Workshop on High Performance Numerical Algorithm and Software for Large-scale Scientific & Engineering Applications

Vanburgh Hotel, Guangzhou, China, Jan 14, 2019

Workshop Agenda:

(Each speaker has 25 minutes for presentation and 5 minutes in addition for questions & discussions)

8:25-8:30	**Workshop Introduction**
Session 1. Chair: Xiaowen Xu	
8:30-9:00	**Iwashita, Takeshi**: Development of a high-performance multi-threaded ILU-GMRES solver based on a novel parallel ordering technique
9:00-9:30	**Zhang, Chensong**: Numerical Simulation of Fluid Flows in Carbonate Oil Reservoirs
9:30-10:00	**Liu, Hui**: Numerical Simulations of Thermal Reservoir Model using Parallel Computers
10:00-10:30	**AM Coffee Break & Group Photo**
Session 2. Chair: Linbo Zhang	
10:30-11:00	**Wittum, Gabriel**: TAB
11:00-11:30	**Chen, Rongliang**: Scalable Parallel Methods for Patient-specific Blood Flow Simulations
11:30-12:00	**Lee, Chang-Ock**: Fast Nonoverlapping Block Jacobi Method for the Dual Rudin-Osher-Fatemi Model
12:00-13:30	**Lunch Break**
Session 3. Chair: Chensong Zhang	
13:30-14:00	**Sheen, Dongwoo**: Introduction to the algebraic multiscale method
14:00-14:30	**Logashenko, Dmitry**: Simulation of density-driven groundwater flow with a phreatic surface in complicated geometries
14:30-15:00	**Cai, Jianfeng**: A Framework of Non-Convex Methods for Low-Rank Matrix Reconstruction: Algorithms and Theory
15:00-15:30	**Zhang, Lian**: Decoupling Techniques for Coupled Models in Multi-Physics Supercomputing
15:30-16:00	**PM Coffee Break**
Session 4. Chair: Hui Liu	
16:00-16:30	**Zhang, Linbo**: Implementation of Immersed Finite Element Methods on Tetrahedral Meshes
16:30-17:00	**He, Xin**: Co-designing Computational Fluid Dynamics and Numerical Linear Algebra
17:00-17:30	**Xu, Ran**: JPSOL, a app-oriented parallel suite for numerical algebraic problems arising from PDEs
17:30-17:40	**Closing Remarks**
18:00-20:00	**Dinner at the Vanburgh Hotel**

Invited Speakers, Titles, and Abstracts:

1. Cai, Jianfeng (HKUST, Hong Kong)

***Short Bio*:** Jian-Feng Cai is an associate professor from Department of Mathematics, Hong Kong University of Science and Technology (HKUST). He obtained his Bachelor degree in Computational Mathematics from Fudan University, and PhD degree in Mathematics from Chinese University of Hong Kong. Before joining HKUST in 2015, he has been worked at National University of Singapore, UCLA, and University of Iowa. His research focuses on the design and analysis of algorithms for problems in imaging and data sciences, using tools from computational harmonic analysis, numerical linear algebra, optimization, and high-dimensional probability.

Title: A Framework of Non-Convex Methods for Low-Rank Matrix Reconstruction: Algorithms and Theory

Abstract: Low-rank matrix is a versatile model that describes the structure of many datasets of practical interests arising from machine learning, bioinformatics, computer vision etc. Under this model, it is a fundamental problem how to recover a low-rank matrix from small amount linear samples. We present a framework of non-convex methods for low-rank matrix recovery. Our methods will be applied to several concrete example problems such as matrix completion, phase retrieval, and robust principle component analysis. We will also provide theoretical guarantee of our methods for the convergence to the correct low-rank matrix.

2. Chen, Rongliang (SIAT, CAS, China)

Short Bio: Rongliang Chen, holds an associate professor position in Shenzhen Institutes of Advanced Technology , Chinese Academy of Sciences. He received his PhD in computational mathematics from Hunan University in 2012. He visited the University of Colorado Boulder as a joint PhD student from 09/2009-04/2012 and as a visiting scholar from 09/2014-02/2015 and 07/2017-08/2018. His research interests include high performance computing, computational fluid dynamics, domain decomposition method, and fluid-structure interaction computation.

Title: Scalable Parallel Methods for Patient-specific Blood Flow Simulations

Abstract: 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 methods 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-Schwarz method. Several mathematical, biomechanical, and supercomputing issues will be discussed in detail, and some numerical experiments for the cerebral and coronary arteries will be presented. We will also report the parallel performance of the methods on a supercomputer with a large number of processors.

3. Iwashita, Takeshi (Hokkaido U., Japan)

Short bio: Takeshi Iwashita received a B.E., an M.E., and a Ph.D. from Kyoto University in 1992, 1995, and 1998, respectively. In 1998-1999, he worked as a post-doctoral fellow of the JSPS project in the Graduate School of Engineering, Kyoto University. He moved to the Data Processing Center of the same university in 2000. In 2003-2014, he worked as an associate professor in the Academic Center for Computing and Media Studies, Kyoto University. He currently works as the vice director and a professor in the Information Initiative Center, Hokkaido University. His research interests include high performance computing, linear iterative solver, and electromagnetic field analysis.

Title: Development of a high-performance multi-threaded ILU-GMRES solver based on a novel parallel ordering technique

Abstract: A high-performance multi-threaded ILU-GMRES solver was developed. The ILU-GMRES method is one of the most popular linear solvers for a linear system of equations with an unsymmetric coefficient matrix. It has been used in various applications. In parallelization of the ILU-GMRES solver, a sparse triangular solver involved in the preconditioning step is often problematic. One of well-known techniques to parallelize the sparse triangular solver is parallel ordering. Among various parallel ordering techniques, we focused on the algebraic block multi-color ordering and developed an enhanced version of it, which is applicable for a linear system with an unsymmetric coefficient matrix. The effectiveness of the developed solver was confirmed in numerical tests conducted on latest multi-core and many-core processors.

4. Logashenko, Dmitry (KAUST, Saudi Arabia)

Short Bio: Dmitry Logashenko is a research scientist at the Extreme Computing Research Center of the King Abdullah University of Science and Technology, Saudi Arabia. He received his PhD from Department of Mathematics and Computer Science of the Heidelberg University in 2004. His research interests include development, analysis and implementation of efficient numerical methods for solving the partial differential equations on parallel architectures. The main field of the applications is the density-driven groundwater flow in fractured porous media and with free surfaces.

Title: Simulation of density-driven groundwater flow with a phreatic surface in complicated geometries

Abstract: Presence of a phreatic surface separating saturated and unsaturated parts of an aquifer influences the groundwater flow essentially. Macroscopically, this interface can be modeled as a moving boundary which is tracked with the flow. We represent it by the level-set method and use the ghost-fluid method to impose the boundary conditions for the flow model in the saturated part. This technique is applied to the density-driven haline groundwater flow in real hydrogeological formations. These 3d domains have complicated, anisotropic, layered geometries and curved boundaries, that should be accurately resolved by unstructured grids consisting mainly of prisms. The non-linear model is discretized by a finite volume method. The linearized systems are solved by the geometric multigrid method with ILU smoothing. The high resolution of the grid motivates the parallelization is of the computations. In the talk, we present examples of these simulations.

5. He, Xin (ICT, CAS, China)

Short Bio: Dr. Xin He is an associate professor in the Institute of Computing Technology, Chinese Academy of Sciences. Dr. He got the PhD degree from Uppsala University, Sweden and then worked as a post-doctoral researcher at Delft University of Technology, the Netherlands. The main research consists of computational fluid dynamics, numerical linear algebra and high performance computing.

Title: Co-designing Computational Fluid Dynamics and Numerical Linear Algebra

Abstract: Computational fluid dynamics (CFD) is of key importance in many academic and industrial applications, e.g. maritime industry. In this presentation, I introduce how to use numerical linear algebra and high performance computing to accelerate the procedure of CFD, in particular the fast and efficient solutions of sparse and linear systems arising from CFD.

6. Lee, Chang-Ock (KAIST, South Korea)

Short Bio: Chang-Ock Lee is a Professor of Department of Mathematical Sciences, KAIST. He got his Ph.D from University of Wisconsin-Madison in 1995. His research areas including domain decomposition methods (DDM for optimization problems, Dual iterative substructuring method with a penalty term), Isogeometric Analysis. He is Vice President, Korean Society of Computational Mechanics (2016~), and Chair of Committee for International Exchanges, Korean Society for Industrial and Applied Mathematics (KSIAM) (2017~).

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

Abstract: In this talk, we consider nonoverlapping domain decomposition methods for the total variation minimization. We show that the nonoverlapping relaxed block Jacobi method for the dual Rudin-Osher-Fatemi model have the 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 O(1/n^2). Numerical results for comparison with existing methods are presented.

7. Liu, Hui (Calgary, Canada)

Short Bio: Hui Liu is a researcher in University of Calgary, Canada. Hui is working on numerical methods for reservoir simulations, preconditioning, algorithms and development of parallel reservoir simulators. He received his PhD in computational math and parallel computing in 2010 from Academy of Mathematics and System Sciences, Chinese Academy of Sciences.

Title: Numerical Simulations of Thermal Reservoir Model using Parallel Computers

Abstract: Thermal technologies are the main production processes in Canada, due to the high viscosity of heavy oil, and steam is injected into reservoirs to heat the reservoir and to reduce the viscosity of heavy oil. The cost is high compared with conventional production technologies. Therefore, it is important to study the production plan before applying to actual production. The simulation time could be hours, days or even weeks long is the model size is large or the geological model is complicated. In our work, parallel computers are employed to accelerate the simulation. As we know, the performance of parallel computers is proportional to the number of CPUs. As a result, thermal problems can be solved thousands of times faster using parallel computers. In this talk, numerical methods of thermal model and its parallelization are presented.

8. Sheen, Dongwoo (NSU, South Korea)

Short Bio: Dongwoo Sheen graduated from Seoul National University (SNU) with a Bachelor and Master Degrees in Mathematics in 1981 and 1983. He received his PhD under the guidance of Prof. Jim Douglas, Jr. He was appointed as a postdoctoral research fellow at the University of Pavia, Italy and at Purdue University until he joined SNU in 1993 as an assistant professor. Serving as a professor of Mathematics, he also founded and chaired the Interdisciplinary Program in Computational Science and Technology at SNU for many years. His research interests include Numerical Analysis and Scientific Computation in several application areas including fluid and solid mechanics, electrodynamics, math finance, and math biology. Specifically he has contributed in developing several fundamental Nonconforming Finite Element Methods and parallel algorithms based on Laplace Transform Methods. He is currently the President of the Korean Society of Computational Sciences. He was a Plenary Speaker at the 5th Asian Mathematical Conference, Kuala Lumpur, Malaysia (2009). He received a Certificate of Commendation from the Minister of Science and Technology of Korea in 2012 for his contribution in Supercomputing in Korea.

Title: Introduction to the algebraic multiscale method

Abstract: We introduce an algebraic multiscale method. The idea is motivated from the algebraic multigrid method (AMG) which is an iterative scheme to accurately approximate a linear system. Our approach differs in investigating in how to obtain a rough approximation to the original algebraic system arising from modeling heterogeneous materials. We discuss in detail how macroscopic basis functions can be formulated and result in a reduced macroscopic linear system based on the knowledge of microscopic linear system, with significant reduction of dimension.

9. Wittum, Gabriel (KAUST, Saudi Arabia)

Short Bio: Gabriel Wittum is a professor for Applied Mathematics and Computational Science of the Extreme Computing Research Center of the King Abdullah University of Science and Technology, Saudi Arabia. He got his PhD from University of Heidelberg in 1991. Before he joined KAUST, he is director of Goether Center for Scientific Computing, Frankfurt University. His research focuses on a general approach to modelling and simulation of problems from empirical sciences, in particular using high performance computing (HPC). Particular areas of focus include: the development of advanced numerical methods for modelling and simulation, such as fast solvers like parallel adaptive multi-grid methods, allowing for application to complex realistic models; the development of corresponding simulation frameworks and tools; and the efficient use of top-level supercomputers for that purpose. These methods and tools are applied towards problem-solving in fields including computational fluid dynamics, environmental research, energy research, finance, neuroscience, pharmaceutical technology and beyond.

10. Xu, Ran (IAPCM & CAEP-SCNS, China)

Short Bio: Ran Xu received the B.S. and Ph.D. degrees in computational mechanics from Tsinghua University, Beijing, China, in 2006 and 2012, respectively. He is currently an Associate Professor with the Institute of Applied Physics and Computational Mathematics, Beijing, China. His current interests include fast linear system solver, computational mechanics, massively computation method, and their applications.

Title: JPSOL, an app-oriented parallel suite for numerical algebraic problems arising from PDEs

Abstract: A new parallel numerical solver suite, JPSOL will be introduced in this presentation. JPSOL is founded by Institute of Applied Physics and Computational Mathematics since 2015, and aims to act as a powerful tool for huge numerical algebraic problems arising from scientific and realistically engineering applications. Different with hypre, petsc et. al. well-known packages, JPSOL is constructed by modern C++ language, and provides a more convenient and more natural way for using. It means that user can define and solve linear, non-linear and eigen problems in semantic uniform interfaces. With

matrices and vectors in JPSOL, which are defined as combinations with necessary data and traits, you will feel relaxed to found new algorithm in the natural matrix-vector way of expression. Further more, application can define its characteristic matrix or preconditioner obeying a few behavior standards. For example, a new matrix type is only asking to realize the spMV operator. At the last of the talk, some numerical results of realistic engineering cases achieved with JPSOL will be shown, such as the Sanxia Dam, nuclear plants et al.

11. Zhang, Chensong (AMSS, CAS, China)

Short Bio: Chen-Song Zhang, PhD. Graduated from the Applied Mathematics & Scientific Computing program at the University of Maryland, College Park, US; Worked as a postdoctoral fellow at the Penn State University, University Park, US; Currently working at the Academy of Mathematics and Systems Science, CAS, China. Main research interests include numerical analysis, adaptive methods, petroleum reservoir simulation, complex fluid/flow simulation, and parallel computing.

Title: Numerical Simulation of Fluid Flows in Carbonate Oil Reservoirs

Abstract: Mineral dissolution plays an important role in many subsurface transport processes including water-flooding, geological CO2 sequestration (GCS), and matrix acidizing in carbonate formations. Such a dissolution process could dramatically affect the efficiency of the oil/gas production. Hence a numerical model that accurately describes the dynamic behavior of fracture evolution is essential. In this talk, we introduce a 3-D mathematical model that combines the Stokes--Brinkman equation and reactive-transport equations to describe the coupled processes of fluid flow, solute transport, and chemical reactions in both single and multiple mineral systems. The proposed numerical model can be applied to describe 3-D linear flow and radial flow for different scenarios. We employ a numerical procedure that solves the Stokes--Brinkman equation and the reactive-transport equations by the staggered-grid finite difference method and the control volume finite difference method, respectively, in a sequential fashion. We will also introduce a multiscale hybrid-mixed method for discrete fracture models. The three-dimensional fluid flow in the reservoir and the two-dimensional flow in the discrete fractures are approximated using mixed finite elements. A general system was developed where fracture geometries and conductivities are specified in an input file and meshes are generated using the public domain software GMSH. Several test cases illustrate the effectiveness of the proposed approach comparing the multiscale results with direct simulations.

12. Zhang, Lian (HKUST)

Short Bio: Lian Zhang is a Ph.D student at Department of Mathematics, HKUST. He received B.S. at Zhejiang University in 2015. His current research interests are in the areas of numerical PDE, numerical analysis and multi-physics problems. He mainly work on the numerical simulation and numerical schemes for fluid-structure interaction(FSI) problems.

Title: Decoupling Techniques for Coupled Models in Multi-Physics Supercomputing

Abstract: 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 the fluid-structure interaction (FSI) will be examined. Approximation and stability issues will be addressed, with special attention to the added-mass effect in decoupling FSI computation.

13. Zhang, Linbo (AMSS, CAS, China)

Short Bio: Linbo ZHANG was born in 1962. He graduated from the Mathematics Department of Beijing University in 1982 and received his Ph.D. degree in Mathematics from Universite de Paris-sud, France, in 1987. Currently, he is a professor of Academy of Mathematics and Systems Science of Chinese Academy of Sciences, and the director of State Key Laboratory of Scientific and Engineering Computing. His research interests include numerical algorithms and high performance computing.

Title: Implementation of Immersed Finite Element Methods on Tetrahedral Meshes

Abstract: In this talk I will present algorithms and user interfaces in the open source parallel adaptive finite element toolbox PHG for immersed interface methods, especially a robust numerical quadrature algorithm for high order extended finite element methods, and demonstrate their applications with some benchmark problems. The codes are freely available in the distributions of PHG and can be used in implementations of immersed boundary/interface algorithms on tetrahedral meshes.