The Art of Computational Science, Bridging Gaps

--From Modeling & Algorithm to Simulation & Engineering

The CTPL group (Computational Transport Phenomena Laboratory, KAUST) is holding a workshop themed " The Art of Computational Science, Bridging Gaps--From Modeling & Algorithm to Simulation & Engineering" to highlight the role of computational science as a broad, multidisciplinary science shaping fundamental natural laws and tackling modern engineering problems. Five exhausted vising scholars and engineers, together with three selected members of our group, will give presentations on their latest progress and findings. The total eight talks will cover researches ranging from microscopic molecular dynamics simulations to field scale development process optimizations, from curving thermodynamic phase equilibrium to describing hydrodynamic multiscale flow behaviors, and from concluding current cooperation achievements to remarking potential future collaboration directions.

Location: Room 5220, Building 3, KAUST, Saudi Arabia

Time: 11:30am – 17:00pm, 24th, January, 2019

Local Organizer: CTPL, KAUST

Workshop Chair: Shuyu Sun

Workshop Secretary: Tao Zhang

Agenda

Time	Speaker	Topic
11:30am—12:00pm		Group lunch and free discussion
12:00pm—12:10pm	Shuyu Sun	Opening and welcome
12:10pm—12:40pm	Nilesh Choudhary	Simulating oil-gas interface at the molecular level
12:40pm—13:10pm	Yiteng Li	Isothermal-isochoric phase equilibrium calculation in conventional and unconventional reservoirs by a dynamic model
13:10pm—13:40pm	Yuanqing Wu	The Application of High-dimensional Sparse Grids in Flash Calculations: from Theory to Realization
13:40pm—14:10pm	Qiaolin He	Numerical study of phase transition in Van der Waals and asymptotic stability of solutions of compressible Navier-Stokes-Cahn-Hilliard coupled system
14:10pm—14:30pm		Coffee break and free discussion

14:30pm—15:00pm	Dong Joon Youn	Numerical analysis of the methane degassing from crosslinked polyethylene cable insulation
15:00pm—15:30pm	Mohamed F. El-Amin	Multiscale Time-splitting DFM Modeling of two-phase flow including nanoparticles transport in fractured porous media
15:30pm—16:00pm	Manal Alotibi	GMsFEM for Solving Reduced Darcy Flow Model in Fractured Porous Media
16:00pm—16:30pm	Chenguang Li	Field process and surface process in CPF3, Halfaya Oil Field, Iraq
16:30pm—17:00pm	Shuyu Sun	Wrap up and free discussion

* All presentations will include a short Q&A at the end.

** Lunch will be served at 11:30am, and juice, coffee and water will be provided all the time.

*** A short introduction to each speaker and abstract of each talk are attached in the following pages.

**** The map of KAUST Inn and Discovery Square, as well as of Campus, are illustrated on the last page to guide you to the workshop meeting room and tour around our university.

Simulating oil-gas interface at the molecular level

Name: Nilesh Choudhary

Affiliation: King Abdullah University of Science and Technology, KAUST, Saudi Arabia

Biography: Nilesh Choudhary is working in our group since last six months. He has recently completed Ph.D. in Chemical Engineering from Council for Scientific and Industrial Research-National Chemical Laboratory, Pune, India (CSIR-NCL). Previously, he worked on gas hydrate using molecular dynamics simulation and quantum mechanical calculation. He has explored the effect of additive during gas hydrate formation and decomposition at molecular level.

Abstract: Interfacial properties are one of the decisive properties for the process from crude oil extraction to end user hydrocarbon product where industries deal with multiphase-multicomponent fluids. Therefore, in this work, we performed molecular dynamics simulation for decane-CO2, decane-methane, and decane- a mixture of CO2 and methane at reservoir temperature and pressures. We also report the correlation of MD outcome with Density gradient theory. The obtained results from theory and MD simulation have an agreement with experimental studies. Further, we capture molecular orientation and behavior which is complicated to get from experimental studies.

Isothermal-isochoric phase equilibrium calculation in conventional and unconventional reservoirs by a dynamic model

Name: Yiteng Li

Affiliation: King Abdullah University of Science and Technology, KAUST, Saudi Arabia

Biography: Mr. Li is now a PhD student in the department of Earth Science and Engineering, joining our group since January 2016. In 2012, he got his Bachelor degree in Ocean University of China, Qingdao with the major Material Chemistry. In May 2014, he obtained his master degree in petroleum engineering in University of Southern California, Los Angeles. Currently his research area includes phase equilibrium calculation and multiphase flow in subsurface reservoirs.

Abstract: Phase equilibrium calculation has various applications in petroleum engineering, not only as a standalone calculation for separation process but also an integral component of the compositional reservoir simulation. As the most commonly-used flash technique in popular compositional simulators, the PT flash calculation has been well developed since Michelsen proposed his well-known studies in stability test and phase split calculation in 1982. In today's topic, the phase equilibria problem is modeled by the VT flash formulation due to some inherent advantages over the conventional PT flash formulation. A dynamic model is constructed based on the laws of thermodynamics and Onsager's reciprocal principle to describe the transition process from any non-equilibrium state to the equilibrium state. For illustration of the broad application of our dynamic model, we will discuss the VT flash calculation from two aspects: the bulk phase equilibrium in conventional reservoirs and confined phase equilibrium in unconventional reservoirs, particularly, in the presence of capillary pressure. To reach the equilibrium state, we minimize the Helmholtz free energy in bulk phase equilibria problems, and on the other hand maximize the entropy production for the capillary equilibrium problem. A convex splitting technique is employed to construct a thermodynamically-stable time marching scheme, which achieves the persistent dissipation of the Helmholtz free energy and entropy production without and with capillary effect, respectively. A number of examples, involving the pure substance, multi-component mixtures and even real reservoir fluids, are presented to exhibit the robustness and accuracy of the proposed model. It is found the equilibrium solutions of our dynamic model agree with the published data very well. In addition, we observe similar phase behaviors under the capillary effect, as the observations of published references suggested.

The Application of High-dimensional Sparse Grids in Flash Calculations: from Theory to Realization

Name: Yuanqing Wu

Affiliation: Shenzhen University, China

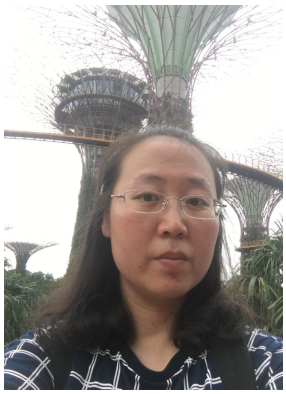
Biography: Yuanqing Wu is now an assistant professor in the College of Mathematics and Statistics, Shenzhen University, China. He got his B.Sc. degree in Statistics and Finance & B.Eng. degree in Computer Science in University of Science and Technology of China in 2005. In 2008, he got his Master Degree in Software Engineering in Peking University, China. He joined our group in 2010, as a founding student of KAUST and got his Ph.D degree in Applied Mathematics and Computational Science in 2015. Currently his research area includes phase equilibrium calculation and multiphase flow in subsurface reservoirs, sparse grids, high performance computing, etc.

Abstract: Flash calculations are a performance bottleneck of compositional flow simulations. Some work has demonstrated the feasibility of using sparse grid techniques to remove the bottleneck, but a complete realization of the idea is still not available. Thus, this work fills the niche. By introducing a new concept of layer to sparse grid points, the sparse grid construction can become much efficient. As a result, a much easier data structure the array can be used to store the sparse grids. Compared with the popular data structures to store the sparse grids such as the hash table and the tree, the array can minimize the space size and the traversing time, and at the same time reduce the number of points in the sparse grids by removing the architecture ancestors in the tree, which in turn makes parallelization of flash calculations come true. All of them are not only contributions to flash calculations, but also contributions to existing sparse grid techniques. Moreover, both of the sparse grid construction and interpolation algorithms can be done in parallel. Different from the former parallel algorithms in sparse grid techniques, which have troubles in decomposing the domain equally and keeping load balance among the processors, our parallel algorithm can achieve load balance easily among the threads for any sparse grid configurations. Lastly, multicomponent experiments are also carried out to demonstrate the accuracy, correctness and efficiency of the algorithms.

Numerical study of phase transition in Van der Waals and asymptotic stability of solutions of compressible Navier-Stokes-Cahn-Hilliard system

Name: Qiaolin He

Affiliation: Sichuan University, China



Biography: Prof. He is now an Associate Professor in School of Mathematics, Sichuan University, China. In 2003, she got her Master degree in Sichuan University. Afterwards, she obtained her Ph.D. degree of Mathematics in The Hong Kong University of Science and Technology, under the supervision of Prof. Xiaoping Wang. Before joining Sichuan University, she has worked with Prof. Xiaoping Wang as a postdoc for three years. Her current research interests include Adaptive Methods for Singular Problems and Numerical Methods for Complex Fluid Dynamics.

Abstract: In this talk, we use a relaxation scheme for conservation laws to study liquid-vapor phase transition modeled by the van der Waals equation, which introduces a small parameter ϵ and a new variable. In the case of diffuse interface model for two immiscible fluids, in order to understand the motion of the interfaces between immiscible fluids, we use a relaxation scheme coupled with convex splitting method to solve a compressible Navier-Stokes-Cahn-Hilliard system. Numerical results are given.

Numerical analysis of the methane degassing from crosslinked polyethylene cable insulation

Name: Dong Joon Youn

Affiliation: King Abdullah University of Science and Technology, KAUST, Saudi Arabia

Biography: Dr. Youn is now a postdoc in our group. He got his Bachelor and Master degree in Civil Engineering at Konkuk University, South Korea, and Ph. D degree in Civil Engineering at Colorado School of Mines, USA. He is the Member of ASCE (The American Society of Civil Engineers), SPE (The Society of Petroleum Engineering) and SME (The Society of Mining, Metallurgy & Exploration). He was awarded as the best paper given by Korean Geotechnical Society in 2007. Currently his research interests include Petroleum Geomechanics, Hydraulic fracturing, Numerical simulation on Unconventional hydro carbon production.

Abstract: Methane is a major byproduct chemically produced during the peroxide crosslinking process of the polyethylene insulation in high and extra-high voltage cables. Due to the environmental and safety issues, efficient removal of the methane, namely byproduct degassing, must be performed carefully during the cable manufacturing process. Several analytical and numerical techniques have been applied to analyze the efficiency of the methane transport within the cable, but our current understanding about the degassing process is still very limited due to the overly simplified degassing conditions applied for the previous researches. In contrast to the previous researches, we conducted a series of numerical studies considering the realistic degassing conditions such as thermal-diffusion coupling, internal holes in the conductor, diffusion coefficient variations between the XLPE and semiconductor, and non-uniform distribution of the methane concentration within the XLPE. From the results, we confirmed that the internal holes in the conductor play a significant role in the cable degassing, although the thermal-diffusion coupling effect is extremely small due to the substantial temperature increase during the initial degassing period. Because of the holes in the conductor, we also found that the amount of the methane stored within the conductor must be included in the degassing analysis to determine the completion of the degassing process. Additionally, the diffusion coefficient of the semiconductors and the non-uniform distribution of the methane within the XLPE are pretty essential factors influencing the degassing efficiency, while the effect of the non-uniform distribution of the methane on the degassing largely depends on the degassing time.

Multiscale Time-splitting DFM Modeling of two-phase flow including nanoparticles transport in fractured porous media

Name: Mohamed F. El-Amin

Affiliation: Effat University, Jeddah, Saudi Arabia

Biography: Mohamed F. El-Amin is a Full Professor at Effat University, Jeddah, Saudi Arabia and a Visiting Professor at King Abdullah University of Science and Technology (KAUST) in Saudi Arabia, and he also was a Professor at Aswan University, Egypt. As a mathematician, he has over 23 years of research experience in the field of computational mechanics, applied mathematics, reservoir simulation, heat and mass transfer, fluid dynamics, transport phenomena, and turbulence. After obtaining his PhD in applied mathematics in 2001, he held research positions in several universities including South Valley University (Egypt), Stuttgart University (Germany), and Kyushu University (Japan). He is a fellow of Alexander von Humboldt (AvH), and JSPS. The research of Dr. El-Amin has resulted in around 140 journal and conference papers and book chapters; and three edited books. He is a referee and a guest editor of some specialized journals.

Abstract: In this talk, we consider a two-phase immiscible incompressible flow including nanoparticles transport in fractured heterogeneous porous media. The system of the governing equations consists of water saturation, Darcy's law, nanoparticles concentration in water, deposited nanoparticles concentration on the pore-wall, and entrapped nanoparticles concentration in the pore-throat, as well as, porosity and permeability variation due to the nanoparticles deposition/entrapment on/in the pores. The discrete-fracture model (DFM) is used to describe the flow and transport in fractured porous media. Moreover, multiscale time-splitting strategy has been employed to manage different time-step sizes for different physics, such as saturation, concentration, etc. Numerical examples are provided to demonstrate the efficiency of the proposed multi-scale time splitting approach

GMsFEM for Solving Reduced Darcy Flow Model in Fractured Porous Media

Name: Manal Alotibi

Affiliation: Taif University, Taif, Saudi Arabia

Biography: Manal Alotibi is now an assistant professor in Department of Mathematics, Taif University in Saudi Arabia. She got her Ph. D degree of Mathematics at Numerical Analysis in Texas A& M University, USA, under the supervision of Prof. Yalchin Efendiev. During her long-time teaching experience in Taif University, she has taught various classes including Calculus I, II, III, Topology, Algebra, Numerical Analysis, Partial Differential equations, Complex Variable, Differential Equations and Group Theory. Currently, Prof. Alotibi is interested in researches focusing on Multiscale Finite Element Methods in Fractured Porous Media.

Abstract: In this talk I will present a reduced model for Darcy flow in fractured porous media. We solve this reduced model using Generalized Multiscale Finite Element Method (GMsFEM). Our approach is based on modeling the fracture flow in one dimension and the matrix flow in two dimensions. And then the GMsFEM is used to construct, efficiently, a lower dimension space that approximates the coupled Darcy flows in the matrix and the fracture. The advantage of using GMsFEM is representing the fracture effects on a coarse grid via multiscale basis functions constructed using local spectral problem. Solving local problem leads to consider small scale information in each coarse grid. On another hand, the multiscale basis functions generated offline following GMsFEM framework can be re-used for any input parameter to solve the problem in the online stage. Our goal is to combine GMsFEM with a reduced model for Darcy flow in fractured porous media. In this work, we consider a general case for the permeability in both fracture and matrix domain. Here, we would like to note that other research considered special case when the fracture permeability is much larger than the matrix permeability. Our experiment, at current stage, shows that the finite element solution for the matrix pressure in the case when the fracture permeability being much larger than the matrix permeability is almost continuous, while in the opposite case we will have discontinuity along the fracture.

Field process and surface process in CPF3, Halfaya Oil Field, Iraq

Name: Chenguang Li

Affiliation: China National Oil and Gas Exploration and Development Corporation, CNODC, China

Biography: Mr. Li is currently a process engineer for CNODC, China National Oil and Gas Exploration and Development Corporation. He got his bachelor degree in China University of Petroleum, Beijing and joined Worley-Parsons to start his career as an assistant piping engineer. In 2014, he decided to further his education by studying in UK and was awarded an MBA degree in oil and gas management from the Coventry University in the year of 2016 and then joined CNODC. In 2017 he was dispatched to Australia to work in an joint venture between Petrochina and Shell on a coal seam gas development project which Petrochina owns 50% of the natural gas from production. Since mid 2018 he has been transferred to Halfaya oil field which is jointly developed by Petrochina, Total, Petronas, Missan Oil Company and South Oil Company based in Iraq and this is an oil service contract mode. Now, Mr. Li is working on the process management and optimization of CPF3 in Halfaya Oil Field.

Abstract: Halfaya oil field is situated in the southern part of Iraq, in the Missan Governorate, 35 km southeast of Amarah city. The field is a NW-SE trending anticline structure about 30 km long, 10 km wide, total area is about 288km2. It was discovered in 1976 and significant oil accumulations have been discovered in the Tertiary Jeribe/Euphrates/ Upper Kirkuk formations and the Cretaceous Sa'di/Tanuma/Khasib, Mishrif, Nahr Umr and Yamama formations. Production 400,000BOPD, the PPT of Halfaya oilfield, was planned to achieve in the three Phases. Production 70,000-100,000BOPD for Phase I, based on the approved PDP, was achieved in June of Year 2012. For Phase II, the construction was completed according to the approved SPDP and total production of 200,000 BOPD was achieved in August of Year 2014. For Phase III, total production of 400,000BOPD (PPT) was planned to be achieved in December of Year 2016 based on MFDP and to maintain for 16 years. In this talk, Mr. Li will introduce Halfaya Oil Field, CNPC (China National Petroleum Cooperation), as well as CNODC and then report on his current work as a process engineer living and working at site.

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