive level set method based on two-level uniform meshes and its application to dislocation dynamics	RM3
16:10–16:35	MS	**Wu, Xinming** Fudan University	Error Estimates of the Finite Element Method for Interior Transmission Problem and Interior Transmission Eigenvalue Problem	RM3
16:35–17:00	MS	**Xie, Manting** Tianjin University	Adaptive Multigrid Methods for the Ground State Solution of Bose-Einstein Condensates	RM3
17:00–17:25	MS	**Wang, Jun** Flatiron Institute	Fast boundary integral solvers for Stokes flows: quadrature, periodization and adaptivity	RM3
17:25–17:50	MS	**Jiang, Chaolong** Yunnan University of Finance and Economics	Linearly implicit structure-preserving exponential integrators for the nonlinear Klein-Gordon equations	RM3
MS12		**Chair: Guangming Tan**		
15:45–16:10	MS	**Nakajima, Kengo** Information Technology Center, The University of Tokyo	Parallel Multigrid with Adaptive Multilevel hCGA on Manycore Clusters	RM4
16:10–16:35	MS	**Li, Shishun** Henan Polytechnic University, China	Highly parallel space-time domain decomposition methods for parabolic problems	RM4

16:35–17:00	MS	**He, Xin** Institute of Computing Technology, Chinese Academy of Sciences	Efficient and scalable solvers for linear systems arising from Computational Fluid Dynamics on CPU+GPU Clusters	RM4
17:00–17:25	MS	**Zhang, Peng** CAEP Software Center for High Performance Numerical Simulation	Performance Optimization Study of Several HPC Codes: Experience and Generalization	RM4
19:00–21:00	**Reception**			

13 of August, Tuesday

Plenary Talks	**Chair: Zeyao Mo**			
8:30–9:20	PT	**Zikatanov, Ludmil** Penn State Univ, State College, USA	Geometric, Algebraic, and Abstract MultiGrid Methods	RM1
9:20–10:10	PT	**Vogel, Andreas** Ruhr University Bochum	Parallel and adaptive geometric multigrid in UG4	RM1
10:10–10:20	**Group Photo**			
10:20–10:30	**Coffee Break, 3rd Floor**			
MS09, Part 1	**Chair: Zhiming Chen**			
10:30–10:55	MS	**Lu, Ya Yan** Department of Mathematics, City University of Hong Kong	Vertical mode expansion method for applications in photonics	RM1
10:55–11:20	MS	**Chen, Junqing** Department of Mathematics, Tsinghua University	An inverse eddy current problem and its finite element approximation	RM1
11:20–11:45	MS	**Chen, Yongpin** University of Electronic Science and Technology of China	Domain Decomposition Method for the Efficient Analysis of Multiscale Electromagnetic Scattering	RM1
11:45–12:05	MS	**Cui, Tao** LSEC & NCMIS, AMSS, CAS	Parallel 3-D Adaptive Finite Element Method and its Application on EDA tools	RM1

MS06, Part 2		**Chair: Hehu Xie**		
10:30–10:55	MS	**Hu, Xiaozhe** Tufts University	Spectral Graph Distance for Biological Networks	RM2
10:55–11:20	MS	**Duan, Huoyuan** Wuhan University, China	New Mixed Elements for Maxwell Equations	RM2
11:20–11:45	MS	**Dai, Xiaoying** LSEC & NCMIS, AMSS, CAS	Convergence and optimal complexity of the adaptive Fourier-Galerkin method for eigenvalue problems	RM2
MS 07		**Chair: Ulrike Meier Yang**		
10:30–10:55	MS	**Yang, Ulrike Meier** Lawrence Livermore National Laboratory	Designing a semi-structured algebraic multigrid solver	RM3
10:55–11:20	MS	**Mitchell, Wayne** Universitaet Heidelberg	Parallel Performance of Algebraic Multigrid Domain Decomposition (AMG-DD)	RM3
11:20–11:45	MS	**Wolfson-Pou, Jordi** Georgia Institute of Technology, U.S.	Asynchronous Multigrid Methods	RM3
11:45–12:10	CT	**Jodlbauer, Daniel** RICAM, Linz, Austria	Parallel Matrix-Free Multigrid Applied to Phase-Field Fracture Problems	RM3
MS16, Part 1		**Chair: Gabriel Wittum**		
10:30–10:55	MS	**Höllbacher, Susanne** AMCS, KAUST	Gradient-consistent finite element spaces for problems with immersed interfaces	RM4
10:55–11:20	MS	**Larisch Lukas** AMCS, KAUST and G-CSC Frankfurt	3D Modeling and Simulation of a Harpsichord	RM4
11:20–11:45	MS	**Kühn, Arlene** G-CSC Frankfurt University	Simulation of flow in a forward osmosis membrane device from a desalination plant	RM4
11:45–12:10	MS	**Wang, Junxi** G-CSC, Frankfurt University	UG4 Application in Skin Problem: Homogenized modeling of Microscopic Anisotropic Diffusion for Effective Diffusivities in Stratum Corneum	RM4
12:15–14:00	**Lunch Break**			
MS09, Part 2		**Chair: Weiying Zheng**		

14:00–14:25	MS	**Jiang, Xue** Beijing University of Technology	Cartesian PML method for Maxwell's equations in a two-layer medium	RM1
14:25–14:50	MS	**Lai, Jun** Zhejiang University	A fast algorithm for electromagnetic scattering from axis-symmetric objects	RM1
14:50–15:15	MS	**Li, Buyang** Department of Applied Mathematics, The Hong Kong Polytechnic University	Optimal control in a bounded domain for wave propagating in the whole space: coupled through boundary integral equations	RM1
15:15–15:40	MS	**Lu, Wangtao** Zhejiang University	Error Analysis of the UPML-method for analyzing Helmholtz equation in a layered medium with a compact source	RM1
MS08, Part 1		**Chair: Xiaoping Xie**		
14:00–14:25	MS	**Wei, Huayi** Xiangtan University	An adaptive virtual element method for the self-consistent field theory on general domains	RM2
14:25–14:50	MS	**Huang, Xuehai** Shanghai University of Finance and Economics	Nonconforming Virtual Element Method for $2m$-th Order Partial Differential Equations in $\mathbb{R}^n$ with $m \geq n$	RM2
14:50–15:15	MS	**Chen, Gang** College of Mathematics, Sichuan University	An HDG Method for Dirichlet Boundary Control of Convection Dominated Diffusion PDES	RM2
15:15–15:40	MS	**Chen, Long** University of California at Irvine	Bridging Virtual Element Methods and Immersed Finite Element Methods for Interface Problems	RM2
MS02, Part 1		**Chair: Hengbin An**		
14:00–14:25	MS	**He, Xin** Institute of Computing Technology, Chinese Academy of Sciences	The adapted augmented Lagrangian preconditioner for the turbulent incompressible Navier-Stokes equations discretized by a finite volume method	RM3
14:25–14:50	MS	**Jing, Yan-Fei** University of Electronic Science and Technology of China	Promising strategies for accelerating the Scheduled Relaxation Jacobi method	RM3

14:50–15:15	MS	**Xie, Hehu** LSEC & NCMIS, AMSS, CAS	A Multigrid Method for Semilinear Problems	RM3
MS21, Part 1		**Chair: Jun Hu**		
14:00–14:25	MS	**Wu, Haijun** Nanjing University, China	A Pure Source Transfer Domain Decomposition Method for Helmholtz Equations in Unbounded Domain	RM4
14:25–14:50	MS	**Chen, Long** University of California at Irvine, USA	From differential equation solvers to optimization methods	RM4
14:50–15:15	MS	**Huang, Jianguo** Shanghai Jiao Tong University, China	Two-level Arrow-Hurwicz methods for steady incompressible Navier-Stokes equations	RM4
15:15–15:40	MS	**Huang, Xuehai** Shanghai University of Finance and Economics, China	A nonoverlapping DDM for general elastic body-plate problems discretized by the P1-NZT FEM	RM4
15:40–16:00	**Coffee Break, 2nd Floor & 3rd Floor**			
MS09, Part 3		**Chair: Chunxiong Zheng**		
16:00–16:25	MS	**Wu, Haijun** Nanjing University	An Unfitted Interface Penalty Finite Element Method for Elliptic Interface Problems	RM1
16:25–16:50	MS	**Wu, Yumao** Fudan University	The efficient algorithm for electromagnetic scattering by the electrically large and mutiscale scatterers	RM1
16:50–17:15	MS	**Zheng, Weiying** Academy of Mathematics and Systems Science, Chinese Academy of Sciences	Multigrid method for inductionless MHD equations	RM1
Contributed Talk		**Chair: Weiying Zheng**		
17:20–18:00	CT	**Joachim Heinze** Springer, Verlag	How the Web, Open Access and Artificial Intelligence are changing the Exchange of Scientific Information	RM1
MS08, Part 2		**Chair: Xuehai Huang**		

16:00–16:25	MS	**Wang, Fei** Xi'an Jiaotong University	Virtual Element Methods for Variational and Hemivariational Inequalities	RM2
16:25–16:50	MS	**Wu, Yongke** University of Electronic Science and Technology of China	Energy-preserving mixed finite element methods for the elastic wave equation	RM2
16:50–17:15	MS	**Huang, Jianguo** Shanghai Jiao Tong University	Virtual element methods for elliptic variational inequalities of the second kind	RM2
17:15–17:40	MS	**Xie, Xiaoping** SCU, China	A locking-free hybridizable discontinuous Galerkin method for linear elasticity with strong symmetric stress and continuous displacement trace approximation	RM2
MS02, Part 2		**Chair: Hehu Xie**		
16:00–16:25	MS	**An, Hengbin** Inst. of Appl. Phys. and Comp. Math. & CAEP	Preconditioning for thermo-mechanical-contact coupled applications	RM3
16:25–16:50	MS	**Yue, Xiaoqiang** Xiangtan University, China	Several multilevel iterative algorithms for multi-group radiation diffusion equations	RM3
16:50–17:15	MS	**Zhu, Shengxin** Xi'an Jiaotong Liverpool University, China	Acceleration for heterogeneous high throughput data analysis	RM3
17:15–17:40	MS	**Yue, Meiling** Beijing Technology and Business University	A Multigrid Method for the Ground State Solution of Bose-Einstein Condensates Based on Newton Iteration	RM3
MS21, Part 2		**Chair: Shuonan Wu**		
16:00–16:25	MS	**Ma, Suna** Peking University, China	Efficient Spectral Methods for Some Singular Eigenvalue Problems	RM4
16:25–16:50	MS	**Wang, Hua** Peking University, China	Anisotropic Finite Element Methods for Interface Problems	RM4
16:50–17:15	CT	**Schwalsberger, Martin** JKU Linz	A parallel space-time multigrid method for the Eddy-Current equation	RM4

14 of August, Wednesday

Plenary Talks		**Chair: Ulrike Meier Yang**		
8:30–9:20	PT	**Yserentant, Harry** Technische Universität Berlin	On the expansion of solutions of Laplace-like equations into traces of separable higher dimensional functions	RM1
9:20–10:10	PT	**Xu, Xiaowen** Inst. of Appl. Phys. and Comp. Math.	The efficiency issues of AMG solver for large-scale realistic simulations	RM1
10:10–10:30	**Coffee Break, 2nd Floor**			
MS18, Part 1		**Chair: Yingzhou Li**		
10:30–10:55	MS	**Li, Xiaoye S.** Lawrence Berkeley National Laboratory	Optimal complexity direct solver for Kernel Ridge Regression	RM1
10:55–11:20	MS	**Yang, Chao** Lawrence Berkeley National Laboratory	A Greedy Algorithm for Solving Large-scale Eigenvalue Problem	RM1
11:20–11:45	MS	**Gao, Weiguo** Fudan University	Alternating Semidefinite Programing for Block Bi-clustering	RM1
11:45–12:10	MS	**Chen, Wenguang** Tsinghua University	Bridge the Gap between Neural Networks and Neuromorphic Hardware with a Neural Network Compiler	RM1
MS10		**Chair: Liuqiang Zhong**		
10:30–10:55	MS	**Cui, Jintao** The Hong Kong Polytechnic University	A two-grid finite difference algorithm for compressible Darcy-Forchheimer model in porous media	RM2
10:55–11:20	MS	**Hu, Xianliang** School of Mathematical Sciences, Zhejiang University	A multi-mesh phase-field approach for optimal shape design of incompressible flows	RM2
11:20–11:45	MS	**Xie, Manting** Tianjin University	A Cascadic Multigrid Method for Nonsymmetric Eigenvalue Problem	RM2

11:45–12:10	MS	**Zheng, Haibiao** School of Mathematical Sciences, East China Normal University	Local and parallel finite element algorithm based on the partition of unity for incompressible flows	RM2
MS01, Part 1		**Chair: Martin Gander**		
10:30–10:55	MS	**Ciaramella, Gabriele** University of Konstanz	Substructured two-level and multi-level domain decomposition methods	RM3
10:55–11:20	MS	**Kwok, Felix** Department of Mathematics, Hong Kong Baptist University	Optimized Schwarz-based nonlinear preconditioning for elliptic PDEs	RM3
11:20–11:45	MS	**Leng, Wei** LSEC & NCMIS, AMSS, CAS	An Additive Overlapping Domain Decomposition Method for the Helmholtz Equation	RM3
11:45–12:10	MS	**Martin, Gander** University of Geneva, Switzerland	Diagonalization-Based Parareal and Waveform Relaxation Algorithms	RM3
MS16, Part 2		**Chair: Andreas Vogel**		
10:30–10:55	MS	**Nägel, Arne** G-CSC Frankfurt	Efficient solution of transient non-linear flow problems in the subsurface	RM4
10:55–11:20	MS	**Logashenko, Dmitry** King Abdullah University of Science and Technology	Simulation of propagation of uncertainties in density-driven groundwater flow	RM4
11:20–11:45	MS	**Yahyaei, Saberi** Ruhr University Bochum, Germany	Multigrid Solvers for the Finite Cell Method	RM4
11:45–12:10	MS	**Junker, Philipp** Ruhr University Bochum	Adaptive mesh refinement and geometric multigrid for brittle damage simulations	RM4
12:15–14:00		**Lunch Break**		
MS18, Part 2		**Chair: Tao Cui**		
14:00–14:25	MS	**Li, Yingzhou** Duke University	Approximate Tensor Ring Decomposition	RM1
14:25–14:50	MS	**Fan, Yuwei** Stanford University	Multiscale Neural Network for PDEs	RM1
MS04, Part 1		**Chair: Jingrun Chen**		
14:00–14:25	MS	**Chen, Jingrun** Suzhou University	Second-order semi-implicit methods for Landau-Lifschitz equation	RM2

14:25–14:50	MS	**Chen, Huangxin** Xiamen University	Physics-preserving algorithms for flow and transport in porous media	RM2
14:50–15:15	MS	**Chen, Rongliang** Shenzhen Institutes of Advanced Technology, CAS	Parallel Domain Decomposition Preconditioners for Large-scale Patient-specific Blood Flow Simulations	RM2
15:15–15:40	MS	**Han, Fei** Dalian University of Technology	A hybrid local/nonlocal continuum mechanics modeling for fracture simulation	RM2
MS01, Part 2		**Chair: Gabriele Ciaramella**		
14:00–14:25	MS	**Halpern, Laurence** Université Paris 13	Optimized Schwarz methods for complex elliptic problems	RM3
14:25–14:50	MS	**Zhang, Hui** Zhejiang Ocean University	Optimized Schwarz method for the convection-diffusion problem with an interface	RM3
14:50–15:15	MS	**Ciaramella, Gabriele** University of Konstanz	Analysis of the parallel Schwarz method for growing chains of fixed-sized subdomains	RM3
15:15–15:40	MS	**Chen, Long** University of California at Irvine	Randomized method of subspace corrections with machine learning	RM3
MS03, Part 1		**Chair: Shuo Zhang**		
14:00–14:25	MS	**Xie, Hehu** AMSS, CAS	Fast eigenpairs computation with operator adapted wavelets and hierarchal subspace correction	RM4
14:25–14:50	MS	**Ma, Dingjiong** The University of Hong Kong	A multiscale finite element method for the Schrödinger equation with multiscale potentials	RM4
14:50–15:15	MS	**Zheng, Hui** Huazhong University of Science and Technology, Wuhan, China	Multiscale simulation method for the elastic wave equation and Biot equation	RM4
15:40–16:00		**Coffee Break, 2nd Floor & 3rd Floor**		
MS18, Part 3		**Chair: Yuwei Fan**		
16:00–16:25	MS	**Wang, Han** Inst. of Appl. Phys. and Comp. Math.	Deep Learning for Multiscale Molecular Modelling	RM1

16:25–16:50	MS	**Chen, Wei** Beihang University, Beijing, China	IMRank: Influence Maximization via Finding Self-Consistent Ranking	RM1
16:50–17:15	MS	**Guo, Ling** Shanghai Normal University	Quantifying total uncertainty in physics-informed neural networks for solving forward and inverse stochastic problems	RM1
17:15–17:40	MS	**Li, Lei** Shanghai Jiaotong University	Random Batch Method and its applications	RM1
MS04, Part 2		**Chair: Fei Han**		
16:00–16:25	MS	**Wang, Hao** Sichuan University	A Simplified a Posteriori Error Estimation for a Consistent Atomistic-to-continuum Coupling Method in 2D	RM2
16:25–16:50	MS	**Yang, Zihao** Northwestern Polytechnical University	Stochastic multiscale heat transfer analysis of heterogeneous materials with multiple random configurations	RM2
16:50–17:15	CT	**Oberhuber, Tomas** Czech Technical University in Prague	Template numerical library for modern parallel architectures	RM2
MS05, Part 1		**Chair: Mingchao Cai**		
16:00–16:25	MS	**Mu, Mo** Hong Kong University of Science and Technology	Decoupling Multi-physics Computation with Intrinsic Robin Condition	RM3
16:25–16:50	MS	**Chen, Jinru** Nanjing Normal University, China	Nonconforming Nitsche's Extended Finite Element Methods for Interface Problems	RM3
16:50–17:15	MS	**Wang, Feng** School of Mathematical Sciences, Nanjing Normal University	On a weak virtual element element method for the poroelasticity problem	RM3
17:15–17:40	MS	**Wang, Shufen** Fudan University	Numerical simulations and analysis for epitaxial thin film models	RM3
MS03, Part 2		**Chair: Shuo Zhang**		
16:00–16:25	MS	**Jiang, Lijian** Tongji University	A model reduction for nonlinear multiscale parabolic problems	RM4

16:25–16:50	MS	**Wang, Yaohong** Tianjin University	Brownian motion of a nano-ellipsoid in a cylindrical vessel flow	RM4
16:50–17:15	MS	**Chen, Jingrun** Suzhou University	An efficient multigrid strategy for large-scale molecular mechanics optimization	RM4
17:15–17:40	CT	**Rong, Yao** Harbin Institute of Technology, Shenzhen	Grad-div stabilization method for magnetohydrodynamic flows at low magnetic Reynolds numbers	RM4
19:00–21:00	**Scientific Committee Meeting**			

15 of August, Thursday

Plenary Talks	**Chair: Rolf Krause**			
8:30–9:20	PT	**Gander, Martin** Université de Genève	Multigrid and Domain Decomposition: Similarities and Differences	RM1
9:20–10:10	PT	**Grasedyck, Lars** RWTH Aachen University	Distributed HT-Tensor Multigrid	RM1
10:10–10:30	**Coffee Break, 2nd Floor**			
MS19, Part 1	**Chair: Juncai He**			
10:30–10:55	MS	**Zhang, Shijun** National University of Singapore	Deep Network Approximation Characterized by Number of Neurons	RM1
10:55–11:20	MS	**Dong, Bin** Beijing International Center for Mathematical Research Peking University	Learning and Learning to Solve PDEs	RM1
11:20–11:45	MS	**Lin, Rongrong** Sun Yat-sen University	Machine Learning in Reproducing Kernel Banach Spaces	RM1
11:45–12:10	MS	**Li, Yingzhou** Duke University	Variational training of neural network approximations of solution maps for physical models	RM1

MS14, Part 1		Chair: Chensong Zhang		
10:30–10:55	MS	**Sheen, Dongwoo** Seoul National University, Korea	Comments on Beavers-Joseph-Saffman conditions on the Brinkman-Stokes-Darcy Interface Problems	RM2
10:55–11:20	MS	**Lee, Youngju** Texas State University, USA	Locally conservative finite elements for axisymmetric Stokes equation	RM2
11:20–11:45	MS	**Jeon, Youngmok** Ajou University	The immersed hybrid difference method for elliptic interface problems	RM2
11:45–12:10	MS	**Zhang, Chen-Song** LSEC & NCMIS, AMSS, CAS	Numerical Methods for Problems with Moving Interfaces	RM2
MS05, Part 2		**Chair: Mo Mu**		
10:30–10:55	MS	**Razzaqa, Mudassar** Lahore University of Management Sciences, Pakistan	Numerical study of flow across an ellipse and a circle placed in a uniform stream of infinite extent	RM3
10:55–11:20	MS	**Huang, Jian** Xiangtan University, China	Multigrid Methods for a Mixed Finite Element Method of the Darcy–Forchheimer Model	RM3
11:20–11:45	MS	**Qin, Fangfang** Nanjing University of Posts and Telecommunications, China	A Cartesian grid nonconforming immersed finite element method for planar elasticity interface problems	RM3
11:45–12:10	MS	**Cai, Mingchao** Department of Mathematics, Morgan State University	Some Algorithms for Biot Model with Applications in Brain Swelling Simulation	RM3
MS20		**Chair: Gillian Queisser**		
10:30–10:55	MS	**Queisser, Gillian** Temple University	A smooth subdivision multigrid method	RM4
10:55–11:20	MS	**Krause, Rolf** Institute of Computational Science, Switzerland	Multilevel strategies for non-standard contact formulations	RM4

11:20–11:45	MS	**Trotti, Ken** University of Insubria, University of Italian Switzerland	Anisotropic multigrid preconditioners for space-fractional diffusion equations	RM4
12:15–14:00	**Lunch Break**			
MS19, Part 2	**Chair: Bin Dong**			
14:00–14:25	MS	**He, Juncai & Xu, Jinchao** Penn State University, USA	MgNet: A Unified Framework of Multigrid and Convolutional Neural Networks	RM1
14:25–14:50	MS	**Zhang, Lian** Penn State University, USA	Make ℓ_1 Regularization Effective in Training Sparse CNN	RM1
14:50–15:15	MS	**Chen, Yuyan** Peking University	Linear data-feature mapping in different grids in classical CNN models	RM1
15:15–15:40	MS	**Siegel, Jonathan** Penn State University	Sparse Training Algorithms for Neural Networks	RM1
MS14, Part 2	**Chair: Dongwoo Sheen**			
14:00–14:25	MS	**Lu, Benzhuo** Chinese Academy of Sciences	Adaptive grid in Modeling of Biomolecular Electrostatics and Diffusion using FEM/BEM	RM2
14:25–14:50	MS	**Hoang, Viet Ha** Nanyang Technological University, Singapore	High dimensional finite elements for multiscale Maxwell wave equations	RM2
14:50–15:15	MS	**Moon, Minam** Korea Military Academy, Koera	Multiscale Hybridizable Discontinuous Galerkin method for porous media flow	RM2
15:15–15:40	MS	**Cho, Kanghun** Seoul National University	Algebraic multiscale methods	RM2
MS13, Part 1	**Chair: Yajuan Sun**			
14:00–14:25	MS	**Wu, Yongke** University of Electronic Science and Technology of China	Energy-preserving mixed finite element methods for the Hodge wave equation	RM3
14:25–14:50	MS	**Hu, Kaibo** University of Minnesota	Finite elements for curvature	RM3
14:50–15:15	MS	**Qiu, Weifeng** City University of Hong Kong	Convergence of a B-E based finite element method for MHD models on Lipschitz domains	RM3

15:15–15:40	MS	**Lee, Youngju** Texas State University	Helicity conservative finite element discretizations	RM3
MS11, Part 1		**Chair: Chang-Ock Lee**		
14:00–14:25	MS	**Park, Eun-Hee** Kangwon National University	A non-overlapping DD method for heterogeneous elliptic problems	RM4
14:25–14:50	MS	**Kim, Seungil** Kyung Hee University	Convergence analysis of a double sweep preconditioner for solving the Helmholtz equation in waveguide	RM4
14:50–15:15	MS	**Kim, Hyea Hyun** Kyung Hee University	An adaptive BDDC algorithm for three dimensional elliptic problems with an enhanced edge eigenvalue problem	RM4
15:40–16:00	**Coffee Break, 2nd Floor**			
MS13, Part 2		**Chair: Kaibo Hu**		
16:00–16:25	MS	**Sun, Yajuan** LSEC & NCMIS, AMSS, CAS	Construction of contact numerical methods and implementation in Fokker-Planck system	RM3
16:25–16:50	MS	**Wu, Shuonan** Peking University	On the robust discretization and fast solver for the H(curl) and H(div) convection-diffusion problems	RM3
MS11, Part 2		**Chair: Hyea Hyun Kim**		
16:00–16:25	MS	**Lee Chang-Ock** KAIST	Fast Nonoverlapping Block Jacobi Method for the Dual Rudin-Osher-Fatemi Model	RM4
16:25–16:50	MS	**Xie, Manting** Tianjing University	A fast multilevel algorithm for total variation minimization problems	RM4
Plenary Talks		**Chair: Gabriel Wittum**		
17:00–17:50	PT	**Bank, Randolph E.** UC San Diego, USA	A Semi-Algebraic 2-Level Solver	RM1
17:50–18:00	**Closing Remarks, Chair: Gabriel Wittum**			
19:15–21:00	**Conference Banquet, RM1**			

16 of August, Friday

08:30–08:40	**Opening Remarks**			
Solver2019	**Chair: Shi Shu**			
08:40–09:00	EM	**Li, Yingzhou** Duke University, USA	Distributed-Memory Hierarchical Matrix Algebra	RM4
09:00–09:20	EM	**Li, Shengguo** National University of Defense Technology, China	Challenge and opportunities for some rank-structured algorithm and eigen-solvers on exascale supercomputers	RM4
09:20–09:40	EM	**Zhang, Hui** Zhejiang Ocean University, China	Domain Decomposition Methods for the Helmholtz Equation: A Review	RM4
09:40–10:00	EM	**Hu, Shaoliang** CAEP Software Center for High Performance Numerical Simulation	Numerical algorithms for time-harmonic Maxwell equation arising from integrated microelectronics system	RM4
10:00–10:20	**Workshop Group Photo and Coffee Break, 3rd Floor**			
Solver2019	**Chair: Xiaowen Xu**			
10:20–10:40	EM	**Yue, Xiaoqiang** Xiangtan University, China	Convergence analysis and HPC results of the Parareal and MGRIT algorithms for time dependent problems	RM4
10:40–11:00	EM	**Wang, Yinshan** Institute of Computing Technology, CAS	Performance Optimization of the HPCG Benchmark on the SUGON 7000 supercomputer	RM4
11:00–11:20	EM	**Li, Shishun** Henan Polytechnic University, China	Some space-time Schwarz algorithms for solving parabolic problems	RM4
11:20–12:00	EM	**Xu, Xiaowen** Inst. of Appl. Phys. and Comp. Math.	Discussion	RM4
12:00–14:00	**Lunch**			

List of Abstracts

Short courses, Aug 11th–Aug 12th

An Introduction to GMG and AMG

Zikatanov, Ludmil

SC

Penn State University, State College, PA, USA

Multigrid methods (MGs) is a name used for a suite of advanced techniques for the solution of linear systems. We will introduce the basic components of geometric multigrid methods (GMGs) and algebraic multigrid methods (AMGs) such as smoothing via iterative methods, coarsening using adjacency graphs and the combination of these tools which give rise to several well known methods. We will also present some of the adaptive AMG techniques which construct iteratively better and better coarse spaces.

Introduction to Convolutional Neural Networks

Zhu, Zhanxing

SC

Peking University, Beijing, China

In this short tutorial, I will provide a comprehensive introduction to the convolutional neural networks (CNNs). CNNs are the most successful deep learning architectures and have been wildly used in many AI tasks and scientific domains. I will introduce (1) the basic components of CNNs, (2) popular architectures, including LeNet, AlexNet, ResNet, etc, (3) applications of CNNs in various tasks, (4) visualization of CNNs, (5) instability of CNN and (6) some regularization strategies. The tutorial requires some basic mathematical background and assumes no prior knowledge of machine learning or deep learning.

An Integrated Introduction to Multigrid and Deep Learning

Xu, Jinchao

SC

Penn State University, State College, PA, USA

In this short course, an integrated introduction will be given to both multigrid methods and machine learning based on deep neural networks. The presentation will be elementary as it assumes little prior knowledge on both subjects and yet advanced as it will quickly reach to core issues in the relevant algorithm/model formulation, mathematical understanding and practical applications. Practice problems will be given to both theoretical analysis and practical applications that uses iFEM (for multigrid) and TensorFlow or Pytorch (for Deep Learning).

Plenary Talks

An adaptive high-order unfitted finite element method for elliptic interface problems

Chen, Zhiming PT

LSEC & NCMIS, Academy of Mathematics and Systems Sciences, CAS

We design an adaptive unfitted finite element method on the Cartesian mesh with hanging nodes. We derive an hp-reliable and efficient residual type a posteriori error estimate on K-meshes. A key ingredient is a novel hp - domain inverse estimate which allows us to prove the stability of the finite element method under practical interface resolving mesh conditions and also prove the lower bound of the a posteriori error estimate. Numerical examples are included. This talk is based on a joint work with Ke Li and Xueshuang Xiang.

Geometric, Algebraic, and Abstract MultiGrid Methods

Zikatanov, Ludmil PT

Penn State University, State College, PA, USA

We review of several key theoretical results in multigrid theory which are in the foundation of the classical and also modern multigrid methods. We further present a unified framework that can be used to derive and analyze different geometric and algebraic multigrid methods in a coherent manner. We also discuss the modern trends in multigrid such as adaptive and bootstrap multigrid techniques. This is a joint work with Jinchao Xu (Penn State, USA).

Parallel and adaptive geometric multigrid in UG4

Vogel, Andreas PT

High Performance Computing in the Engineering Sciences, Ruhr University Bochum, Germany

Geometric multigrid allows for a highly-scalable implementation on distributed machines due to the existing coarse grid hierarchy that can be balanced among the processes. In addition, adaptive mesh refinement can help to account for highly localized features and speed up the computation by saving non-required degrees of freedom. We present an overview about our implementations in the massively parallel simulation framework UG4 (unstructured grids). The applicability for largest high-performance computing clusters is demonstrated on a variety of problems including PDE continuum model simulations and numerical optimization.

On the expansion of solutions of Laplace-like equations into traces of separable higher dimensional functions

Yserentant, Harry **PT**

Technische Universität, Berlin

The talk deals with the equation $-\Delta u + \mu u = f$, μ a positive constant, on high-dimensional spaces $\mathbb{R}^m$. If the right-hand side f is a rapidly converging series of separable functions, the solution u can be represented in the same way. These constructions are based on approximations of the function $1/r$ by sums of exponential functions. I will present results of similar kind for more general right-hand sides $f(x) = F(Tx)$ that are composed of a separable function on a space of a dimension n greater than m and a linear mapping given by a matrix T of full rank. These results are based on the observation that in the high-dimensional case the euclidian norm of $T^t\omega$ behaves for ω in most of the $\mathbb{R}^n$ like the euclidian norm of ω.
Reference: H. Yserentant, On the expansion of solutions of Laplace-like equations into traces of separable higher dimensional functions. arXiv:1807.05340 [math.NA]

The efficiency issues of AMG solver for large-scale realistic simulations

Xu, Xiaowen **PT**

Institute of Applied Physics and Computational Mathematics, China Academy of Engineering Physics

As one of the most frequently used preconditioning strategies for solving large-scale sparse linear systems in realistic numerical simulations, algebraic multigrid (AMG) methods are facing challenges in efficiency due to the increasingly complicated problems involved in real-world applications and the extreme concurrency in modern supercomputers. This talk will discuss the approaches for improving the efficiency of AMG solver in the context of large-scale computing, including application-driven components, automatic-tuning procedures, etc. Numerical results for some typically realistic problems in laser fusion simulation are included.

Multigrid and Domain Decomposition: Similarities and Differences

Gander, Martin **PT**

University of Geneva, Switzerland

Both multigrid and domain decomposition methods are so called optimal solvers for Laplace type problems, but how do they compare? I will start by showing in what sense these methods are optimal for the Laplace equation, which will reveal that while both multigrid and domain decomposition are iterative solvers, there are fundamental differences between them. Multigrid for Laplace's equation is a standalone solver, while classical domain decomposition methods like the additive Schwarz method or Neumann-Neumann and FETI methods need Krylov acceleration to work. I will explain in detail for each case why this is so, and then also present modifications so that Krylov acceleration is not necessary any more. This leads to a second fundamental difference, namely the coarse space. Good coarse spaces in domain decomposition methods are very different from coarse spaces in multigrid, due to the very aggressive coarsening in domain decomposition. I will introduce the concept of optimal coarse spaces for domain decomposition in a sense very different from the optimal above, and then present approximations of this coarse space. Together with optimized transmission conditions, this leads to a two level domain decomposition method of Schwarz type which is competitive with multigrid for Laplace's equation in wallclock time.

Distributed HT-Tensor Multigrid

Grasedyck, Lars PT

RWTH Aachen University, Germany

In this talk we consider tensor structured systems as they arise in the context of PDE discretizations with possibly many (stochastic or deterministic) parameter dependencies. The PDE discretization is typically highly adaptive and far from tensor structured. It will lead to a large scale system and we assume that a multigrid hierarchy is readily available. The parameters that enter the problem e.g. via stochastic quantities in the PDE or via optimization / control variables, are responsible for a high dimensionality. We overcome this curse of dimension by use of a hierarchical low rank representations of all involved vectors and matrices. The large scale is handled by a fast multigrid method coupled with low rank representations and a quasi-optimal SVD based truncation. All parts of the solver are executed on a distributed memory architecture so that we can exploit parallelity in time, space, and parameters.

A Semi-Algebraic 2-Level Solver

Bank, Randolph E. PT

University of California at San Diego, USA

We develop a simple semi-algebraic 2-level solver built on traditional multigrid ideas. It is designed to be easily incorporated into existing simulation software. It exhibits good convergence for many classes of challenging problems including discontinuous diffusion, convection-diffusion, and Helmholtz equations. It has built-in structure that makes it simple to generalize to a hierarchical basis multigrid solver.

MS01: New trends in domain decomposition methods

Organizers: Gabriele Ciaramella, Martin J. Gander

Substructured two-level and multi-level domain decomposition methods

Ciaramella, Gabriele[1], **Vanzan, Tommaso**[2]

MS

[1] University of Konstanz, Germany
[2] Université de Genève, Switzerland

Two-level domain decomposition methods are very powerful techniques for the efficient numerical solution of partial differential equations (PDEs). A two-level domain decomposition method requires two main components: a one-level pre-conditioner (or its corresponding smoothing iterative method), which is based on domain decomposition techniques, and a coarse correction step, which relies on a coarse space. The coarse space must properly represent the error components that the chosen one-level method is not capable to deal with. In the literature most of the works introduced efficient coarse spaces obtained as the span of functions defined on the entire space domain of the considered PDE. Therefore, the corresponding two-level preconditioners and iterative methods are defined in volume. In this talk, a new class of substructured two-level methods is introduced, for which both domain decomposition smoothers and coarse correction steps are defined on the interfaces. This approach has several advantages. On the one hand, it allows one to use some of the well-known efficient coarse spaces proposed in the literature. On the other hand, the required computational effort is cheaper than the one required by classical volumetric two-level methods. Moreover, our new substructured framework can be efficiently extended to a multi-level framework, which is always desirable when the high dimension or the scarce quality of the coarse space prevent the efficient numerical solution. Numerical experiments demonstrate the effectiveness of the proposed new numerical framework.

Optimized Schwarz-based nonlinear preconditioning for elliptic PDEs

Kwok, Felix

MS

Department of Mathematics, Hong Kong Baptist University

One way to accelerate the numerical solution of a nonlinear elliptic problem is to use nonlinear preconditioning, which replaces the original discretized problem by an equivalent but easier one. A well-known domain decomposition-based nonlinear preconditioner is the Additive Scwharz Preconditioned Inexact Newton (ASPIN) method, which was introduced by Cai and Keyes (2002). More recently, Dolean et al. (2016) derived the Restricted Additive Schwarz Preconditioned Exact Newton (RASPEN) method by considering the fixed point form of the nonlinear Restricted Additive Schwarz method, and showed that it compares favourably with existing methods. In this talk, we will study the performance of a version of RASPEN that uses optimized transmission conditions. We show that a good choice of Robin parameters can lead to a significant reduction in the number of GMRES iterations required by the outer Newton loop. We motivate this choice by studying a linear model problem with discontinuous diffusion coefficients, where we show that the contraction rate can be made independent of the size of the jump in the diffusion coefficient. Numerical experiments on both linear and nonlinear problems illustrate the effectiveness of our approach.

An Additive Overlapping Domain Decomposition Method for the Helmholtz Equation

Leng, Wei MS

LSEC & NCMIS, Academy of Mathematics and Systems Sciences, CAS

An additive domain decomposition method (DDM) for solving the Helmholtz equation with the Sommerfeld radiation condition is proposed and analyzed. In the proposed method, the computational domain is partitioned into structured subdomains along all spatial directions, and at each step, all subdomain PML problems are solved concurrently and then the horizontal, vertical, and corner directional residuals on each subdomain are passed to their corresponding neighbor subdomains as the sources for the next step. This DDM is efficient in nature and theoretically shown to produce the exact solution for the PML problem with constant medium defined in the whole two-dimensional space. Various numerical experiments in two and three dimensions are conducted to verify the theoretical results and demonstrate excellent performance of the proposed method as an iterative solver or a preconditioner.

Diagonalization-Based Parareal and Waveform Relaxation Algorithms

Gander, Martin[1], **Wu, Shulin**[2] MS

[1] University of Geneva, Switzerland
[2] Northeast Normal University, Changchun, China

The diagonalization technique is an interesting idea for solving time-dependent PDEs in parallel. It can be used alone resulting in a direct parallel-in-time (PinT) algorithm and it can be also used as a component for the parareal algorithm and waveform relaxation algorithms. We explain in this talk how this combination is realized and show the advantages of the new PinT algorithms for solving linear and nonlinear wave propagation problems.

Optimized Schwarz methods for complex elliptic problems

Halpern, Laurence MS

Université Paris 13, France

The Schwarz method (Schwarz, 1872) is an overlapping domain decomposition algorithm whose properties are now well-known and widely used in the context of parallel computations. But the convergence of low frequency components deteriorates with the size of the overlap. Optimized Schwarz methods have been developed in the last twenty years, which improve drastically the convergence of the method. They involved transmission conditions at the interfaces of Robin type. The Robin coefficient is solution of a best approximation problem, which has been solved in various cases, when the search reduces to a somewhat real problem. We present here a study of a really complex problem, arising in many applications, like the control of elliptic problems or the solution of waves in conductive bodies.

Optimized Schwarz Methods for Thermal Contact Problems

Zhang, Hui

MS

Zhejiang Ocean University, China.

Heat conduction between two bodies may have a temperature jump proportional to the heat flux. The ratio coefficient is called thermal contact resistance. For many reasons, it becomes convenient to solve the heat equation in the two bodies separately. This gives rise to new questions for domain decomposition methods because of the unusual interface conditions. In this talk, we discuss the new transmission conditions suitable for the thermal contact problem. The optimized two-sided Robin parameters are derived. Numerical experiments show the fast convergence by using the optimized parameters.

Analysis of the parallel Schwarz method for growing chains of fixed-sized subdomains

Ciaramella, Gabriele

MS

University of Konstanz, Germany

A new class of Schwarz methods was recently presented in the literature for the solution of solvation models, where the electrostatic energy contribution to the solvation energy can be computed by solving a system of elliptic partial differential equations [1,2]. Numerical simulations have shown an unusual convergence behavior of Schwarz methods for the solution of this problem, where each atom corresponds to a subdomain: the convergence of the Schwarz methods is independent of the number of atoms [1], even though there is no coarse grid correction. Despite the successful implementation of Schwarz methods for this solvation model, a rigorous analysis for this unusual convergence behavior is required. In this talk, we analyze the behavior of the Schwarz method for the solution of chains of subdomains and show that its convergence does not depend on the number of subdomains in many cases [3,4]. Moreover, we will present new recent results that study the behavior of the Schwarz method in the cases its convergence depends on the number of subdomains [5].

References
[1] Domain decomposition for implicit solvation models, Cancs, Maday, Stamm, J. of Chem. P. (2013).
[2] Fast Domain Decomposition Algorithm for Continuum Solvation Models, F. Lipparini et al., J. Chem. Theory Comput. (2013).
[3] Analysis of the PSM for the solution of chains of atoms: Part I, Ciaramella and Gander, SIAM J. Num. An. (2017).
[4] Analysis of the PSM for the solution of chains of atoms: Part II, Ciaramella and Gander, SIAM J. Num. An. (2018).
[5] On the Scalability of the Parallel Schwarz Method, Ciaramella, Hassan and Stamm, submitted (2019).

Randomized method of subspace corrections with machine learning

Chen, Long[1], **Xu, Jinchao**[2]

MS

[1] University of California at Irvine, USA
[2] Penn State University, USA

In this talk, I will touch upon the following three main components in a general framework of method of subspace correction consists: the space decomposition, the subspaces solvers and the ordering of subspace corrections. I will first briefly recall some traditional theory and then present some new results and new ideas on using randomization and machine learning in the design and analysis methods of subspace corrections, in particular multigrid and domain decomposition methods.

MS02: Application-driven preconditioning

Organizers: Hengbin An, Hehu Xie

The adapted augmented Lagrangian preconditioner for the turbulent incompressible Navier-Stokes equations discretized by a finite volume method

He, Xin MS

Institute of Computing Technology, Chinese Academy of Sciences

The augmented Lagrangian (AL) preconditioner and its variants have been successfully applied to solve saddle point systems arising from the incompressible Navier-Stokes equations discretized by the finite element method. Attractive features are the purely algebraic construction and robustness with respect to the Reynolds number and mesh refinement. In this work, we reconsider the application of the AL preconditioner in the context of the stabilized finite volume methods and present the extension to the Reynolds-Averaged Navier-Stokes (RANS) equations, which are used to model turbulent flows in industrial applications. Furthermore, we propose a new variant of the AL preconditioner, obtained by substituting the approximation of the Schur complement from the SIMPLE preconditioner into the inverse of the Schur complement for the AL preconditioner. This new variant is applied to both Navier-Stokes and RANS equations to compute laminar and turbulent boundary-layer flows on grids with large aspect ratios. Spectral analysis shows that the new variant yields a more clustered spectrum of eigenvalues away from zero, which explains why it outperforms the existing variants in terms of the number of the Krylov subspace iterations.

Promising strategies for accelerating the Scheduled Relaxation Jacobi method

Jing, Yan-Fei MS

School of Mathematical sciences/Institute of Computational Science, University of Electronic Science and Technology of China

Elliptic equations are encountered in many areas of computational physics such as fluid mechanics and heat transfer. Discretization of elliptic partial differential equations (ePDEs) using second-order finite-difference method leads to a linear system of equations with a banded matrix representing the bonding among the variables, and the right-hand side being associated to the source term. ePDEs must be solved numerically in many circumstances, which generates a growing demand for efficient and highly parallel algorithms to deal with their computational solution. The Jacobi iteration is outstanding for such kind of linear systems because of its tremendous simplicity and potential for massive parallelization. While the Scheduled Relaxation Jacobi (SRJ) method, as a generalization of the weighted Jacobi method, is an attractive strategy to greatly improve the convergence rate. In this talk, we illustrate two promising strategies for accelerating the SRJ method to resulting in two algorithms. Numerical results demonstrate our proposed algorithms are competitive for solving large, sparse linear systems while maintaining the simplicity of the Jacobi method.

Circulant preconditioner for the fractional American option pricing model

Yin, Junfeng MS

Tongji University, Shanghai, China

After discretation by the finite volume method, the numerical solution of fractionalAmerician option pricing model leads to a large, positive definite linear systems or linear complementarity with Toeplitz-like structure. Motivated by the idea of ADI scheme, we proposed a class of positive-definite splitting iteration method, as well as the preconditioner From the implementation, circulant approximation and FFT are applied. Numerical experiment verifed the convergence of the proposed methods and the efficiency of the preconditioners is compared with the existing approaches.

A Multigrid Method for Semilinear Problems

Xie, Hehu MS

LSEC & NCMIS, Academy of Mathematics and Systems Sciences, CAS

In this talk, we will introduce a way to design the multigrid method for the seminlinear problems based on the multilevel correction technique. With the help of a special low dimensional space, this solution of the semilinear problems in the finest level of mesh can be transformed to the solution of the standard elliptic problems in the finest level of mesh and the solution of the semilinear problem which is defined on the low dimensional space. This type of multigrid method has obvious uniform convergence rate which improve the solving efficiency overfull. When the nonlinear term is polynomial function, we will also introduce a type of implementation scheme such that the computational work is absolute asymptotically optimal.

Preconditioning for thermo-mechanical-contact coupled applications

An, Hengbin MS

[1] Software Center for High Performance Numerical Simulation, CAEP
[2] Institute of Applied Physics and Computational Mathematics

In the application of thermo-mechanical-contact coupled simulations, it is very difficult to solve the discretized linear system because the linear equations contains multi-physics coupling, the scale is very large, and the coefficient matrix is non-symmetric. When an algebraic multi-grid preconditioned Krylov method, such as GMRES or BiCGStab method, is employed to solve the linear system, the iteration is usually difficult to converge. We propose a kind of preconditioning method by analyzing the character of thermo-mechanical-contact coupled applications. The preconditioning operator has diagonal block structure with each block a diffusion operator, which is very friendly for multi-grid method. By using the preconditioner, a real application model of Tianshengqiao with 1.1 billion DOFs was simulated on Tianhe-2 with 10 thousands cores.

Several multilevel iterative algorithms for multi-group radiation diffusion equations

Yue, Xiaoqiang MS

Xiangtan University, Xiangtan, China

This talk focuses on developing and studying efficient multilevel iterative algorithms (including adaptive combined preconditioners, additive and semi-multiplicative substructuring preconditioners with a simple coarse space) for the large-scale sparse linear systems arising from fully coupled and implicit cell-centered finite volume discretizations of two- and three-dimensional multi-group radiation diffusion equations.

Acceleration for heterogeneous high throughput data analysis

Zhu, Shengxin MS

Xi'an Jiaotong Liverpool University, Xi'an, China

In this talk, we will talk about the challenges related to some heterogeneous data analysis with linear mixed model. Several techniques are used to reduce the computational complexity, and transform an seemingly computational prohibitive procedure salable.

A Multigrid Method for the Ground State Solution of Bose-Einstein Condensates Based on Newton Iteration

Yue, Meiling MS

Beijing Technology and Business University, China

In this talk, we introduce a new kind of multigrid method for the ground state solution of Bose-Einstein condensates based on Newton iteration method. Instead of treating eigenvalue λ and eigenvector u separately, we regard the eigenpair (λ, u) as one element in the composite space $\mathbb{R} \times H_0^1(\Omega)$ and then Newton iteration method is adopted for the nonlinear problem. Thus in this multigrid scheme, we only need to solve a linear discrete boundary value problem in every refined space, which can improve the overall efficiency for the simulation of Bose-Einstein condensations.

MS03: Multigrid methods for multiscale problems

Organizers: Jingrun Chen, Pingbing Ming, Shuo Zhang

A multiscale finite element method for the Schrödinger equation with multiscale potentials

Ma, Dingjiong MS

The University of Hong Kong

In recent years, an increasing attention has been paid to quantum heterostructures with tailored functionalities, such as heterojunctions and quantum metamaterials, in which quantum dynamics of electrons can be described by the Schrödinger equation with multiscale potentials. The model, however, cannot be solved by asymptotic-based approaches where an additive form of different scales in the potential term is required to construct the prescribed approximate solutions. In this paper, we propose a multiscale finite element method to solve this problem in the semiclassical regime. The localized multiscale basis functions are constructed using sparse compression of the Hamiltonian operator, and thus are "blind" to the specific form of the potential term. After a one-shot eigendecomposition, we solve the resulting system of ordinary differential equations explicitly for the time evolution. In our approach, the spatial mesh size is $H = \mathcal{O}(\epsilon)$, where ϵ is the semiclassical parameter and the time stepsize k is independent of ϵ. Numerical examples in one dimension with a periodic potential, a multiplicative two-scale potential, and a layered potential, and in two dimension with an additive two-scale potential and a checkboard potential are tested to demonstrate the robustness and efficiency of the proposed method. Moreover, first-order and second-order rates of convergence are observed in H^1 and L^2 norms, respectively.

Multiscale simulation method for the elastic wave equation and Biot equation

Zheng, Hui MS

School of Mathematics and Statistics, Huazhong University of Science and Technology, Wuhan, China

We propose a multiscale simulation method for the elastic wave equation and Biot equation in the heterogeneous media. This method firstly computes the local basic functions on the fine mesh by the multiscale finite element methods, then computes on the coarse mesh through these local basic functions by a method like the stagger grid method. The numerical results show that the multiscale method proposed can both catch the information on the fine scale and save the cost of computations.

Fast eigenpairs computation with operator adapted wavelets and hierarchal subspace correction

Xie, Hehu MS

Chinese Academy of Mathematics and Systems Science, Chinese Academy of Sciencecs

In this talk, we present a method for the fast computation of the eigenpairs of a bijective positive symmetric linear operator. The method is based on a combination of operator adapted wavelets (gamblets) with hierarchical subspace correction. First, gamblets provide a raw but fast approximation of the eigensubspaces by block-diagonalizing the operator into sparse and well-conditioned blocks. Next, the hierarchical subspace correction method, computes the eigenpairs associated with the Galerkin restriction to a coarse (low dimensional) gamblet subspace, and then, corrects those eigenpairs by solving a hierarchy of linear problems in the finer gamblet subspaces (from coarse to fine, using multigrid iteration). The proposed algorithm is robust to the presence of multiple (a continuum of) scales and is shown to be of near-linear complexity when the operator is an elliptic PDE with rough coefficients This work is collaborated with Lei Zhang and Houman Owhadi.

A model reduction for nonlinear multiscale parabolic problems

Jiang, Lijian MS

Tongji University

In this talk, I present a model reduction technique for solving nonlinear multiscale parabolic problems. The proposed method combines Constraint Energy Minimizing Generalized Multiscale Finite Element Method (CEM-GMsFEM) and Dynamic Mode Decomposition(DMD) to reduce the computational complexity. The CEM-GMsFEM is used to represent the solution on a coarse grid with multiscale basis functions computed offline. Using the CEM-GMsFEM to solve nonlinear multiscale model involves calculating the residual and the Jacobian on a fine grid. This is computationally expensive because the evaluation of the nonlinear term requires computing the full-dimensional model. To overcome the challenge, the DMD method is used to estimate nonlinear term and decomposes the nonlinear system into spatiotemporal coherent structures for short-term future state prediction. The proposed approach avoids the evaluation of the nonlinear term in the online stage. In order to achieve a full coarse model for the nonlinear problem, we utilize a coarse-scale observation in DMD.

Brownian motion of a nano-ellipsoid in a cylindrical vessel flow

Wang, Yaohong MS

Tianjin University

We developed a direct numerical simulation method based on arbitrary Lagrangian-Eulerian (ALE) finite element method with thermal fluctuations to accurately resolve the fluid-nanoparticle interfacial motions. Comprehensive numerical studies of the motion of a buoyant or a nearly neutrally buoyant nano-sized ellipsoidal particle in a fluid filled cylindrical tube with or without the presence of imposed pressure gradients are presented. Brownian interactions in the translational and rotational degrees of freedom for the particle are considered, and the fluctuation-dissipation relation and the principle of thermal equipartition of energy are both satisfied. We focus on capturing the hydrodynamic interactions due to the confining boundaries and report results for the velocity autocorrelations, diffusivity, drag and lift forces for the particle as functions of aspect ratio, inclination angle, and proximity to the wall.

An efficient multigrid strategy for large-scale molecular mechanics optimization

Chen, Jingrun MS

Suzhou University, Suzhou, China

Static mechanical properties of materials require large-scale nonlinear optimization of the molecular mechanics model under various controls. We present an efficient multigrid strategy which approximates solutions on grids in a quasi-atomistic and inexact manner, transfers solutions on grids following a coarse-to-fine (oneway) schedule, and finds physically relevant minimizers with linear scaling complexity in the general situation. For systems with 1,000,000 atoms (over three million degrees of freedom), on average a more than 70

Grad-div stabilization method for magnetohydrodynamic flows at low magnetic Reynolds numbers

Rong, Yao CT

Harbin Institute of Technology, Shenzhen

Magnetohydrodynamics (MHD) is the study of the interaction of electrically conducting fluids in the presence of magnetic fields. MHD applications require substantially more efficient and stable numerical methods than currently exist. The divergence constraint of the incompressible MHD equations might contribute to the pollution of velocity which is caused by the pressure dependent consistency error when the standard mixed finite element is used. Grad-div stabilization is a popular technique which improves the robustness of the standard mixed finite element spaces by adding a penalization with respect to the continuity equation. In this paper, we construct grad-div stabilization algorithm for calculating solutions to the MHD equations at low magnetic Reynolds numbers. Stability and optimal-order convergence of the method are proven. Numerical tests confirm the theory and illustrate the benefits of these algorithms over the standard FE method.

MS04: Multi-scale and multi-physics modeling and simulations in scientific and engineering computing

Organizer: Jizu Huang

Second-order semi-implicit methods for Landau-Lifschitz equation

Chen, Jingrun

MS

Suzhou University, Suzhou, China

In ferromagnets, the intrinsic magnetic order, known as magnetization, makes these materials ideal for information storage and manipulation. From the modeling perspective, magnetization dynamics is described by the Landau-Lifshitz equation with pointwise length constraint. From the numerical perspective, typically, second-order in time schemes are either explicit with strong stability restriction on the stepsize due to the high nonlinearity or implicit with a nonlinear system of equations to be solved at each step. In the talk, we will introduce several second-order semi-implicit schemes based on the second-order backward-differentiation-formula and the one-sided interpolation from former steps with a projection step. For these schemes, we are able to prove the uniqueness of the numerical solution to the linear system of equations at each step. For one of these schemes, we then prove its second-order accuracy under the mild condition that the stepsize in time is proportional to the gridsize in space. Examples in 1D and 3D are given to verify the analysis results. A benchmark problem from National Institute of Standards and Technology is also tested to verify the applicability of these schemes.

Physics-preserving algorithms for flow and transport in porous media

Chen, Huangxin

MS

Xiamen University

Simulation of flow and transport in porous media has wide applications, which include in particular the management of existing petroleum fields and the development of new oil and gas reservoirs. In this talk we will introduce a new efficient IMplicit Pressure Explicit Saturation (IMPES) scheme for the simulation of incompressible and immiscible two-phase flow in heterogeneous porous media with capillary pressure. The new algorithm is locally mass conservative for both phases and also deserves another merit that the total velocity is continuous in the normal direction. Moreover, the new scheme is unbiased with regard to the two phases and the saturations of both phases are bounds-preserving if the time step size is smaller than a certain value. We will also discuss the application of the idea of the new algorithm to develop the fully mass-conservative scheme for the multicomponent compressible flow in porous media. Some interesting examples will be shown to demonstrate the efficiency of the new algorithms.

Parallel Domain Decomposition Preconditioners for Large-scale Patient-specific Blood Flow Simulations

Chen, Rongliang

MS

Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences

Numerical simulation of blood flows in compliant arteries based on patient-specific geometry and parameters can be clinically helpful for physicians or researchers to study vascular diseases, to enhance diagnoses, as well as to plan surgery procedures. In this talk, we will discuss some scalable parallel domain decomposition preconditioners for the simulation of blood flow in compliant arteries on large scale supercomputers. The blood flow is modeled by 3D unsteady incompressible Navier-Stokes equations with a lumped parameter boundary condition, which are discretized with a stabilized finite element based on unstructured meshes in space and a fully implicit method in time. The large scale discretized nonlinear systems are solved by a parallel Newton-Krylov method preconditioned by linear and nonlinear domain decomposition preconditioners. Several mathematical, biomechanical, and supercomputing issues will be discussed in detail, and some numerical experiments for patient-specific arteries will be presented. We will also report the parallel performance of the methods on a supercomputer with a large number of processors.

A hybrid local/nonlocal continuum mechanics modeling for fracture simulation

Han, Fei

MS

Dalian University of Technology

The classical continuum mechanics which leads to a local continuum model, encounters challenges when the discontinuity appears, while the peridynamics that falls into the category of nonlocal continuum mechanics, suffers from a high computational cost. A hybrid model coupling classical continuum mechanics with peridynamics can avoid both disadvantages. This work describes the hybrid model and its adaptive coupling approach which dynamically updates the coupling domains according to crack propagations for brittle materials. Then this hybrid local/nonlocal continuum model is applied to fracture simulation. Some numerical examples like a plate with a hole, Brazilian disk, notched plate and beam, are performed for verification and validation.

A Simplified a Posteriori Error Estimation for a Consistent Atomistic-to-continuum Coupling Method in 2D

Wang, Hao

MS

Sichuan University

Atomistic-to-continuum coupling methods are a class of computational multiscale methods which combine the accuracy of the atomistic model and the efficiency of the continuum model for the computation of defects in crystal solids. Such methods can be efficiently implemented by adaptivity and achieve (quasi-)optimal balance between accuracy and efficiency. In this talk, we will present a simplified a posteriori error estimator for a consistent a/c coupling method in 2D. Such error estimator is essentially a simplified version of the residual based error estimator for the a/c method which avoids the computation of model error in the continuum bulk. We will show both analytically and numerically that the model error in the continuum region, which is expensive in computational due to the discrepency of the finite element mesh and the reference lattice, is of higher order compared with other sauce of error and thus can be omitted. Numerical experiments are also given to demonstrate the efficiency of the simplified error estimator compared with the classical residual based error estimator for the adaptive computation of crystal defects.

Stochastic multiscale heat transfer analysis of heterogeneous materials with multiple random configurations

Yang, Zihao MS

Northwestern Polytechnical University

This study presents a new stochastic multiscale analysis approach to analyze the heat transfer performance of heterogeneous materials with random structures at different length scales. The heterogeneities of the materials are taken into account by periodic layouts of unit cells, consisting of randomly distributed inclusion dispersions and homogeneous matrix on the microscale and mesoscale. Based on the reiterated homogenization, a novel unified micro-meso-macro stochastic multiscale formulation is established and the scale gap is correlated by means of two-scale asymptotic expansions. Also, the stochastic multiscale formulae for computing the effective thermal property and temperature field are derived successively. Then, the stochastic prediction algorithm coupled with the finite element method is brought forward in details. The accuracy of the implemented stochastic multiscale analysis is verified by comparing the results against the experimental data for three scales heterogeneous materials with several different material combinations. The comparison demonstrates the usability of the proposed stochastic multiscale method for the determination of the thermal behaviors. This study offers a unified multiscale framework that enables heat transfer behavior analysis of heterogeneous materials with multiple random configurations.

Template numerical library for modern parallel architectures

Oberhuber, Tomas CT

Czech Technical University in Prague

We will present a new Template Numerical Library (TNL, www.tnl-project.org) with native support of modern parallel architectures like multi–core CPUs and GPUs. The library offers an abstract layer for accessing these architectures via unified interface tailored for easy and fast development of numerical solvers of PDEs. Once the user implements the solver, it can be executed on any supported architecture. The library is written in C++ and it benefits from template meta–programming techniques. Currently, it supports regular rectangular numerical grids and unstructured conforming meshes. We demonstrate the use of TNL on the MHFEM method for multiphase flow in porous media. We also present scalability on multi–core CPUs and speed–up on GPUs with CUDA.

MS05: Algorithms for multiphysics models

Organizer: Mingchao Cai

Decoupling Multi-physics Computation with Intrinsic Robin Condition

Mu, Mo MS

Department of Mathematics, Hong Kong University of Science and Technology

We discuss decoupling issues for numerical computation with coupled PDE models in large scale simulation of multi-physics systems. An abstract mathematical framework is presented for devising effective and efficient decoupled numerical methods. Applications in mixed fluid-porous media flows and fluid-structure interactions (FSI) will be examined. Approximation and stability issues will be addressed, with special attention to the added-mass effect in decoupling FSI computation. Stable decoupling techniques are proposed based on the intrinsic Robin condition.

Nonconforming Nitsche's Extended Finite Element Methods for Interface Problems

Chen, Jinru MS

School of Mathematical Sciences, Nanjing Normal University

We study P_1 nonconforming Nitsche's extended finite element methods with interfaceunfitted meshes for elliptic/Stokes interface problems. By adding some penalty terms defined on the transmission edges to the discrete form, the stability of the discrete problems and optimal error estimates are derived in spite of the low regularity of the elliptic/Stokes interface problems. For the elliptic interface problems, it is shown that all results are independent of not only the diffusion parameters but also the position of the interface with respect to the mesh without other assumption for the interface. For the Stokes interface problems, all results are independent of the viscosity parameters. Numerical experiments validate theoretical results.

On a weak virtual element element method for the poroelasticity problem

Wang, Feng MS

School of Mathematical Sciences, Nanjing Normal University

In this talk, we shall present a weak virtual element element method for the two-field poroelasticity problem. The displacement is discretized by the H(div) virtual element, while the pressure is approximated by the piecewise constant. Besides, we use additional spaces on element boundaries for both variables, and introduce weak gradients correspondingly. We

will show that the discrete problem is well-posed, and that the a priori error estimate will not deteriorate when the Lame constant $\lambda \to \infty$. A series of numerical experiments are reported to verify the theoretical results and show the method is free of pressure oscillations.

Numerical simulations and analysis for epitaxial thin film models

Wang, Shufen MS

Fudan University

There have been quite a few works focused on the numerical simulations and analysis for the thin film epitaxy models. In this talk, a review will be given on the related results. In a recent one, an energy stable, second-order mixed finite element scheme is proposed and analyzed for the thin film epitaxial growth model with slope selection. The second-order backward differentiation formula (BDF) scheme with a second-order stabilized term, which guarantees the long time energy stability was applied to approximate the continuous model. In terms of the convergence analysis, the key difficulty to derive an optimal rate spatial estimate is associated with the appearance of the gradient operator in the nonlinear terms, which may lead to a loss of optimal accuracy order. To overcome this well-known difficulty, some auxiliary techniques over triangular elements were used, consequently, an optimal convergence rate $O(h^{q+1} + t^2)$, in comparison with $O(h^q + t^2)$ rate from a standard projection estimate was obtained.

Numerical study of flow across an ellipse and a circle placed in a uniform stream of infinite extent

Razzaqa, Mudassar MS

Department of Mathematics, School of Science and Engineering, Lahore University of Management Sciences, Opposite Sector U, DHA, Lahore Cantt., 54792, Pakistan

As an example of aerodynamics prototypical study, we examine a two-dimensional low Reynolds number flow over obstacles immersed in a stream of infinite extent. The Navier Stokes equation is being discretized by nonconforming finite element method approach. The resulting discretized algebraic system is being solved by using the Newton method for nonlinear part and Multigrid method for the linear subproblem. The magnitude of the uniform upstream velocity under the study of the problem for Reynolds number in the range $1 \leq Re \leq 100$ and the angle of attack of the upstream velocity at $\alpha = -5°, 0°, 5°$ performed. Analysis of the resulting drag and lift forces acting on obstacles with respect to the angle of attack of the upstream velocity and the Reynolds number is made. Which determine the influence of one obstacle onto the resulting drag and lift coefficients of other obstacles.

Multigrid Methods for a Mixed Finite Element Method of the Darcy-Forchheimer Model

Huang, Jian

MS

School of Mathematics and Computational Science, Xiangtan University, China

In this talk, we will introduce an efficient nonlinear multigrid method for a mixed finite element method of the Darcy-Forchheimer model. A Peaceman-Rachford type iteration is used as a smoother to decouple the nonlinearity from the divergence constraint. The nonlinear equation can be solved element-wise with a closed formula. The linear saddle point system for the constraint is reduced into a symmetric positive definite system of Poisson type. Furthermore, an empirical choice of the parameter used in the splitting is proposed and the resulting multigrid method is robust to the so-called Forchheimer number which controls the strength of the nonlinearity. By comparing the number of iterations and CPU time of different solvers in several numerical experiments, our multigrid method is shown to convergent with a rate independent of the mesh size and the Forchheimer number and with a nearly linear computational cost.

A Cartesian grid nonconforming immersed finite element method for planar elasticity interface problems

Qin, Fangfang

MS

College of Science, Nanjing University of Posts and Telecommunications, Nanjing, China

In this talk, a new nonconforming immersed finite element (IFE) method on triangular Cartesian meshes is developed for solving planar elasticity interface problems. The proposed IFE method possesses optimal approximation property for both compressible and nearly incompressible problems. Its degree of freedom is much less than those of existing finite element methods for the same problem. Moreover, the method is robust with respect to the shape of the interface and its location relative to the domain and the underlying mesh. Both theory and numerical experiments are presented to demonstrate the effectiveness of the new method. Theoretically, the unisolvent property and the consistency of the IFE space are proved. Experimentally, extensive numerical examples are given to show that the approximation orders in L2 norm and semi-H1 norm are optimal under various Lame parameters settings and different interface geometry configurations.

Some Algorithms for Biot Model with Applications in Brain Swelling Simulation

Cai, Mingchao

MS

Department of Mathematics, Morgan State University

Biot's model has been widely used in Biomechanics, for example, brain swelling simulation and modeling of cancellous bones. In this work, we present some algorithms for Biot's model. To solve the resulting saddle point linear systems, some preconditioners and iterative methods are proposed. In the preconditioners, the Schur complement approximation is derived by using a Fourier analysis approach. These preconditioners are implemented exactly or inexactly using Multigrid or domain decomposition methods. We also discuss a multiphysics reformulation of the Biot model. From the reformulation, the Biot model can be viewed as a generalized Stokes subproblem combining with a reaction-diffusion subproblem. Then, we discuss the algorithms based on the multiphysics reformulation.

MS06: Multilevel algorithms for eigenvalue problems

Organizers: Xiaoying Dai, Hehu Xie

A Multilevel Correction Method for Interior Transmission Eigenvalue Problem

Wu, Xinming MS

Fudan University

In this talk, we give a numerical analysis for the transmission eigenvalue problem by the finite element method. A type of multilevel correction method is proposed to solve the transmission eigenvalue problem. The multilevel correction method can transform the transmission eigenvalue solving in the finest finite element space to a sequence of linear problems and some transmission eigenvalue solving in a very low dimensional spaces. Since the main computational work is to solve the sequence of linear problems, the multilevel correction method improves the overfull efficiency of the transmission eigenvalue solving. Some numerical examples are provided to validate the theoretical results and the efficiency of the proposed numerical scheme.

A Type of Parallel Augmented Subspace Method for Eigenvalue Problems

Xu, Fei MS

Beijing Institute for Scientific and Engineering Computing, Beijing University of Technology

A parallel multilevel correction method is proposed for eigenvalue problems. The main idea is to transform the solution of the eigenvalue problem into a series of solutions of the corresponding linear boundary value problems on the sequence of finite element spaces and eigenvalue problems on a very low dimensional space. The computational efficiency can be improved since we do not need to solve the eigenvalue problems in the fine space directly. Besides, for different eigenvalues, the corresponding boundary value problem and low dimensional eigenvalue problem can be solved in the parallel way since they are independent for each other and no data exchanging. This property means that we do not need to do the orthogonalization in the high dimensional spaces.

Local and parallel finite element algorithms for fourth-order differential operator eigenvalue problems

Bi, Hai MS

School of Mathematical Sciences, Guizhou Normal University

Local and parallel computation is a general and powerful computing approach that can be used for a variety of partial differential problems. In 2000, Xu and Zhou (Math. Comput., 2000) combine the two-grid finite element discretization scheme with the local defect-correction technique to propose this technique for elliptic boundary value problem. Later, this technique has been used and developed by many scholars. Our work explores the local and parallel finite element algorithms for Helmholtz transmission eigenvalue problem and the biharmonic eigenvalue problem of plate buckling/vibration. We propose the local and parallel computational schemes, present a complete error analysis and implement numerical experiments. Theoretical analysis and numerical experiments indicate that local and parallel algorithms can solve the eigenvalue problems with local low smoothness or singularity efficiently.

Two-scale finite element approximations for semilinear parabolic equations

Liu, Fang MS

School of Statistics and Mathematics, Central University of Finance and Economics, Beijing 100081, China

To reduce computational cost, we study some two-scale finite element approximations with the backward Euler scheme for the semilinear parabolic equations. First, a basic two-scale finite element method with the backward Euler scheme is proposed. A Boolean sum of some existing finite element approximations for the semilinear system on a coarse grid and some univariate fine grids is calculated. Second, a linearized two-scale finite element method with the backward Euler scheme is introduced. A semilinear system is solved on a coarse grid and then some linear systems are solved on some univariate fine grids. Both the two new two-scale finite element approximations with the backward Euler scheme not only have the less degrees of freedom but also achieves a good accuracy of approximation.

Spectral Graph Distance for Biological Networks

Hu, Xiaozhe MS

Tufts University

Recently, diffusion state distance (DSD) was introduced for protein-protein interaction networks and used for protein function prediction. In this talk, we study the DSD metric via spectral analysis. We develop theoretical fundations that provides guarantees on the behavior of DSD for data exhibiting multiscale structure. In addition, multilevel algorithm for approximating DSD efficiently are also proposed. Applications to the protein-protein networks are presented and possible generalizations will be discussed.

New Mixed Elements for Maxwell Equations

Duan, Huoyuan MS

School of Mathematics and Statistics, Wuhan University, Wuhan 430072, China

New inf-sup stable mixed elements are proposed and analyzed for solving the Maxwell equations in terms of electric field and Lagrange multiplier. Nodal Lagrange elements of any order on simplexes in two- and three- dimensions can be used for the electric field. The multiplier is compatibly approximated always by the discontinuous piecewise constant elements. A general theory of stability and error estimates is developed; in particular, when applied to the eigenvalue problem, we prove the key property of discrete compactness, and we show that the proposed mixed elements are spectral-correct and spurious-free. Essentially optimal error bounds (only up to an arbitrarily small constant) are obtained for eigenvalues and for both singular and smooth eigenfunction solutions. Numerical experiments are performed for Maxwell eigenvalue problem in nonsmooth domains to illustrate the theoretical results.

Convergence and optimal complexity of the adaptive Fourier-Galerkin method for eigenvalue problems

Dai, Xiaoying MS

LSEC & NCMIS, Academy of Mathematics and Systems Sciences, CAS

In this talk, we will propose an adaptive Fourier-Galerkin method for multiple eigenvalues of second-order elliptic partial equations. Inspired by the technique for the adaptive finite element analysis, we prove that the adaptive Fourier-Galerkin method has the linear convergence rate and optimal complexity. This is a joint work with Y. Pan, B. Yang, and A. Zhou.

MS07: Parallel multigrid methods

Organizer: Ulrike Meier Yang

Designing a semi-structured algebraic multigrid solver

Yang, Ulrike Meier

MS

Lawrence Livermore National Laboratory, USA

Multigrid methods are well suited to large massively parallel computer architectures, because they are mathematically optimal and display excellent parallelization properties. Since current architecture trends are favoring regular compute patterns to achieve high performance, the ability to express structure has become much more important. An alternative to standard sparse matrix classes expressed with row and column indices is a semi-structured matrix class that is primarily described in terms of stencils and logically rectangular grids is. The definition of semi-structured rectangular matrices, which are a needed as prolongation operators in algebraic multigrid, is however nontrivial. We will discuss our efforts on the new semi-structured matrix class and introduce a semi-structured algebraic multigrid solver built upon it.

Parallel Performance of Algebraic Multigrid Domain Decomposition (AMG-DD)

Mitchell, Wayne

MS

Universitaet Heidelberg

Algebraic multigrid (AMG) is a widely used and highly scalable solver and preconditioner for large-scale linear systems resulting from the discretization of a wide class of elliptic PDEs. The need for constant communication between processors in order to perform matrix-vector multiplications during a multigrid cycle is often a significant bottleneck for AMG in parallel, however. This talk examines the design, implementation, and parallel performance of a novel algorithm designed specifically to limit communication, Algebraic Multigrid Domain Decomposition (AMG-DD). The goal of AMG-DD is to provide a low-communication alternative to standard AMG V-cycles by enabling significantly more independent computational work to be done between communication steps. Thus, AMG-DD is particularly well suited to computational environments where the cost of communication is high compared to the cost of computation. Parallel performance results for AMG-DD are shown for a variety of algorithm design choices and for a variety of elliptic PDE problems in 2 and 3 dimensions.

Asynchronous Multigrid Methods

Wolfson-Pou, Jordi MS

Georgia Institute of Technology, U.S.

Reducing synchronization in iterative methods for solving large sparse linear systems may become one of the most important goals for such solvers on exascale computers. Research in asynchronous iterative methods has primarily considered basic iterative methods. In this talk, we examine how multigrid methods can be executed asynchronously. We introduce models of asynchronous additive multigrid methods, and we present parallel implementations of asynchronous multigrid. Our implementations use OpenMP and MPI, and we generate the prolongation, restriction and coarse grid matrices using the BoomerAMG package. Our experimental results show that asynchronous multigrid can exhibit grid-size independent convergence and can be faster than classical multigrid in terms of solve wall-clock time.

Parallel Matrix-Free Multigrid Applied to Phase-Field Fracture Problems

Jodlbauer, Daniel CT

The Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria

Matrix-based finite element methods tend to require lots of memory, in particular, for higher-order discretizations and 3d problems. This gets even worse when we apply algebraic (AMG) or geometric multigrid (GMG) solvers, as we need to store the coarse level matrices as well. Fortunately, geometric multigrid methods are suitable for a matrix-free implementation. Within such a matrix-free approach, we aim to assemble the matrix-vector product on the fly instead of using the standard way of assembling, storing, and performing matrix-vector multiplication. In this talk, we apply the matrix-free framework to a monolithic quasi-static phase-field fracture model. The equations of interest are nonlinear and need to satisfy a variational inequality. This imposes several challenges for the implementation, which will be discussed throughout this talk. Finally, several numerical examples are presented to show the applicability and parallel scalability of the matrix-free GMG solver.

MS08: Advances in numerical methods on polytopal meshes and solvers

Organizers: Xuehai Huang, Xiaoping Xie, Shiquan Zhang

An adaptive virtual element method for the self-consistent field theory on general domains

Wei, Huayi MS

Xiangtan University

Block copolymers provide a wonderful platform in the study of soft condensed matter systems. Many fascinating ordered structures have been discovered in bulk and confined systems. Among various theories, the self-consistent field theory (SCFT) has been proven to be a powerful tool for studying the equilibrium ordered structures. Many numerical methods have been developed to solve the SCFT model. In this work, we developed a adaptive element method for the self-consistent field theory on general domains, which can be applied to study the phase behaviors of block copolymers on general domains accurately.

Nonconforming Virtual Element Method for $2m$-th Order Partial Differential Equations in $\mathbb{R}^n$ with $m \geq n$

Huang, Xuehai MS

Shanghai University of Finance and Economics

A unified construction of the H^m-nonconforming virtual elements of any order k is developed on any shape of polytope in $\mathbb{R}^n$ with constraints $m \geq n$ and $k \geq m$. As a vital tool in the construction, a generalized Green's identity for H^m inner product is derived. The H^m-nonconforming virtual element methods are then used to approximate solutions of the m-harmonic equation. After establishing a bound on the jump related to the weak continuity, the optimal error estimate of the canonical interpolation, and the norm equivalence of the stabilization term, the optimal error estimates are derived for the H^m-nonconforming virtual element methods.

An HDG Method for Dirichlet Boundary Control of Convection Dominated Diffusion PDES

Chen, Gang MS

College of Mathematics, Sichuan University

We first propose a hybridizable discontinuous Galerkin (HDG) method to approximate the solution of a convection dominated Dirichlet boundary control problem without constraints.

Dirichlet boundary control problems and convection dominated problems are each very challenging numerically due to solutions with low regularity and sharp layers, respectively. Although there are some numerical analysis works in the literature on diffusion dominated convection diffusion Dirichlet boundary control problems, we are not aware of any existing numerical analysis works for convection dominated boundary control problems. Moreover, the existing numerical analysis techniques for convection dominated PDEs are not directly applicable for the Dirichlet boundary control problem because of the low regularity solutions. In this work, we obtain an optimal a priori error estimate for the control under some conditions on the domain and the desired state. We also present some numerical experiments to illustrate the performance of the HDG method for convection dominated Dirichlet boundary control problems.

Bridging Virtual Element Methods and Immersed Finite Element Methods for Interface Problems

Chen, Long MS

University of California at Irvine

This talks presents an improvement to the existing immersed finite element (IFE) methods for solving the second order elliptic interface problems. A virtual body-fitted mesh is generated using the intersection points of the interface and the underlying shape regular triangulation and the corresponding linear finite element space is used as a virtual element space. By using the norm equivalence from virtual element method (VEM), it is shown that the extra degree of freedom on the intersection points can be eliminated from the stabilization term and the resulting scheme is equivalent to an edge penalized term. This approach not only provides a more concise convergence proof of partially penalized IFE method, but also brings connection between various methods such as body-fitted FEM, IFE, VEM, etc. This is a joint work with Shuhao Cao and Frank Lin.

Virtual Element Methods for Variational and Hemivariational Inequalities

Wang, Fei MS

Xi'an Jiaotong University

As an extension of the finite element method, the virtual element method (VEM) can handle very general polygonal meshes, which makes it very suitable for h-adaptive strategy. We study VEMs for solving different variational and hemivariational inequalities, such as obstacle problem, simplified frictional problem, Kirchhoff plate contact problem, contact problem with nonconvex friction term. We derive a priori error estimates for these virtual elements, and show that they achieve optimal convergence order for the lowest-order case. Some numerical results are reported to confirm the theoretical predictions of the convergence order. This talk is based on the joint works with Prof. Wei Huayi (Xiangtan University), Dr. Zhao Jikun (Zhengzhou University) and Prof. Weimin Han (University of Iowa).

Energy-preserving mixed finite element methods for the elastic wave equation

Wu, Yongke

MS

School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu 611731, China

In this talk, the mixed finite element corresponding to $\mathbf{H}(curl)$, $\mathbf{H}(div)$ and L^2 spaces is employed to construct a second order space-time geometric method for the elastic wave equation, which combine finite element exterior calculus (FEEC) and symplectic methods. The semi-discrete method conserves the system energy. Our fully discrete methods employing a second order symplectic Runge-Kutta method in time which exactly conserve the actual energy functional. Furthermore, the uniformly stability and optimal convergence order of semi and fully discrete methods are given. Numerical experiments confirm the theoretical results.

Virtual element methods for elliptic variational inequalities of the second kind

Huang, Jianguo

MS

Shanghai Jiao Tong University

In this talk, we are concerned with virtual element methods for solving elliptic variational inequalities (EVIs) of the second kind. First, a general framework is provided for the numerical solution of the EVIs and for its error analysis. Then virtual element methods are applied to solve two representative EVIs: a simplified friction problem and a frictional contact problem. Optimal order error estimates are derived for the virtual element solutions of the two representative EVIs, including the effects of numerical integration for the non-smooth term in the EVIs. A fast solver is introduced to solve the discrete problems. Several numerical examples are included to show the numerical performance of the proposed methods. This is a joint with Fang Feng from Shanghai Jiao Tong University and Weimin Han from University of Iowa.

A locking-free hybridizable discontinuous Galerkin method for linear elasticity with strong symmetric stress and continuous displacement trace approximation

Xie, Xiaoping

MS

School of Mathematics, Sichuan University, Chengdu, 610064, China

In this talk, we consider a new hybridizable discontinuous Galerkin (HDG) for 2- and 3-dimensional linear elasticity problems on simplex meshes. This HDG method uses discontinuous piecewise-polynomial approximations of degrees k (≥ 0) for the stress, $k+1$ for the displacement, and a continuous piecewise-polynomial approximation of degree $k+1$ for the displacement trace on the inter-element boundaries, respectively. A special stabilized term is added to ensure locking-free approximations. After the local elimination of unknowns defined in the interior of elements, the proposed method leads to an SPD system where the unknowns are only the degrees of freedom describing the continuous trace approximation. The new HDG method is shown to be robust in the sense that the derived a priori error estimates are optimal and uniform with respect to the Lame constant λ. Numerical experiments confirm the theoretical results. This is joint work with Gang Chen.

MS09: Mathematical modeling of practical problems, numerical methods, and efficient preconditioners for solving discrete problems

Organizers: Zhiming Chen, Liwei Xu, Weiying Zheng

Vertical mode expansion method for applications in photonics

Lu, Ya-Yan MS

Department of Mathematics, City University of Hong Kong

To simulate lightwaves propagating in, scattered by, or radiated from a photonic device, it is necessary to solve the 3D Maxwell's equations on structures with complicated geometric and material features. The problem can be very difficult, since the structures often have subwavelength features, sharp edges and corners, and metallic components, and they could be much larger than the wavelength in some spatial directions. Numerical solutions must be sufficiently accurate to resolve strong local fields and field singularities, and must satisfy the correct physical condition, such as the outgoing radiation condition, at infinity. Fortunately, photonic devices are often locally layered, since they are designed to avoid fabrication difficulties. The vertical mode expansion method is a special hybrid method for locally layered structures, where the electromagnetic field in each layered region is expanded in 1D vertical modes with unknown coefficients that are functions of the two horizontal variables. It is a hybrid method, since it uses boundary integral equations or cylindrical wave expansions to treat the unknown functions that depend on the two horizontal variables. The method is illustrated by numerical examples including metallic bowtie structures, bull's eye structures, nanogaps in metal films, and photonic crystal slabs.

A direct sampling method for inverse scattering problem in waveguide

Chen, Junqing MS

Department of Mathematics, Tsinghua University

I will introduce a direct sampling method for inverse scattering problem in rectangular waveguide. The method is similar to the reverse time migration method, it is simple and easy to implement. The resolution is analyzed, some numerical examples are provided to show the efficiency of the proposed method.

Domain Decomposition Method for the Efficient Analysis of Multiscale Electromagnetic Scattering

Chen, Yongpin MS

University of Electronic Science and Technology of China

The domain decomposition method (DDM) has received intensive study in the computational electromagnetics community in recent years. By invoking the spirit of divide and conquer, a complicated solution domain can be decomposed into several smaller and easily solvable sub-domains. Proper transmission conditions are then designed to transfer the electromagnetic information between adjacent sub-domains to guarantee an accurate overall solution. In this talk, the-state-of-the-art DDM schemes based on both surface integral equations (SIE) and finite element method (FEM) are first reviewed. A hybrid non-conformal FEM-DDM and discontinuous Galerkin integral equation (DGIE) is then developed for the efficient analysis of electromagnetic scattering from multiscale, composite and electrically-large objects. In this method, a closed exterior boundary domain and an interior volume domain are first generated at level-1 decomposition. The exterior and interior domains are then respectively decomposed into smaller partitions in the level-2 procedure according to the local feature of the geometry and material distribution. Consequently, the FEM is applied for the interior volume sub-domains, whereas the DGIE is utilized for the exterior boundary sub-domains. The information in different domains are exchanged by the Robin transmission conditions (RTCs). The proposed method allows for non-conformal discretization between any touching sub-domains, hence much eases the geometrical preparation. Moreover, since each sub-domain can be easily solved, the solution can be applied to precondition the global system in the Krylov subspace iterative solvers. Several numerical results will be presented to validate the accuracy and demonstrate the versatility of the proposed method.

Parallel 3-D Adaptive Finite Element Method and its Application on EDA tools

Cui, Tao MS

Academy of Mathematics and Systems Science, Chinese Academy of Sciences

Electronic design automation (EDA), also referred to as electronic computer-aided design (ECAD), is a category of software tools for designing electronic systems such as integrated circuits and printed circuit boards. As the VLSI technology scales down to nanoscale and the circuit's frequency reaches GHz, EDA tools play a more and more important role in today's integrated circuits (IC) industry. The finite element method (FEM) is a powerful tool for the numerical simulation of a wide range of problems. In this talk, the parallel adaptive finite element method for parasitic extraction of large scale interconnects and thermomechanical stress evaluation of 3D IC is developed to provide extremely high parallel scalability and numerical accuracy. Numerical results of some large scale adaptive finite element simulations with up to 1 billion degrees of freedom and using up to ten thousand CPU cores are presented to demonstrate that our adaptive method is robust and scalable for analysis of very complicated geometries.

Cartesian PML method for Maxwell's equations in a two-layer medium

Jiang, Xue

MS

Beijing University of Technology

The perfectly matched layer (PML) method is a very efficient approach for solving exterior scattering problems. It provides a highly-accurate approximation to the radiation condition on the truncation boundary. This talk presents the Cartesian PML method for solving electromagnetic scattering problem in a two-layer medium. By extending the Cagniard-de Hoop transformation to complex coordinates and using the reflection extension of function, we proved the stability and exponential convergence of the solution of the PML problem.

A fast algorithm for electromagnetic scattering from axis-symmetric objects

Lai, Jun

MS

Zhejiang University

Fast, high-accuracy algorithms for electromagnetic scattering from axisymmetric objects are of great importance when modeling physical phenomena in optics, materials science (e.g. meta-materials), and many other fields of applied science. In this talk, we develop an FFT-accelerated separation of variables solver that can be used to efficiently invert integral equation formulations of Maxwell's equations for scattering from axisymmetric bodies. Using a standard variant of Müller's integral representation of the fields, our numerical solver rapidly and directly inverts the resulting second-kind integral equation. The solver is also extended to geometries with non-smooth generating curves and the scattering from large cavities.

Optimal control in a bounded domain for wave propagating in the whole space: coupled through boundary integral equations

Li, Buyang

MS

Department of Applied Mathematics, The Hong Kong Polytechnic University

This paper is concerned with an optimal control problem in a bounded-domain 0 under the constraint of a wave equation in the whole space. The problem is regularized and then reformulated as an initial-boundary value problem of the wave equation in a bounded domain Ω coupled with a set of boundary integral equations taking account of wave propagation through the boundary. The well-posedness and stability of the reformulated problem are proved. A fully discrete finite element method is proposed for solving the reformulated problem. In particular, the wave equation in the bounded domain is discretized by an averaged central difference method in time, and the boundary integral equations are discretized in time by using the convolution quadrature generated by the second-order backward difference formula. The finite and boundary element methods are used for spatial discretization of the wave equation and the boundary integral equations, respectively. The stability and convergence of the numerical method are also proved. Finally, the spatial and temporal convergence rates are validated numerically in 2D.

Error Analysis of the UPML-method for analyzing Helmholtz equation in a layered medium with a compact source

Lu, Wangtao MS

Zhejiang University

In this talk, I will report a recent result on using UPML method for analyzing the Helmholtz equation in a layered medium with a compact source. We will show that based on a nearly sharp condition regarding the PML, the PML-truncated solution converges to the true solution exponentially as we increase the PML absorbing power or the PML thickness.

An Unfitted Interface Penalty Finite Element Method for Elliptic Interface Problems

Wu, Haijun MS

Nanjing University, China

An unfitted interface penalty finite element method (UIPFEM) is proposed for the elliptic interface problems. Both the convergence rate of the UIPFE solution and the condition number of the algebraic system are optimal and independent of the interface position. Furthermore the error estimates do not depend on the ratio of the discontinuous coefficients. Numerical examples are also given to confirm the theoretical results.

The efficient algorithm for electromagnetic scattering by the electrically large and mutiscalescatterers

Wu, Yumao MS

Key Laboratory for InformationScience of Electromagnetic Waves (MoE), School of Information Science and Technology, Fudan University

Fast and accurate solver of high frequency electromagnetic physical optics scattered fields is always important problems in computational electromagnetic area. Recently, we have comprehensively studied the physical optics scattered fields from the quadratic patch scatterers. On invoking the numerical steepest descent path method on the complex plane, we have calculated the high frequency physical optics scattered fields efficiently. Then, we have further applied the proposed numerical steepest descent path method to the electrically large target. Next, we have considered the diffraction problems from the electrically large scatterers. With the numerical steepest descent path method, we have achieved the improvement on the accuracies of the electromagnetic scattered fields from both the perfect conductor and dielectric scatterers. Importantly, the scattered fields from the convex scatterer, like the creeping wave fields are achieved accurately. We have then adopted the high frequency method together with the full wave integral equation method and finite element method to mutiphysicscalculations. Meanwhile, we have considered the periodic and quasi-periodic structures. By the integral equation method, we have calculated the electromagnetic scattered fields from the layered medium structures.

Multigrid method for inductionless MHD equations

Zheng, Weiying

MS

Academy of Mathematics and Systems Science, Chinese Academy of Sciences

In this talk, I will present a geometric multigrid (MG) method for the inductionless magnetohydrodynamic (MHD) equations on tetrahedral meshes. The model is of the Stokes type, meaning that it consists of the Stokes equations and the Poisson equation of the electrostatic potential. I will show the uniform convergence and compare the performances of the geometric MG method and the algebraic MG method.

MS10: Two-grid method and its applications

Organizers: Liuqiang Zhong, Hehu Xie

A two-grid finite difference algorithm for compressible Darcy-Forchheimer model in porous media

Cui, Jintao MS

The Hong Kong Polytechnic University

In this work, a two-grid finite difference method is proposed to solve the compressible Darcy-Forchheimer model which describes the high speed non-Darcy flow in porous media. The discretized nonlinear problem on the fine grid is solved in two steps: first solving a small nonlinear system on the coarse grid; then solving a modified nonlinear problem on the fine grid. On the coarse grid, the coupled term of pressure and velocity is approximated by using the fewest number of nodes. On the fine grid, the original nonlinear term is modified with a small parameter to construct a linear block-centered finite difference scheme. Optimal order error estimates for pressure and velocity are obtained. The two-grid finite difference scheme is proved to be unconditionally convergent without any time step restriction. The theoretical results are confirmed by numerical experiments.

A multi-mesh phase-field approach for optimal shape design of incompressible flows

Hu, Xianliang MS

School of Mathematical Sciences, Zhejiang University

Optimal design for the shapes of fluid flow is very useful in various applications, and different approaches have been proposed to solve it numerically, such as the density-based approach, the level set method and the phase field method. In this talk, a multi-mesh scheme of phase field simulations for fluid-based shape optimization will be introduced. In our scheme, the fluid flow is governed by the incompressible Navier-Stokes equations, and a phase field variable is used to indicate material distributions, as well as the optimized shape of the fluid, which could be obtained by minimizing the certain regularized objective functional. Meshes with different element sizes are used for the finite element calculations on solving different partial differential equations. Numerical results show that our multi-mesh approach saves the computational efforts significantly without losing in accuracy.

A Cascadic Multigrid Method for Nonsymmetric Eigenvalue Problem

Xie, Manting MS

Tianjin University, China

In this talk, we proposed a cascadic multigrid method to solve nonsymmetric eigenvalue problems. Based on the multilevel correction method, the proposed method transforms a nonsymmetric eigenvalue problem solving on the finest finite element space to linear smoothing steps on a sequence of multilevel finite element spaces and some nonsymmetric eigenvalue problems solving in a very low dimensional space. Choosing the sequence of finite element spaces and the number of smoothing steps appropriately, we obtain the optimal convergence rate with the optimal scale of computational work. Some numerical examples are provided to validate the theoretical results and the efficiency of this proposed scheme.

Local and parallel finite element algorithm based on the partition of unity for incompressible flows

Zheng, Haibiao

MS

School of Mathematical Sciences, East China Normal University

By combining two-grid method with domain decomposition method, a new local and parallel finite element algorithm based on the partition of unity is proposed for the incompressible flows. The interesting points in this algorithm lie in (1) a class of partition of unity is derived by a given triangulation, which guides the domain decomposition (2) the globally fine grid correction step is decomposed into a series of local and parallel linearized residual problems on some subdomains constructed according to the partition of unity functions. Some numerical simulations are presented to demonstrate the high efficiency and flexibility of the new algorithm.

MS11: Domain decomposition methods for high performance computing

Organizers: Hyea Hyun Kim, Chang-Ock Lee

A non-overlapping DD method for heterogeneous elliptic problems

Park, Eun-Hee MS

Division of Liberal Studies, Kangwon National University

In this talk we will discuss a non-overlapping domain decomposition (DD) method for heterogeneous elliptic problems. There are two key ingredients in the proposed DD method: one is a subspace decomposition of the finite element space and the other is a procedure based on the dual-primal finite element tearing and interconnecting approach. The performance of DD methods as iterative solvers is mainly determined by the condition number of the resulting linear system. From this point of view, numerical results are presented, which illustrate the performance of the proposed DD method. This talk is based on joint work with Susanne C. Brenner and Li-yeng Sung.

Convergence analysis of a double sweep preconditioner for solving the Helmholtz equation in waveguide

Kim, Seungil MS

Kyung Hee University, Koera

In this talk we will discuss a double sweep preconditioner for solving the Helmholtz equation in waveguides. The double sweep preconditioner is defined in terms of transmission conditions based on high order absorbing boundary conditions such as PML (perfectly matched layer) or CRBC (complete radiation boundary condition). It seeks for an approximate solution in $\prod_{j=1}^{J} H^1(\Omega_j)$, which is discontinuous across interfaces of nonoverlapped subdomains Ω_j. We discuss the convergence of approximate solutions to the problem in both continuous level and discontinuous level.

An adaptive BDDC algorithm for three dimensional elliptic problems with an enhanced edge eigenvalue problem

Kim, Hyea Hyun MS

Kyung Hee University, Koera

An adaptive BDDC algorithm is developed for three dimensional elliptic problems with random and high contrast coefficients. For such model problems, generalized eigenvalue problems on faces and edges are often used to select problematic eigenvectors, that are used when forming coarse components for the BDDC preconditioner. In many previous works, face eigenvalue problems are shown to give quite effective coarse components while those for edges are not satisfactory. In this work, a new edge eigenvalue problem is proposed by utilizing prior selected coarse components and it is shown to give more effective coarse components than those from previous studies. Numerical results are also presented.

Fast Nonoverlapping Block Jacobi Method for the Dual Rudin-Osher-Fatemi Model

Lee, Chang-Ock

MS

Korea Advanced Institute of Science and Technology

We consider nonoverlapping domain decomposition methods for the Rudin-Osher-Fatemi (ROF) model, which is one of the standard models in mathematical image processing. The image domain is partitioned into rectangular subdomains and local problems in subdomains are solved in parallel. Local problems can adopt existing state-of-the-art solvers for the ROF model. We show that the nonoverlapping relaxed block Jacobi method for a dual formulation of the ROF model has the $\mathcal{O}(1/n)$ convergence rate of the energy functional, where n is the number of iterations. Moreover, by exploiting the forward-backward splitting structure of the method, we propose an accelerated version whose convergence rate is $\mathcal{O}(1/n^2)$. The proposed method converges faster than existing domain decomposition methods both theoretically and practically, while the main computational cost of each iteration remains the same. We also provide the dependence of the convergence rates of the block Jacobi methods on the image size and the number of subdomains.

A fast multilevel algorithm for total variation minimization problems

Xie, Manting, Duan, Yuping

MS

Tianjing University

We present a fast multilevel domain decomposition method for total variation minimization problems such as the convex Chan-Vese model, Rudin-Osher-Fatami model. We use the piecewise constant function spanned subspace correction to design a multilevel method for directly solving the total variation minimization problems. On each level, non-overlapping domain decomposition is implemented to realize the parallel computation. Supporting numerical results are presented to demonstrate our method is more efficient for large-scale minimization problems.

MS12: Recent achievements on numerical algorithms and performance optimization for large-scale scientific and engineering computing

Organizers: Xin He, Guangming Tan, Xiaowen Xu

Parallel Multigrid with Adaptive Multilevel hCGA on Manycore Clusters

Nakajima, Kengo

MS

Information Technology Center, The University of Tokyo

A multigrid is a scalable multilevel method for solving linear equations and preconditioning Krylov iterative linear solvers, and is especially suitable for large-scale problems because of its scalable feature. The parallel multigrid method is expected to be one of the most powerful tools on exa-scale systems. In the previous work (K. Nakajima, IEEE ICPADS 2014), we have already developed an FVM code for 3D Groundwater Flow through Heterogenous Porous Media (pGW3D-FVM) with MGCG solvers (Multigrid Preconditioned Conjugate Gradient) using OpenMP/MPI with RCM (Reverse Cuthill-Mckee), and it is ready for exa-scale systems by hCGA (Hierarchical Coarse Grid Aggregation). hCGA provided significant improvement of performance (60 % in weak scaling, 600 % in strong scaling) for 3D FVM application on 4,096 nodes of Oakleaf-FX for problems with 1.8×10^{10} DOF. Because the hCGA can only handle 2-hierarchica-levels, we are developing AM-hCGA (Adaptive Multilevel hCGA) for multiple hierarchical levels (more than three). In this presentation, we will present preliminary results of AM-hCGA on the Oakforest-PACS, Joint Center for Advanced High Performance Computing (JCAHPC), which consists of 8,208 nodes of Intel Xeon Phi (Knights Landing).

Highly parallel space-time domain decomposition methods for parabolic problems

Li, Shishun

PT

Henan Polytechnic University, China

Abstract: In the past few years, massively parallel computers with millions of processors have been developed since increase in clock speed is stagnating but the number of processors is going up rapidly. To increase the degree of parallelization, some parallel-in-time algorithms have been developed. In this talk, we present in detail some space-time multiplicative Schwarz methods for solving parabolic partial differential equations. The optimal convergence theory shows that the convergence rate is bounded independent of the mesh parameters, the number of subdomains and the window size. Some numerical experiments carried out on a parallel computer with a large number of processor cores for parabolic problems are given

to show the parallel scalability of the methods. Finally, we provide a comparison of the space-time algorithms with a traditional algorithm that is parallelized only in space.

Efficient and scalable solvers for linear systems arising from Computational Fluid Dynamics on CPU+GPU Clusters

He, Xin MS

Institute of Computing Technology, Chinese Academy of Sciences

In the field of Computational Fluid Dynamics, efficient and accurate solutions of large and sparse linear systems arising linearization and discretization of governing equations are of key importance in terms of overall performance. This project is meant to provide portable and scalable solvers for non-symmetric and symmetric systems, including BICGStab and CG Krylov subspace methods, with focus on exploring fine-grained parallelism, targeting modern processors and accelerators including multi/many-core CPU and GPU platforms. Regarding the solvers, the following optimizations are considered. First, we propose improved variants of the solvers such that all inner products of a single iteration step are independent and communication time required for inner product can be overlapped efficiently with computation time of vector updates. Therefore, the cost of global communication which represents the bottleneck of the parallel performance can be significantly reduced. Second, to fully explore the power of GPU accelerators, we move the computational efforts to GPUs as much as possible and leave the CPUs to be in charge of communications. The data transformation between device and host is minimized. Last, the calculations of three components of the velocity unknown, accomplished by solving the non-symmetric systems with the same coefficient matrix but different right hand-side vectors by three times, are simultaneously realized due to the large amount of computing units on GPUs. The efficiency and scalability of the solvers are demonstrated by numerical results carried out on a massively parallel distributed CPU+GPU system. In addition, the comparison with the well-known library PETSc in terms of the computational time and parallel scalability is evaluated and reported.

Performance Optimization Study of Several HPC Codes: Experience and Generalization

Zhang, Peng MS

CAEP Software Center for High Performance Numerical Simulation

Performance optimization is of great importance for HPC applications today. On one hand, many existed applications were developed by domain scientists who cares little about performance, leading to potential performance problem. On the other hand, modern processors are more and more complicated, thus making good performance is not easy to obtain. In this talk, I will first introduce our recent work in performance optimization study of three practical scientific applications. Detail performance analysis and optimization techniques will be both described. Then, some general experience we learn from these case studies will be discussed. At last, I will show our thoughts and some early trials to make application-driven performance optimization study more systematic.

MS13: Geometric numerical methods for fluids and electromagnetic fields

Organizers: Kaibo Hu, Yajuan Sun

Energy-preserving mixed finite element methods for the Hodge wave equation

Wu, Yongke MS

School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu 611731, China

In this talk, mixed finite element methods corresponding to de Rham complex are considered for the first-order formulation of the Hodge wave equation. The semi-discrete method conserves the system energy. A full discrete method employing the second order symplectic Runge-Kutta time method (i.e., Crank-Nicolson) in time exactly conserves the actual energy. In addition to prove the optimal convergence order, we also construct a quasi-interpolation operator based on the Hodge decomposition, which has optimal approximation order and is stable in both $L^2\Lambda$ and $H\Lambda$ norms. Numerical experiments confirm the theoretical results.

Finite elements for curvature

Hu, Kaibo MS

University of Minnesota, USA

We review the elasticity (linearized Calabi) complex, and its potential applications in continuum dislocation theory and differential geometry. We construct discrete finite element complexes. In particular, this leads to new finite element discretization for the Riemannian tensor and the linearized curvature operator. Compared with the classical discrete geometric approaches, e.g., the Regge calculus, the new elements are conforming. The construction is based on a Bernstein-Gelfand-Gelfand type diagram chase with various Stokes type complexes, or new Poincaré type path integral operators for the elasticity complex, which thus mimics the standard Nedlec and Raviart-Thomas elements for the de Rham complex. This is a joint work with Snorre H. Christiansen.

Convergence of a B-E based finite element method for MHD models on Lipschitz domains

Qiu, Weifeng MS

City University of Hong Kong

We discuss a class of magnetic-electric fields based finite element schemes for stationary magnetohydrodynamics (MHD) systems with two types of boundary conditions. We establish a key L^3 estimate for divergence-free finite element functions for a new type of boundary conditions. With this estimate, we rigorously prove the convergence of Picard iterations and the finite element schemes with weak regularity assumptions. These results demonstrate the convergence of the finite element methods for singular solutions.

Helicity conservative finite element discretizations

Lee, Youngju

MS

Texas State University

We present finite element methods for the magnetohydrodynamics (MHD) system where the magnetic and cross helicity, the energy law and the magnetic Gauss law are globally and locally preserved at the discrete level. New scheme will lead the simulation in which he topology and knot structures of the MHD flow can thus be preserved. The variables are discretized as discrete differential forms fitting in a discrete de Rham complex. Some sample numerical test will be presented for demonstration.

Construction of contact numerical methods and implementation in Fokker-Planck system

Sun, Yajuan

MS

LSEC & NCMIS, Academy of Mathematics and Systems Sciences, CAS

In this talk, we study the contact system and establish the connection between the contact transformation and its generating function. We present the generalized Hamilton-Jacobi equation for the generating function. By truncating the generating function, we construct the numerical methods which can preserve the contact structure of the given contact system. We implement the contact numerical methods in solving the Fokker-Planck system and give the numerical experiments.

On the robust discretization and fast solver for the H(curl) and H(div) convection-diffusion problems

Wu, Shuonan

MS

Peking University

In this talk, we present robust discretization and fast solver for H(curl) and H(div) convection-dominated PDEs discretized on unstructured simplicial grids. The derivation of this schemes

makes use of some intrinsic properties of differential forms and in particular some crucial identities from differential geometry. Both theoretical analysis and numerical experiments show that the new upwind finite element schemes provide an accurate and robust discretization and fast solver in many applications and in particular for simulation of magnetohydrodynamics systems.

MS14: Multiscale, multiphysics, and interface problems and related fields

Organizers: Youngju Lee, Dongwoo Sheen, Chen-Song Zhang

Comments on Beavers-Joseph-Saffman conditions on the Brinkman-Stokes-Darcy Interface Problems

Sheen, Dongwoo MS

Department of Mathematics, Seoul National University, Seoul 08826, Korea

The interface conditions for flow interaction between fluid and porous regions have been well established [1, 2, 3] for these two decades. In this lecture we review several fundamental theoretical results, such as well-posedness and regularity, on these conditions. Also numerical aspects on these conditions will be addressed.

References

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[2] A. Mikelic and W. Jäger. On the interface boundary condition of Beavers, Joseph, and Saffman. SIAM Journal on Applied Mathematics, 60(4):1111-1127, 2000.

[3] P. G. Saffman. Boundary condition at surface of a porous medium. Studies in Applied Mathematics.

Locally conservative finite elements for axisymmetric Stokes equation

Lee, Youngju MS

Texas State University, USA

In this talk, we shall consider the mixed finite element approximation of the axisymmetric Stokes problem (ASP) on a bounded polygonal domain in the rz-plane. Standard stability results on mixed methods do not apply due to the singular coefficients in the differential operator and due to the singular or vanishing weights in the associated function spaces. We develop new finite element analysis in these weighted spaces, and propose macroelement conditions that are sufficient to ensure the well-posedness of the mixed methods for the ASP. These conditions are local, relatively easy to verify, and therefore will be useful for validating the stability of a variety of mixed finite element methods. These new conditions can not only re-verify existing stable mixed methods for the ASP, but also lead to the discovery of new stable conservative mixed methods. In particular, we report newly discovered, locally conservative finite elements for axisymmetric Stokes equation, numerical test results that confirm the theory and applications.

The immersed hybrid difference method for elliptic interface problems

Jeon, Youngmok MS

Ajou University, Korea

We propose an immersed hybrid difference (IHD) method for elliptic interface problems. When deriving the IHD method we consider a virtual overlapping of two solutions on interface cells. To recover the real solution from the virtually extended solutions we introduce the virtual to real transformation, which is derived from the interface conditions in addition to the mass conservation property. The method is easy to be implemented and high order methods are conveniently derived. Numerical tests on several types of interfaces with low and high order methods are presented, which demonstrate efficiency of the suggested method.

Numerical Methods for Problems with Moving Interfaces

Zhang, Chen-Song MS

LSEC & NCMIS, Academy of Mathematics and Systems Sciences, CAS

Many important multiphysics applications involve time-dependent interfaces, which could cause significant regularity deterioration of the solution. Such a nonlinear feature also make numerical treatment more challenging. In this talk, we discuss a few numerical methods for multiphysics problems with evolving interfaces. To treat moving domains, we will mainly focus on the arbitrary Lagrangian-Eulerian method and the fictitious domain method.

Adaptive grid in Modeling of Biomolecular Electrostatics and Diffusion using FEM/BEM

Lu, Benzhuo MS

Chinese Academy of Sciences

The Poisson-Boltzmann equation and Poisson-Nernst-Planck equations are two common models used in simulating molecular electrostatics and ion transport in ionic solution. Molecular interface problem, singular charge distribution, the nonlinear coupled system, and meshing are issues to be addressed in numerical solutions of these equations. We will present our works on fast boundary element methods for solution of the linear PB equation, and stable finite element methods for solution of the PNP equations. Case studies are performed on calculations of macromolecular electrostatics, current-voltage curve of ion channels/nanopores, etc.

High dimensional finite elements for multiscale Maxwell wave equations

Hoang, Viet Ha MS

Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, 937371

We develop an essentially optimal numerical method for solving multiscale Maxwell wave equations in a domain D in $\mathbb{R}^d$. The problems depend on $n+1$ scales: one macroscopic scale and n microscopic scales. Solving the macroscopic multiscale homogenized problem, we obtain all the desired macroscopic and microscopic information. This problem depends on $n+1$ variables in $\mathbb{R}^d$, one for each scale that the original multiscale equation depends on, and is thus posed in a high dimensional tensorized domain. The straightforward full tensor product finite element (FE) method is exceedingly expensive. We develop the sparse tensor product FEs that solve this multiscale homogenized problem with essentially optimal number of degrees of freedom, that is essentially equal to that required for solving a problem posed in a domain in $\mathbb{R}^d$ only, for obtaining a required level of accuracy. The problems are more complicated than multiscale scalar wave equations due to the noncompact embedding of the space $H(curl, D)$ in $L^2(D)$ and the low regularity of the solution. Numerical correctors are constructed from the FE solution. For two sale problems, we show a rate of convergence for the numerical corrector in terms of the microscopic scale and the FE mesh width. Numerical examples confirm our analysis.

Multiscale Hybridizable Discontinuous Galerkin method for porous media flow

Moon, Minam MS

Department of Mathematics, Korea Military Academy, Seoul 01805, KOREA

Flows in porous media have wide ranging applications in many fields of industry, science, engineering and the environment. In many applications, flows are in highly heterogeneous media with properties that vary with different scales and have disparate values. Motivated by applications to numerical simulation of flows in porous media, we design a multiscale model reduction framework within the hybridizable discontinuous Galerkin finite element method. As the problem is expected to be solved for many input parameters such as source terms, boundary conditions, spatial heterogeneities, and porocity. Our approach uses local snapshot space and local spectral decomposition following the concept of Generalized Multiscale Finite Element Method. We propose several multiscale finite element spaces on the coarse edges that provide a reduced dimensional approximation for numerical traces within the HDG framework. We provide a general framework for systematic construction of multiscale trace spaces. We investigate the stability and derive error estimates for the methods and further experimentally study their performance on a representative number of numerical examples.

Algebraic multiscale methods

Cho, Kanghun

MS

Seoul National University

We introduce an algebraic multiscale method, which is a matrix-based approach based on the generalized multiscale finite element method(GMsFEM). First, nonconforming GMsFEM is briefly reviewed. In each macro domain,snapshot spaces are constructed by solving local spectral problems and offline spaces are obtained by applying a suitable dimension reduction technique. Moment functions are introduced to impose continuity between offline functions in neighboring macro elements. Nonconforming GMsFE spaces are then generated by those glued offline functions. Second, the algebraic multiscale method based on DSSY(Douglas-Santos-Sheen-Ye) nonconforming rectangular element is derived. Multiscale basis functions are constructed by using only algebraic information on the micro-scale matrix system. Some representative numerical examples are presented to confirm the efficiency of the proposed method.

MS15: Design of efficient and higher order numerical methods for PDE

Organizers: Hanquan Wang, Yong Zhang

An adaptive level set method based on two-level uniform meshes and its application to dislocation dynamics

Wang, Hanquan MS

Yunnan University of Finance and Economics

In this paper, we present an adaptive level set method for motion of high codimensional objects (e.g., curves in three dimensions). This method uses only two (or a few fixed) levels of meshes. A uniform coarse mesh is defined over the whole computational domain. Any coarse mesh cell that contains the moving object is further divided into a uniform fine mesh. The coarse-to-fine ratios in the mesh refinement can be adjusted to achieve optimal efficiency. Refinement and coarsening (removing the fine mesh within a coarse grid cell) are performed dynamically during the evolution. In this adaptive method, the computation is localized mostly near the moving objects; thus, the computational cost is significantly reduced compared with the uniform mesh over the whole domain with the same resolution. In this method, the level set equations can be solved on these uniform meshes of different levels directly using standard high-order numerical methods. This method is examined by numerical examples of moving curves and applications to dislocation dynamics simulations. This two-level adaptive method also provides a basis for using locally varying time stepping to further reduce the computational cost.

Error Estimates of the Finite Element Method for Interior Transmission Problem and Interior Transmission Eigenvalue Problem

Wu, Xinming MS

Fudan University, Shanghai, China

The interior transmission problem (ITP) plays an important role in the investigation of the inverse scattering problem. In this talk we propose the finite element method for solving the ITP and the corresponding transmission eigenvalue problem. A type of multilevel correction method is proposed to improve the overfull efficiency of the eigenvalue solving. Some numerical examples are provided to validate the theoretical results and the efficiency of the proposed numerical scheme.

Adaptive Multigrid Methods for the Ground State Solution of Bose-Einstein Condensates

Xie, Manting MS

Tianjin University, China

In this talk, we propose two types of adaptive multigrid methods for the ground state solution of Bose-Einstein Condensates (BEC). Different from the classical adaptive finite element method applied to BEC which needs to solve the nonlinear eigenvalue model on each adaptive space directly, our first scheme requires to solve a linear boundary value problem on current refined mesh and a nonlinear eigenvalue model on a quite low dimensional space. Since there is no nonlinear eigenvalue model to be solved directly on the adaptive spaces, the solving efficiency can be improved evidently. The second scheme is based on the first scheme and adaptive multigrid method. In this algorithm, the linear boundary value problems involved in the first scheme are solved by some adaptive multigrid iteration steps. Thus the efficiency is further improved. In addition, the convergence and complexity analysis of the proposed adaptive algorithms are derived theoretically and numerically.

Fast boundary integral solvers for Stokes flows: quadrature, periodization and adaptivity

Wang, Jun MS

Flatiron Institute

We consider in the talk the simulation of spatially periodic suspensions in shear flows. This is an important problem in rheology that is studied extensively by experiments. Applications include industrial processes, complex fluids (e.g. lattice of fibers into page), and the design of electro-rheology devices. However there exists little accurate numerical simulation for general shapes. Boundary integral equation (BIE) method, when combined with suitable fast solvers, provides a highly accurate and efficient solver for such problems. In this talk, we review different aspects of our numerical method, including numerical quadrature for weakly singular integrals, a new framework of periodization, and adaptivity.

Linearly implicit structure-preserving exponential integrators for the nonlinear Klein-Gordon equations

Jiang, Chaolong MS

Yunnan University of Finance and Economics

Inspired by the recent paper (Li and Wu, SIAM J. Sci. Comput., 2016), where the authors proposed an exponential energy-preserving integrator for conservative systems. In this paper, taking the nonlinear Klein-Gordon equations as an example, we aim at developing a novel exponential structure-preserving integrator for conservative systems by combing the idea of the exponential integrator and the scalar auxiliary variable approach (see e.g., Shen et al. J. Comput. Phys., 2018), which is more recently developed to construct efficient and robust energy stable schemes for gradient systems. We show that the proposed exponential integrator can exactly preserve the energy of the system. In comparison with the exponential energy-preserving method proposed by Li and Wu, the new exponential integrator is linearly implicit and forms a linear system with a constant coefficient matrix at each time step, which can be solved efficiently. Finally, several numerical results are addressed to demonstrate the high efficiency and energy preservation of the proposed scheme.

MS16: Multi-grid and modelling

Organizer: Gabriel Wittum, Andreas Vogel

Gradient-consistent finite element spaces for problems with immersed interfaces

Höllbacher, Susanne

MS

AMCS, KAUST

For applications like multiphase flow, free surface flow or diffusion problems with discontinuous density, boundary conditions need to be imposed on a so called immersed boundaries whose location can also change in time. In order to avoid costly remeshing, well known techniques like XFEM or CutFEM introduce enriched finite element spaces in order to impose the boundary conditions. We also follow the idea of enriched finite element spaces on elements cut by the immersed interface. We propose gradient-consistent finite element spaces. Instead of purely enriching the number of DoFs on cut elements, our aim is a good approximation of normal forces or fluxes being present at the immersed boundary. This is motivated by the prominent issue within multiphase flows where spurious oscillations arise near the interface due to a bad approximation of the pressure. The derivation of the gradient-consistent spaces is inspired by the Petrov-Galerkin weak formulation of the finite volume method (box method). Within a finite volume formulation the boundary fluxes naturally arise. We will show, that the gradients of the resulting finite element spaces are consistent with the physical problem. The gradient-consistent enrichment finally results in a fitted approach. Therefore, the discrete system is symmetric and intrinsically stable. In particular, there is no need for additional penalty terms to guarantee stability. Our computations show, that the spurious pressure oscillations were eliminated by the new method. The results therefore demonstrate that the enriched spaces describe the physics of the discrete interface appropriately.

3D Modeling and Simulation of a Harpsichord

Larisch, Lukas[1], Lemke, Babett[2], Wittum, Gabriel[2]

MS

[1] Lemke G-CSC, Frankfurt
[2] AMCS, KAUST and G-CSC Frankfurt

The mathematical characterization of the sound of a musical instrument still follows Schumann's laws [2]. According to this theory, the resonances of the instrument body, the formants, filter the oscillations of the sound generator (e.g. string) and produce the characteristic "timbre" of an instrument. This is a strong simplification of the actual situation: It applies to a point source and can be easily performed by a loudspeaker, disregarding the three dimensional structure of music instruments. To describe the effect of geometry and material of the instruments, we set up a three dimensional model and simulate it using the simulation system UG4 [3, 1]. In our talk, we present FEM based numerical simulations of a harpsichord. We aim to capture the oscillation behavior of eigenfrequencies of its soundboard. We resolve the complicated geometry by an unstructured 3d grid and take into account the anisotropy of wood. The eigenvalue problem is solved using the PINVIT method with an efficient GMG preconditioner. The latter allows us to resolve the harpsichord with a high resolution grid, which is required to capture fine modes of the simulated eigenfrequencies. To verify our results, we compare them with measurement data obtained from an experimental modal analysis of the harpsichord that we have modeled. We finally investigate the impact of various aspects of the geometry on the computed eigenfrequencies.

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Simulation of flow in a forward osmosis membrane device from a desalination plant

Kühn, Arlene MS

G-CSC Frankfurt University

In this talk, we present the simulation of the water flow in the intake area of a membrane device used in a seawater desalination plant. The focus is on the modelling geometry and generating an appropriate grid. Especially the grid quality is investigated. In addition to the flow lines, the three-dimensional model also takes into account the velocity from the inflow to the outflow and the associated pressure. With the numerical simulations we were able to show that the grid quality has a huge effect on the result, so that the grid should not have small dihedral angles. In addition, the behaviour of the water flow can be understood better. The proposed mathematical model helps to understand the flow in the seawater desalination plant in order to finally increase the efficiency and quantity of the desalinated water.

UG4 Application in Skin Problem: Homogenized modeling of Microscopic Anisotropic Diffusion for Effective Diffusivities in Stratum Corneum

Wang, Junxi MS

G-CSC, Frankfurt University

In pharmacy, mathematical models of molecular diffusion through the stratum corneum (SC) layer can be greatly used to predict transdermal delivery of drugs and to risk assessment of chemical exposures. The membrane microstructure is generally accepted as a periodic arrangement of corneocytes embedded in an anisotropic lipid matrix. We show how the effective diffusivity can be calculated in UG4 using mathematical models from homogenization theory. Numerical results are expressed in the dimensionless effective diffusivity tensor $\bar{A}^{SC}$, which is a function of homogenization results χ_i in each field. χ_i is determined by the dimensionless parameters, λ and γ. λ is the ratio of transbilayer to lateral flows in a lipid bilayer and γ is the ratio of permeability in the corneocyte phase $K^{cor/w}D^{cor}$, to that in the lipid phase, $K^{lip/w}D_{\|}^{lip}$. The effective diffusion tensors are finally calculated for a classical and a spatial "brick-and-mortar" structures and a tetrakaidekahedral-shaped cell. A comparison with a previous study confirms that transdermal and lateral diffusivities are strongly influenced by λ due to the barrier function of the lipid phase against transbilayer flow. The lateral diffusivities of poorly water-soluble drugs are limited by γ in contract to transdermal diffusivity. Furthermore, the differences in the various geometries are evident for effective lateral diffusivities of drugs that diffuse much more difficultly in the corneocyte phase than in the lipid phase, i.e. $\gamma < 10^{-5}$. This presented method may more precisely and more intensively predict the drug permeability and evaluate the membrane microstructure.

Efficient solution of transient non-linear flow problems in the subsurface

Nägel, Arne MS

G-CSC Frankfurt

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 often also non-linear. Developing efficient solvers is a delicate task, since one must to 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 take an application oriented approach, and discuss problems from poroelasticity and density-driven-flow. For these two classes, we describe a unified framework, using linearly-implicit time integration and parallel adaptive multilevel solvers, and provide numerical results.

Simulation of propagation of uncertainties in density-driven groundwater flow

Logashenko, Dmitry[1], Litvinenko, Alexander, Tempone, Raul, Wittum, Gabriel MS

King Abdullah University of Science and Technology, Saudi Arabia

Accuracy of prediction of the groundwater flow in geological aquifers is restricted by the precision of the hydrogeological parameters of the porous media whose measurements are often problematic. In this talk, we present a numerical approach for estimation of the propagation of the uncertainty from the parameters to the solution in the subsurface density-driven flow models. We consider an Elder-like problem with random fields for porosity and permeability to model the limited knowledge of the data. Basing on this essentially non-linear benchmark, we construct low-cost generalized polynomial chaos (gPC) expansion surrogate model. Computation of the gPC coefficients is performed by projection on sparse and full tensor grids. Parallelization is applied to both the numerical solution of the deterministic problems (realizations) and the high-dimensional quadrature over the parametric space. We present results of numerical experiments in 2d and 3d.

Multigrid Solvers for the Finite Cell Method

Yahyaei, Saberi MS

Hight Performance Computing in Engineering Sciences, Ruhr University Bochum, Germany

The generation of appropriate computational meshes for complex geometries is a challenging task and constitutes a significant portion of a finite element simulation workflow. The finite cell method is a fictitious domain approach with adaptive integration and weak boundary conditions and essentially eliminates the need for conforming meshes by shifting the workload to the assembling process. However, the solution of the resultant system of equations is one of the most computationally costly parts of the solution procedure. In this talk, we present a study for the convergence behavior of geometric multigrid solvers for finite cell simulations and investigate its suitability to this type of discretization method.

Adaptive mesh refinement and geometric multigrid for brittle damage simulations

Junker, Philipp MS

Ruhr University Bochum, Germany

Effective geometric multigrid schemes are beneficial for many problems that arise from mechanical investigations. One important example is damage modeling in which mechanical stiffness is lost after some threshold value in terms of external loads is exceeded. From a mathematical perspective, the problem formulation becomes ill-posed with the onset of damage. Hence, appropriate regularization is unavoidable. Particularly, brittle damage evolution evolves locally both in time and space, demanding sophisticated regularization schemes and evoking numerical challenges. In the current talk, we present an adaptive finite element treatment to accurately resolve the localization when a gradient-enhanced regularization is employed. We propose further a novel discretization of the Laplace term for regularization which is implemented into a geometric multigrid solver. Several numerical examples reveal extraordinary convergence reducing any numerical noise, allowing the maximum load to be investigated as sole function of the regularization parameter.

MS17: Advances in multilevel methods: from PDEs to data intensive studies

Organizers: Long Chen, Xiaozhe Hu, Ludmil Zikatanov

Preconditioners for multi-physics and multi-scale problems

Mardal, Kent-Andre MS

Department of Mathematics, University of Oslo, Norway

In this talk we will present some recent results for monolithic schemes for multi-physics and multi-scale problems. In particular, we will consider coupled Darcy-Stokes problems and multi-scale 3D-1D couplings. In order to achieve robust preconditions, independent of material parameters, we employ the operator preconditioning technique, deriving stability estimates in interpolation spaces. Furthermore, to handle the interface conditions we propose the use of fractional Laplacians of mixed type to handle the transfer between the physical systems. The theoretical results are confirmed by numerical experiments, as will be shown.

Multigrid method for fourth order eigenvalue problem

Zhang, Shuo MS

Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and System Sciences, and National Centre for Mathematics and Interdisciplinary Sciences, Chinese Academy of Sciences

For practical and theoretical reasons, multigrid schemes for eigenvalue problems are of wide interests. In this talk, we would like to present some multigrid finite element schemes for the fourth order eigenvalue problems. Motivated by the works by Xu-Zhou (Math. Comp. 2001) and Lin-Xie (Math. Comp. 2015), we will firstly rewrite certain fourth order eigenvalue problems to equivalent order-reduced formulations which admit nested discretization. Then a proper application of the routine, namely to solve an eigenvalue problem on coarse grid and to be followed by fine-grid correction, may be able to lead to optimal multigrid schemes for the eigenvalue problems. The idea onto two basic model problems, i.e., the biharmonic equation and the Helmholtz transmission eigenvalue problem, and some expected performance and some unexpected surprising phenomena are observed.

Multigrid Methods for Hellan-Herrmann-Johnson Mixed Method of Kirchhoff Plate Bending Problems

Huang, Xuehai MS

Shanghai University of Finance and Economics

A V-cycle multigrid method for the Hellan-Herrmann-Johnson (HHJ) discretization of the Kirchhoff plate bending problems is developed in this paper. It is shown that the contraction number of the V-cycle multigrid HHJ mixed method is bounded away from one uniformly with respect to the mesh size. The uniform convergence is achieved for the V-cycle multigrid method with only one smoothing step and without full elliptic regularity. The key is a stable decomposition of the kernel space which is derived from an exact sequence of the HHJ mixed method, and the strengthened Cauchy Schwarz inequality. Some numerical experiments are provided to confirm the proposed V-cycle multigrid method.

Recovery-type a posteriori error estimation for adaptive virtual element method

Wei, Huayi MS

Xiangtan University

Virtual Element Method is a new numerical discrete method for solving partial differential equations. Compared with traditional Finite Element Method, it is suitable for more general polygonal and polyhedral meshes, with better mesh adaptability and numerical stability. However, as a new method, the theories, algorithms and applications of virtual element method still need to be further developed and improved. In this work, a new recovery type a posterior error estimator for Poisson equation is proposed. Furthermore, the efficiency and reliability of the posterior error estimator is proved. Finally, several numerical tests are presented to confirm the theoretical results.

Finite Elements and ReLU Deep Neural Networks (DNNs)

He, Juncai MS

Peking University and Penn State

In this talk, we will discuss about the connections of finite elements and ReLU deep neural network models with respect to both h-adaptivity and p-adaptivity. For h-adaptivity, we will talk about the relationship between ReLU DNN and linear finite elements and some results which we established during our investigation of their connection. For p-adaptivity, we will introduce the “superconvergence” of ReLU DNN for x^2 from the viewpoint of hierarchical basis. Based on that, some new approximation properties for both smooth and non-smooth functions can be proven.

MS18: Machine learning and high performance computing

Organizers: Tao Cui, Xin Liu, Yingzhou Li, Xueshuang Xiang, Ran Zhang

Optimal complexity direct solver for Kernel Ridge Regression

Li, Xiaoye S. MS

Lawrence Berkeley National Laboratory

We present scalable and memory-efficient algorithm to approximate kernel methods for machining. Namely, we propose to exploit the approximate sub-block rank deficiency of the kernel matrices to build a direct parallel (hybrid shared and distributed) solver, which finds the regression weights on the training stage of the kernel methods. Our method results in optimal $O(r^2n)$ training time due to the underlying advanced linear algebra techniques (hierarchical matrix formats) combined with the delicate use of the geometry of data (which ensures fast and accurate performance of the solver). We demonstrate with extensive large-scale experiments that our approach provides sufficient accuracy to match the state-of-the-art non-approximated kernel regression, and also successfully competes with the known methods exploiting parallel and distributed architectures to work with datasets of 10^7 data points.

A Greedy Algorithm for Solving Large-scale Eigenvalue Problem

Yang, Chao MS

Lawrence Berkeley National Laboratory

The eigenvectors of many large-scale eigenvalue problems have localization properties, i.e., only a few elements of the desire eigenvector are large in magnitude while others are significantly smaller. However, the location of these large elements are unknown in advance. We present a greedy algorithm for identifying the localization and solving the eigenvalue problem efficiently.

Bridge the Gap between Neural Networks and Neuromorphic Hardware with a Neural Network Compiler

Chen, Wenguang MS

Tsinghua University

TBA

Approximate Tensor Ring Decomposition

Li, Yingzhou MS

Duke University

Tensor ring decomposition has been used to compress high dimensional tensors in both deep learning and computational physics. In this work, we study the tensor ring decomposition and its associated numerical algorithms. We establish a sharp transition of algorithmic difficulty of the optimization problem as the bond dimension increases: On one hand, we show the existence of spurious local minima for the optimization energy landscape even when the tensor ring format is much over-parameterized, i.e., with bond dimension much larger than that of the true target tensor. On the other hand, when the bond dimension is further increased, we establish one-loop convergence for alternating least square algorithm for tensor ring decomposition. The theoretical results are complemented by numerical experiments for both local minimum and one-loop convergence for the alternating least square algorithm.

Multiscale Neural Network for PDEs

Fan, Yuwei MS

Stanford University, USA

We constructed a series novel neural network architectures inspired by classical linear algebra algorithms, including the hierarchical matrices, the hierarchical nested bases and BCR's nonstandard wavelet form. The new architectures inherit the multiscale structure of these classical algorithms, thus called multiscale neural network. To construct the neural networks, we first represent the matrix-vector product algorithm of theses algorithms as a linear neural network. Then in order to address nonlinear problems, we propose an extension by replacing each linear sub-network with a deeper and more powerful nonlinear one. Such neural networks are used to solve PDEs in different fields, including density functional theory, homogenization theory and electrical impedance tomography.

Deep Learning for Multiscale Molecular Modelling

Wang, Han MS

Beijing Institute of Applied Physics and Computational Mathematics

We introduce a series of deep learning based methods for molecular modeling at different scales. We discuss this topic in two aspects: model construction and data generation. In terms of model construction, we introduce the Deep Potential scheme based on a many-body potential and inter-atomic forces generated by a carefully crafted deep neural network trained with ab initio data. We show that the proposed scheme provides an efficient and accurate protocol for a variety of systems, including bulk materials and molecules, and, in particular, for some challenging systems like a high-entropy alloy system. We further show how this scheme is generalized to the context of coarse-graining and free energy computation. In terms of data generation, we present a new active learning approach named Deep Potential Generator (DP-GEN), which is an iterative procedure including exploration, labeling, and training steps. By the example system of Al-Mg alloys, we demonstrate that DP-GEN can generate uniformly accurate potential energy models with a minimum number of labeled data.

IMRank: Influence Maximization via Finding Self-Consistent Ranking

Chen, Wei MS

Beihang University, Beijing, China

Influence maximization, fundamental for word-of-mouth marketing and viral marketing, aims to find a set of seed nodes maximizing influence spread on social network. Existing method can not guarantee both high accuracy and low computational cost. We develop an iterative ranking framework, i.e., IMRank, to efficiently solve influence maximization problem under independent cascade model.We provide a last-to-first allocating strategy and a generalization of this strategy are proposed to improve the efficiency of estimating ranking-based marginal influence spread for a given ranking. We find IMRank achieves both remarkable efficiency and high accuracy by leveraging simultaneously the benefits of greedy algorithms and heuristic algorithms. As demonstrated by extensive experiments on large scale real-world social networks, IMRank always achieves high accuracy comparable to greedy algorithms, while the computational cost is reduced dramatically, about 10–100 times faster than other scalable heuristics.

Quantifying total uncertainty in physics-informed neural networks for solving forward and inverse stochastic problems

Guo, Ling MS

Shanghai Normal University

Physics-informed neural networks (PINNs) have recently emerged as an alternative way of solving partial differential equations (PDEs) without the need of building elaborate grids, instead, using a straightforward implementation. In particular, in addition to the deep neural network (DNN) for the solution, a second DNN is considered that represents the residual of the PDE. The residual is then combined with the mismatch in the given data of the solution in order to formulate the loss function. This framework is effective but is lacking uncertainty quanti cation of the solution due to the inherent randomness in the data or due to the approximation limitations of the DNN architecture. Here, we propose a new method with the objective of endowing the DNN with uncertainty quantification for both sources of uncertainty, i.e., the parametric uncertainty and the approximation uncertainty. We first account for the parametric uncertainty when the parameter in the

differential equation is represented as a stochastic process. Multiple DNNs are designed to learn the modal functions of the arbitrary polynomial chaos (aPC) expansion of its solution by using stochastic data from sparse sensors. We can then make predictions from new sensor measurements very efficiently with the trained DNNs. Moreover, we employ dropout to correct the over-fitting and also to quantify the uncertainty of DNNs in approximating the modal functions. We then design an active learning strategy based on the dropout uncertainty to place new sensors in the domain in order to improve the predictions of DNNs. Several numerical tests are conducted for both the forward and the inverse problems to quantify the effectiveness of PINNs combined with uncertainty quantification. This NN-aPC new paradigm of physics-informed deep learning with uncertainty quantification can be readily applied to other types of stochastic PDEs in multi-dimensions.

Random Batch Method and its applications

Li, Lei

MS

Shanghai Jiaotong University

A random algorithm for simulating interacting particle systems that reduces the complexity per time step from $O(N^2)$ to $O(N)$, called Random Batch Method (RBM), will be introduced in this talk. The algorithm is motivated by the mini-batch idea in machine learning and statistics. Under some special conditions, we show the convergence of RBM for the first marginal distribution under Wasserstein distance. Compared with traditional tree code and fast multipole expansion algorithms, RBM works for kernels that do not necessarily decay.

MS19: Multigrid and machine learning

Organizers: Juncai He, Zuowei Shen, Jinchao Xu

Deep Network Approximation Characterized by Number of Neurons

Zhang, Shijun

MS

National University of Singapore

This talk introduces a quantitative and optimal approximation rate of ReLU neural networks in terms of both width and depth simultaneously to approximate continuous functions on a compact domain. The analysis provides a general guide for selecting the width and depth of ReLU networks to approximate continuous functions, especially when the computation is conducted with parallel computing in large-scale applications.

Learning and Learning to Solve PDEs

Dong, Bin

MS

Beijing International Center for Mathematical Research Peking University

Deep learning continues to dominate machine learning and has been successful in computer vision, natural language processing, etc. Its impact has now expanded to many research areas in science and engineering. In this talk, I will particularly focus on some recent impact of deep learning on scientific computing. I will present our recent work on bridging deep neural networks with numerical differential equations. On one hand, I will show how to design transparent deep convolutional networks to uncover hidden PDE models from observed dynamical data and to predict the dynamical behavior accurately. On the other hand, I will present our recent attempt to establish a deep reinforcement learning based framework to solve 1D scalar conservation laws.

Machine Learning in Reproducing Kernel Banach Spaces

Lin, Rongrong

MS

School of Data and Computer Science, Sun Yat-sen University, Guangzhou

Kernel methods have been popular in machine learning for their superior performance on a wide spectrum of learning tasks. In the past decade, there has been emerging interest in theories and applications of reproducing kernel Banach spaces (RKBSs) in machine learning community. In this talk, three topics on RKBSs will be discussed: (i) We propose a unified framework of constructing RKBSs that covers all existing constructions, such as, semi-inner-product RKBSs, RKBSs with the l^1 norm, RKBSs with positive definite functions, p-norm RKBSs via generalized Mercer kernels, etc. (ii) Targeting at sparse multi-task learning, we consider regularization models with an l^1 penalty on the coefficients of kernel functions. In order to provide a kernel method for this model, we construct a class of vector-valued RKBSs with the l^1 norm. (iii) We develop kernel methods in RKBSs of continuous functions. To this end, we explore two fundamental RKBSs: Banach spaces of continuous functions which vanish at infinity, and Sobolev spaces.

Variational training of neural network approximations of solution maps for physical models

Li, Yingzhou MS

Duke University

A novel solve-training framework is proposed to train neural network in representing low dimensional solution maps of physical models. Solve-training framework uses the neural network as the ansatz of the solution map and train the network variationally via loss functions from the underlying physical models. Solve-training framework avoids expensive data preparation in the traditional supervised training procedure, which prepares labels for input data, and still achieves effective representation of the solution map adapted to the input data distribution. The efficiency of solve-training framework is demonstrated through obtaining solutions maps for linear and nonlinear elliptic equations, and maps from potentials to ground states of linear and nonlinear Schrödinger equations.

MgNet: A Unified Framework of Multigrid and Convolutional Neural Networks

He, Juncai[1], **Xu, Jinchao**[2] MS

[1] Peking University & Penn State University
[2] Penn State University

In this talk, we will talk about a unified model, known as MgNet, that simultaneously recovers some convolutional neural networks (CNN) for image classification and multigrid (MG) methods for solving discretized partial differential equations (PDEs). This model is based on close connections that we have observed and uncovered between the CNN and MG methodologies. With such connections and new concept in the unified model, the function of various convolution operations and pooling used in CNN can be better understood. As a result, modified CNN models (with fewer weights and hyperparameters) are developed that exhibit competitive and sometimes better performance in comparison with existing CNN models when applied to both CIFAR-10 and CIFAR-100 data sets.

Make ℓ_1 Regularization Effective in Training Sparse CNN

Zhang, Lian MS

Hong Kong University of Science and Technology & Penn State University

In this talk, we first demonstrate that the commonly used SGD (and variants) training algorithm is not an appropriate match with ℓ_1 regularization and then replace it with a different training algorithm based on a regularized dual averaging (RDA) method. RDA was originally designed specifically for convex problem, but with new theoretical insight and algorithmic modifications (using proper initialization and adaptivity), we have made it an effective match with ℓ_1 regularization to achieve a state-of-the-art sparsity for CNN compared to other weight pruning methods without compromising accuracy (achieving 95% sparsity for ResNet18 on CIFAR-10, for example).

Linear data-feature mapping in different grids in classical CNN models

Chen, Yuyan MS

Peking University

MgNet is a new network structure based on multigrid method. According to multigrid theory, we make an assumption that the data and feature are related by a mapping (which can be either linear or nonlinear) in different scale. The classical CNN model like ResNet and DenseNet can be regard as a specical case of MgNet, which means we can find the data-feature mapping in these models by MgNet theory. Besides, we make some numerical experiments to verify it.

Sparse Training Algorithms for Neural Networks

Siegel, Jonathan MS

Penn State University, USA

In this talk we will analyze a class of optimization algorithms designed for optimizing a sum of two convex functions. We exhibit these methods as a generalization of forward-backward gradient descent and discuss their potential usefulness for the training of sparse neural networks. In addition, we consider their extension to the Banach space setting using the notions of distance generating functions and Bregman distance, which leads to a generalization of forward-backward mirror descent, and show how this idea can be viewed as a non-linear generalization of a preconditioner.

MS20: Non-standard multilevel and domain-decomposition approaches

Organizers: Rolf Krause, Gillian Queisser

A smooth subdivision multigrid method

Queisser, Gillian MS

Temple University

We introduce a smooth subdivision theory-based geometric multigrid method. While theory and efficiency of geometric multigrid methods rely on grid regularity, this requirement is often not directly fulfilled in applications where partial differential equations are defined on complex geometries. Instead of generating multigrid hierarchies with classical linear refinement, we propose the use of smooth subdivision theory for automatic grid hierarchy regularization within a geometric multigrid solver. This subdivision multigrid method is compared to the classical geometric multigrid method for two benchmark problems. Numerical tests show significant improvement factors for iteration numbers and solve times when comparing subdivision to classical multigrid. A second study focusses on the regularizing effects of surface subdivision refinement, using the Poisson-Nernst-Planck equations as a model problem. Various applications to problems in life-sciences are presented.

Multilevel strategies for non-standard contact formulations

Krause, Rolf MS

Institute of Computational Science, Center for Computational Medicine in Cardiology

In this talk, we present and discuss two different multilevel approaches for solving contact problems. The first approach is based on a least-squares finite element formulation. The contact constraints are incorporated into the least square-formulation, as a penalty term, by means of the complementarity condition. For the resulting mixed discretization, a monotone multigrid method is constructed, analyzed in terms of different non-linear contact projections, and its performance investigated. The second approach is based on a symmetric, overconstrained, segment-to-segment formulation for linearized contact, that decouples the multiplier discretization from the displacement discretization and allows a simple implementation of multi-body contact. In contrast to some mortar methods, the resulting discrete QPs cannot be solved efficiently. We consider overlapping Block-Jacobi smoothers for an augmented Lagrangian multigrid, and exploit the high arithmetic density of local QPs to be solved for efficient parallelization. The properties of the approaches are illustrated on several numerical examples.

Anisotropic multigrid preconditioners for space-fractional diffusion equations

Trotti, Ken

MS

University of Insubria, University of Italian Switzerland

Fractional Diffusion Equations (FDEs) are a generalization of the classical Partial Differential Equations (PDEs) obtained replacing standard derivatives with fractional ones. Their recent success is notably due to the non-local behavior of fractional differential operators that translates in the appropriate modeling of anomalous differential phenomena appearing in several applicative fields, like plasma physics or imaging. In this work, we focus on a two-dimensional space-FDE problem discretized by means of a second order finite difference scheme obtained as combination of the Crank-Nicolson scheme and the so-called weighted and shifted Grünwald formula [2]. Efficient multigrid strategies for the resulting Toeplitz-like linear systems have been already introduced in [1]. Therein, a symbol-based study of the coefficient matrices has been used to define a multigrid preconditioner built using either rediscretization or a two-dimensional scaled-Laplacian matrix which is particularly effective when the fractional orders are both close to 2. Here we seek to investigate how multigrid approaches can be efficiently extended to the case where only one of the two fractional order is close to 2, while the other is close to 1. In other words, we consider space-FDE problems that involve an intrinsic anisotropy in the direction corresponding to the minimum fractional order. We design a multigrid preconditioner where the grid transfer operator is obtained with a semicoarsening technique and the smoothing is performed with relaxed Jacobi whose damping parameter is accurately estimated by using the symbol approach. Moreover, for large-sized problems a further improvement in the robustness of the multigrid method can be reached using a V-cycle with semicoarsening as smoother (see [3]). Similarly to the proposal in [1], the scaled-Laplacian matrix is used in the direction where the fractional derivative order is close to 2, while in the other direction a rediscretizationn is adopted. Several numerical results confirm that the resulting multigrid preconditioner is computationally effective and outperforms current state of the art techniques.

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MS21: Fast algorithms for complex and large-scale problems

Organizers: Jun Hu, Shuonan Wu

A Pure Source Transfer Domain Decomposition Method for Helmholtz Equations in Unbounded Domain

Wu, Haijun MS

Nanjing University, China

A pure source transfer domain decomposition method (PST-DDM) for solving the truncated perfectly matched layer (PML) approximation in bounded domain of Helmholtz scattering problem is proposed and analyzed.

From differential equation solvers to optimization methods

Chen, Long MS

University of California at Irvine, USA

Convergence analysis of accelerated first-order methods for convex optimization problems are presented from the point of view of ordinary differential equation (ODE) solvers. Two resolution ODEs are derived for accelerated gradient methods. Numerical discretizations for these resolution ODEs are considered and its convergence analyses are established via tailored Lyapunov functions. The ODE solvers approach can not only cover existing methods, such as Nesterov's accelerated gradient method and FISTA, but also produce a large class of new algorithms that possesses optimal convergence rates.

Two-level Arrow-Hurwicz methods for steady incompressible Navier-Stokes equations

Huang, Jianguo MS

Shanghai Jiao Tong University, China

In this talk, we will design and analyze three kinds of two-level Arrow-Hurwicz (A-H) methods for steady incompressible Navier-Stokes equations. The methods are constructed based on the A-H method and the well-known two-level approach for solving nonlinear partial differential equations. The error analyses of the methods are developed with technical derivation. Several numerical results are reported to illustrate the performance of the numerical methods proposed. This is a joint work with Binbin Du from Shanghai Jiao Tong University.

A nonoverlapping DDM for general elastic body-plate problems discretized by the P1-NZT FEM

Huang, Xuehai MS

Shanghai University of Finance and Economics, China

A nonoverlapping domain decomposition method (DDM) is proposed to solve general elastic body-plate problems, discretized by the P1-NZT finite element method. It is proved in a subtle way that the convergence rate of the method is optimal (independent of the finite element mesh size), even for a regular family of finite element triangulations. This enables us to combine the method with adaptive techniques in practical applications. Some numerical results are included to illustrate the computational performance of the method.

Efficient Spectral Methods for Some Singular Eigenvalue Problems

Ma, Suna MS

Peking University, China

We propose and analyze some efficient spectral/spectral element methods to solve singular eigenvalue problems related to the Schrodinger operator with an inverse-power potential. For the Schrodinger eigenvalue problem with an inverse potential, we first design an efficient spectral method on a ball of any dimension by adopting the Sobloev-orthogonal basis functions with respect to the Laplacian operator to overwhelm the homogeneous inverse potential and to eliminate the singularity of the eigenfunctions. Then we extend this spectral method to arbitrary polygonal domains by the mortar element method with each corner covered by a circular sector and origin covered by a circular disc. Furthermore, for the Schrodinger eigenvalue problem with an inverse-cube potential, we devise a novel spectral method by modifying the former Sobloev-orthogonal bases to overcome the homogeneity of the inverse-cube potential and to fit the strong singularities of the eigenfunctions. As in the case of the inverse potential, this approach can be extended to arbitrary polygonal domains by the Mortar element method as well. Finally, for the singular elliptic eigenvalue problem of the mathematical model of fuel cells on rectangles, we propose a novel spectral method by using tensorial bases composed of the L2- and H1-simultaneously orthogonal functions in the y-direction and the Sobolev-orthogonal functions with respect to the Schrodinger operator with an inverse-square potential in the x-direction. Numerical experiments indicate that all our methods possess exponential orders of convergence, and are superior to the existing polynomial based spectral/spectral element methods and hp-adaptive methods.

Anisotropic Finite Element Methods for Interface Problems

Wang, Hua MS

Peking University, China

A new anisotropic finite element method is proposed for second order elliptic interface problems. Approximation capability of the anisotropic finite element space is analyzed. Finite element errors in H1-norm and L2-norm are proved to be optimal. The resulting systems are usually ill-conditioned, thus we construct an optimal V-cycle multi-grid iterator for it. Numerical experiments are presented to demonstrate our theoretical results.

A parallel space-time multigrid method for the Eddy-Current equation

Schwalsberger, Martin CT

Johannes Kepler University Linz

We present a new parallel space-time multigrid method for solving the Eddy-current equation. Specifically this method enables the use of spatial mesh coarsening during the coarse grid correction step. The key component of this solver is the use of a Helmholz splitting. We first present results of a local Fourier analysis conducted in a 2D setting, which directly reveals the need for an auxiliary space correction. We also confirm that with this additional correction we can restore the usual convergence rates. Systematic numerical experiments in the 3D setting confirm the theoretical results andidentify a parameter, which is used to control if spatial coarsening could be applied. Besides increased convergence rates the ability to apply spatial coarsening almost halves the computational costs and speeds up sequential parts of the algorithm. Finally we present numerical experiments which show the performance of this space-time multigrid method.

Special Contributed Talk

How the Web, Open Access and Artificial Intelligence are changing the Exchange of Scientific Information

Heinze, Joachim

CT

Senior Advisor Mathematical Sciences, Springer Verlag

1. A very short overview of **the History of Scientific Publishing** with some Springer examples is given. "**Numerische Mathematik**" was the first of all SpringerNature Journals ever, over all disciplines to go online in 1994.

2. The change of the **World of Publishing: Generating** (*Scientists*), **Composing** (*Publishers and Scientists*) and **Disseminating** (*Librarians and Publishers*) Mathematical Content in electronic form. **TeX** and "**Online Visibility**" are the buzzwords here.

3.**Open Access** for all mathematical content? "New" initiatives like "**Overlay Journals**", based on the **arXiv**, are briefly discussed, as well as the more recent **Sci-Hub** and **ResearchGate** initiatives.

4. Keep track of what has been published and citied. **MathSciNet** and **zbMATH**, the two big **Math Review Journals** in comparison to other initiatives, like **Google Scholar**, **Scopus**, and **Web of Science**. An initiative from China? **MathSciDoc**.

5. Recent developments in the **Dissemination** of **Scientific information** are discussed. **Social Media** {Scholarly Collaboration Networks (**SCN**)} in Scientific Communication like **Research Gate** and some **Initiatives** such as "Sharedit" and "SciGraph" are briefly reflected. The big Challenge and Opportunity for the Scientific Community: **GlobalAccess2020/2021, Plan S** and the **Deal** give a reason for a controversial dispute. **Artificial Intelligence** and some hope for the future will close the presentation.

Embedded Workshop for Fast Solvers 2019

Organizers: Chunsheng Feng, Shi Shu, Guangming Tan, Hehu Xie, Xiaowen Xu, Chao Yang, Chen-Song Zhang

Distributed-Memory Hierarchical Matrix Algebra

Li, Yingzhou

EM

Duke University, USA

We introduce a distributed-memory algorithm for H-matrix application, composition and other related operations which avoids the need for the $\Omega(p^2)$ scheduling procedure used in previous work, where p is the number of processes. Furthermore, we demonstrate that our algorithm is able to effectively use $O(N)$ processes for $N \times N$ H-matrix and achieve strong scalability to more than an order of magnitude processes than previous results. We also show some recent advance in the large scale iterative solver for H-matrix.

Challenge and opportunities for some rank-structured algorithm and eigen-solvers on exascale supercomputers

Li, Shengguo

EM

National University of Defense Technology, China

The E-level calculation puts great demands and challenges on the performance and scalability of the original parallel algorithm. The eigenvalue problems are very important in many areas. This report will first briefly introduce some recent projects in the development of exascale algorithms (library) in countries such as the United States, Japan, and Europe, and then analyze the bottlenecks and optional countermeasures that the rank structure matrix algorithm may encounter in large-scale parallel computing. Finally, combined with the rank structure matrix algorithm, several linear eigenvalue algorithms suitable for large-scale distributed parallel computing are introduced.

Domain Decomposition Methods for the Helmholtz Equation: A Review

Zhang, Hui

EM

Zhejiang Ocean University, China.

The Helmholtz equation has a simple form but is difficult to solve, for which iterative solvers are still hardly close to linear complexity, not to say the parallel speedup. In this talk, we review the special techniques from domain decomposition methods developed for the Helmholtz equation: one is the interface transmission conditions and the other is the plane wave basis. We will focus on the transmission conditions and discuss the various implementation approaches and their impacts on the convergence and complexity. The talk is mainly about the algorithms and experiments but also complemented with the Fourier analysis for model problems.

Numerical algorithms for time-harmonic Maxwell equation arising from integrated microelectronics system

Hu, Shaoliang EM

CAEP Software Center for High Performance Numerical Simulation

The solution of time-harmonic Maxwell equation plays an important role in the integrated microelectronics system, such as electromagnetic simulations in filters and radio-frequency front-end devices. Due to the wideband frequency of interest for multiport system in the real-world application code, it is hard to solve the resulting discretized linear algebraic systems efficiently. In this talk, we first introduce the background and features of the integrated microelectronics system. Then, we show the numerical results of the investigation for the existing algorithms. Finally, we will discuss some challenges of the fast algorithm for this kind of applications.

Convergence analysis and HPC results of the Parareal and MGRIT algorithms for time dependent problems

Yue, Xiaoqiang EM

Xiangtan University, Xiangtan, China

This talk focuses on developing and analyzing parallel-in-time (PinT) multigrid solvers, including the standard and diagonalization-based Parareal and multigrid-reduction-in-time (MGRIT) algorithms. We applied these PinT algorithms to a popular suite of benchmark problems and compared their parallel performance.

Performance Optimization of the HPCG Benchmark on the SUGON 7000 supercomputer

Wang, Yinshan EM

Institute of Computing Technology, Chinese Academy of Sciences, China

The High Performance Conjugate Gradient (HPCG) benchmark is the well-known algorithm that solves a large sparse linear system using multi-grid pre-conditioner in the CG iterative method. It is designed to better represent modern application workloads that mainly depend on memory system and network performance. SUGON 7000 is a new designed DCU accelerated heterogeneous supercomputer system which is composed of the latest developing HYGON CPUs and DCUs. Therefore, we believe that the HPCG optimization work would be an important prior experience for the later applications porting and optimization. In the present work, the key HPCG optimization skills can be concluded as follows: first, block coloring method is implemented to increase the right vector x memory access locality; second, an improved ELL data format is developed to better utilize the DCU shared memory for the stencil case; last but not least, several algorithm procedure is improved to reduce memory access. Finally, we achieve a high performance of over 1.43 pflops and about 86

Some space-time Schwarz algorithms for solving parabolic problems

Li, Shishun

EM

Henan Polytechnic University, China

Compared with traditional time-stepping algorithms, space-time algorithms increase space-time concurrency and can exploit the full power of supercomputer to solve the large-scale time-dependent problems fast. We will introduce some space-time Schwarz methods including the additive and hybrid versions, i.e., these Schwarz methods are viewed as preconditioners for GMRES in the implementation. The optimal convergence theory show that the convergence rate is bounded independent of the mesh parameters, the number of subdomains and the window size. Numerical experiments carried out on a parallel computer with thousands of processors confirm the theory in terms of the number of iterations, as well as the strong/weak scalability. Moreover, numerical comparison also shows space-time additive Schwarz methods outperform the sequential time stepping method when the number of processors is large.

Useful Information

Conference Venue

Talks will be held at the **Yimay International Conference Hall** of Howard Johnson City of Flower Hotel Kunming Orchid Yuan. The hotel locates near the Changshui international airport, which is about 20 minutes away by car. The hotel address is: **No. 8188, Jinwa Road, Panlong District, Kunming, Yunnan, China**. Dining choices include Chinese and Western restaurants. Business travelers will find meeting facilities and a business center at their disposal. Guests can enjoy free parking and Wi-Fi access in public areas. The hotel website is: `http://flowerkunming.hojochina.com/flower-home.html`.

Transportation

1. From the Airport

Taking a taxi from the airport to the hotel costs about 65RMB. The hotel provide airport shuttle services. Shuttle service costs 25RMB per person. Drop off time, 6:00-19:00. Pick up time, 11:00-21:00. The shuttle bus time table is shown in the following picture.

- **Pickup Location:** 20 meters to the left of domestic arrival gate, Exit 4
- **Reservation telephone:** +86 0871-65036999
- **Url:** `http://flowerkunming.hojochina.com/flower-home.html`

2. From the Kunmingnan Railway Station

- Public Transportation: Subway Line 1 or 2 (the same train) —> DONGFENG Square Station, transfer to Subway Line 3 —> East Coach Station, Exit B —> Walk 100 meters —> Kunming Eastern Bus Station (Bus: k9, 906, z110, 60, 22, k18, 29) —> Flower City Square Bus Station —> Walk 220 meters. Cost about 9RMB, 90 minutes.
- Taxi: About 100RMB, 45 minutes, 33 kilometers

3. From the Kunming Railway Station

- Kunming Railway Station (Yongsheng Rd) Bus Station, Bus 60 —> Flower City Square Bus Station —> Walk 330m. Cost about 2RMB, 60 minutes.
- Taxi: About 45RMB, 30 minutes, 15 kilometers.

4. For Directions

In case needed, you may show the following message to a taxi driver or some local people for directions:

您好！请送我到昆明花之城豪生国际大酒店，谢谢！

Hello! Please take me to Kunming Howard Johnson Flower City Hotel. Thank you!

地址：昆明市盘龙区金瓦路 8188 号花之城豪生国际大酒店

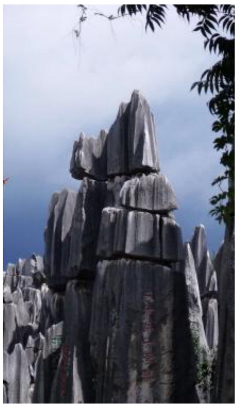
Address: No.8188 Jinwa Road, Huazhicheng (Main Gate), Panlong District, Kunming

电话：400-699-8818，0871-65036999

Telephone: 400-699-8818, 0871-65036999

About Kunming

As the capital of Yunnan Province, **Kunming**, also known as the "City of Eternal Spring", is one of the most pleasant and relaxed cities in China. The city was founded over 2,000 years ago, but it did not gain prominence until it became the eastern capital of the Nanzhao Kingdom in the 8th century. By the time the Mongols swept through in 1274, Kunming, was enough of a flourishing town to have attracted the attention of Marco Polo, who described it as a "very great and noble" capital city. A subtropical location and high elevation (1,864m above sea level) give Kunming a temperate climate year-round. Its days are filled with sunshine, making almost any time good for a visit.



Kunming also has its unique natural and cultural landscapes. The Stone Forests, one of China's four natural scenes, is located in the southwest of Kunming, 80 kilometers away from Kunming. The Stone Forests takes up an area of 350 square kilometers and is the largest and the most complete karst landform existed in the world. There are 26 minorities inhabited in Kunming and the folk customs are pretty colorful.

Other information

Coffee breaks and **lunch buffet** will be offered in the Howard Johnson Hotel. And the **conference banquet** will also be held at the dinning hall of the Howard Johnson Hotel.

Contact information

For more information, contact us via the official e-mail address: `img@multigrid.org`. Emergency contact person: **Dr. Chen-Song Zhang, +86 135-2040-7990**.

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Technical Secretariat and Volunteers

Last Name	First Name	Institute
Cao	Xia	Yunan Co-Creative Center ⋆
Jiang	Chaolong	Yunnan University of Finance and Economics ⋆
Liu	Yuntong	Yunan Co-Creative Center ⋆
Pu	Qiuxian	Yunan Co-Creative Center ⋆
Zhao	Qi	Yunnan University of Finance and Economics ⋆
Zhao	Shenglan	Peking University ⋆
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