



Gate of Industry 4.0, Embracing Artificial Intelligence

-- Tutorial on Machine Learning and Hand-on Coding Training

The CTPL group (Computational Transport Phenomena Laboratory, KAUST) is pleased to announce a workshop themed “Gate of Industry 4.0, Embracing Artificial Intelligence -- Tutorial on Machine Learning and Hand-on Coding Training” to gather our guests from Xi’an Jiaotong University, Virginia Polytechnic Institute and State University, King Fahd University of Petroleum and Minerals, China University of Petroleum, Taif University and Xiamen University, together with our CTPL members to step into the area of machine learning, especially deep learning. A distinguished young scholar, Yu Li, from Computational Bioscience Research Centre (CBRC) will give us a tutorial talk on the basic structure and procedure as well as instructions on the coding using Tensorflow and Matlab. Tao, Yiteng and Jingfa from CTPL will discuss on our current application of deep learning on optimizing engineering computations.

Location: Room 4214, Building 1, KAUST, Saudi Arabia

Time: 12:00pm – 16:00pm, 4th, March, 2019

Workshop Chair: Shuyu Sun

Workshop Secretary: Tao Zhang

Agenda

Time	Speaker	Topic
12:00pm—12:30pm		Group lunch and free discussion
12:30pm—12:40pm	Shuyu Sun	Opening and welcome
12:40pm—13:10pm	Yu Li	Introduction on the Machine Learning and Deep Learning
13:10pm—13:40pm	Tao Zhang	Application of Deep Learning on accelerating flash calculations
13:40pm—14:10pm	Yiteng Li	Further application of deep learning on more complex phase equilibrium problems
14:10pm—14:30pm		Coffee break and free discussion
14:30pm—15:00pm	Jingfa Li	A review on machine learning approach for efficient uncertainty quantification using multiscale methods
15:00pm—15:15pm	Haiyi Wu	Predicting Effective Diffusion in Porous Media from Their images by Deep Learning
15:15pm—16:00pm	Yu Li	Hand-on training on coding

2019 CTPL Workshop on Machine Learning

- * All presentations will include a short Q&A at the end.
- ** Lunch will be served at 12:00pm, 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.
- ***** It is highly suggested that the attendees could set up Tensorflow and Matlab in advance.
- ***** It is recommended that the attendees could finish the Matlab Onramp Course at <https://www.mathworks.com/learn/tutorials/matlab-onramp.html>
- ***** The time is shown in Saudi Arabia time zone (GMT+3)

Guest Attendees

Name	Affiliation
Prof. Rui Qiao	Virginia Polytechnic Institute and State University, the USA
Prof. Bo Yu	Beijing Institute of Petrochemical Technology, China
Prof. Jie Chen	Xi'an Jiaotong University, China
Prof. Liang Gong	China University of Petroleum, Qingdao, China
Prof. Huangxin Chen	Xiamen University, China
Prof. Manal Alotibi	Taif University, Saudi Arabia
Prof. Xianbin Luo	Guizhou University, China
Dr. Gang Lei	King Fahd University of Petroleum and Minerals, Saudi Arabia

Introduction on the Machine Learning and Deep Learning

Name: Yu Li

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

Biography: Mr. Li is now a PhD student at KAUST, majoring in Computer Science. He is a member of Structural and Functional Bioinformatics (SFB) Group, which is led by Dr. Xin Gao. He got Master degree in Computer Science at KAUST in December 2016. Before that, he got Bachelor degree in Biosciences at University of Science and Technology of China (USTC) in 2015. His research interests are Deep Learning, Bioinformatics and Machine Learning.



Abstract:

Machine learning algorithms, especially deep learning, have achieved great successes in recent years across different fields. In this talk, I will give a brief introduction on machine learning and deep learning. Because of the impressive potential of artificial intelligence, the related terminologies, such as ‘artificial intelligence (AI)’, ‘machine learning (ML)’, ‘deep learning (DL)’, have been abused in media, which can inevitably cause incorrect usages and people’s misunderstanding, who are not in the field. So, I will start from clarifying the basic concepts of ‘AI’, ‘ML’ and ‘DL’. After that, I will introduce the main tasks of machine learning, including classification, regression, clustering and dimensionality reduction. Then, I will give a brief introduction to neural networks, touching some interesting models, including convolutional neural networks (CNN), recurrent neural networks (RNN), graph convolutional neural networks (GCN) and generative models, such as generative adversarial networks (GAN).

Application of Deep Learning on accelerating flash calculations

Name: Tao Zhang

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

Biography: Mr. Zhang is now a PhD student in the department of Earth Science and Engineering, joining our group since August 2016. In 2013, he got his Bachelor degree in China University of Petroleum, Beijing with the major Oil & Gas Storage and Transportation. In June 2016, he obtained his master degree in the same major and university. Currently his research area includes multiphase flow simulation in different continuum scales.



Abstract:

In the past two decades, researchers have made remarkable progress in accelerating flash calculation, which is very useful in a variety of engineering processes. In this talk, general phase splitting problem statements and flash calculation procedures using the Successive Substitution Method are reviewed, while the main shortages are pointed out. Two acceleration methods, Newton's method and the Sparse Grids Method are presented afterwards as a comparison with the deep learning model proposed in this presentation. A detailed introduction from artificial neural networks to deep learning methods is provided here with the authors' own remarks. Factors in the deep learning model are investigated to show their effect on the final result. A selected model based on that has been used in a flash calculation predictor with comparison with other methods mentioned above. It is shown that results from the optimized deep learning model meet the experimental data well with the shortest CPU time. More comparison with experimental data has been conducted to show the robustness of our model.

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. Previously, a majority of studies focus on the safety rather than the efficiency. It has been reported that the equation-of-state based flash calculation consumes an enormous amount of computational time, up to 70%, in compositional simulation, making it the bottleneck for the extensive application of compositional simulators. As a result, the acceleration of flash calculations without much compromise in accuracy becomes an active research topic in the last two decades. In today's topic, the phase equilibria problem is modeled based on the NVT flash formulation. Based on the laws of thermodynamics and Onsager's reciprocal principle, mole and volume evolutionary equations are constructed to describe the dynamic process from any non-equilibrium state to the equilibrium state. Benefiting from its great capacity, we incorporate stability test and phase splitting calculation together, both of which constitute the phase equilibrium calculation, and accomplish them by a single deep learning model. It differs from the conventional flash framework where stability testing precedes phase splitting calculation, as most of the researches in flash speedup by machine learning follow. A number of simulation results are presented to show the accuracy and efficiency of the proposed deep neural network model.

A review on machine learning approach for efficient uncertainty quantification using multiscale methods

Name: Jingfa Li

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

Biography: Jingfa Li currently works as a postdoctoral fellow at Computational Transport Phenomena Laboratory (CTPL) at KAUST. He received the Bachelor degree from Southwest Petroleum University in 2012 and the PhD degree from China University of Petroleum (Beijing) in 2017 both in Petroleum Storage & Transportation Engineering. His research interests focus on FVM, model reduction method, and uncertainty qualification.



Abstract: In this talk, I will review a machine learning approach for the estimation of coarse scale basis functions in multiscale finite volume method. In this approach, a neural network predictor fitted using a set of solution samples from which it learns to generate subsequent basis functions at a lower computational cost than solving the local problems is developed. The computational advantage of this approach is realized for uncertainty quantification tasks where a large number of realizations has to be evaluated. The proposed approach is evaluated on elliptic problems yielding very promising results.

Predicting Effective Diffusion in Porous Media from Their images by Deep Learning

Name: Haiyi Wu

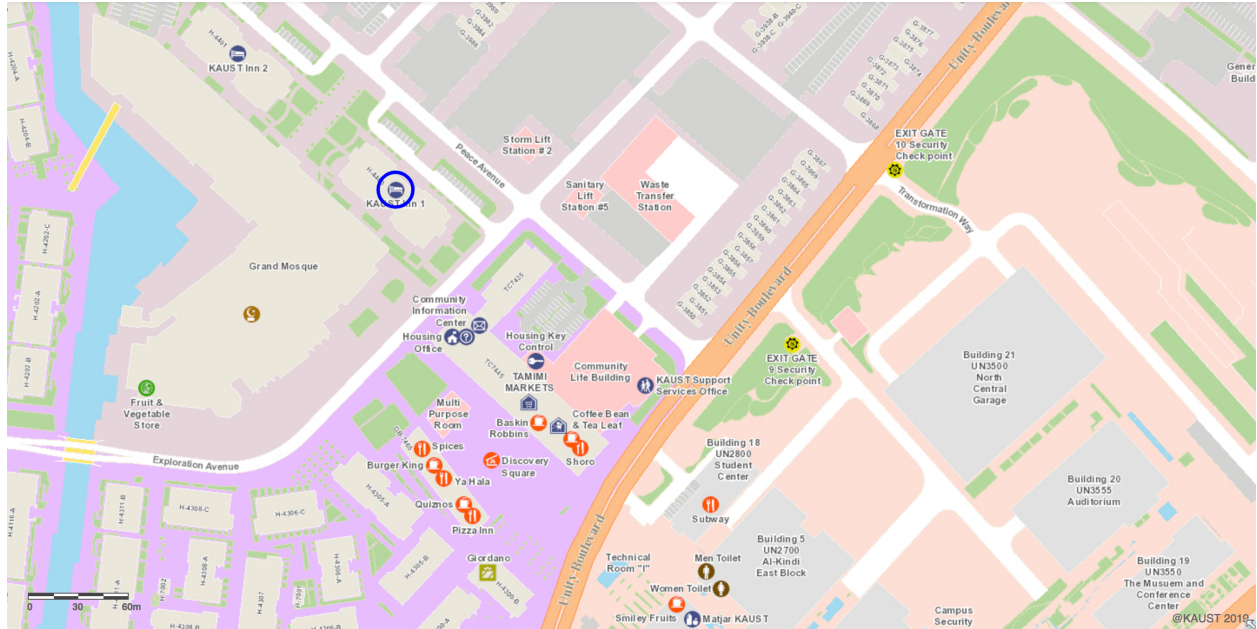
Affiliation: Virginia Polytechnic Institute and state University,
the USA

Biography: Mr. Wu is now a PhD student at Virginia Tech, majoring in Mechanical Engineering. He is a member in Laboratory of Transport Phenomena for Advanced Technology, which is led by Prof. Rui Qiao. He got Bachelor degree in Modern Mechanics at University of Science and Technology of China in 2015. His research interests are multiscale and multiphase transport phenomena in porous media.



Abstract: This work aims to test the application of machine learning for predicting the effective diffusion of a porous medium from its geometry and to improve machine learning performance by combining it with field knowledge. The general framework includes two parts. In the first part, a dataset for the diffusion coefficient in porous media is generated using the Lattice Boltzmann method. In the second part, machine learning method is used to process the datasets generated in the first step and to predict the diffusion coefficient of given porous structure. The convolutional neural networks (CNN) is used to train the dataset. Comparison with the ground truths indicates the excellent predictive performance by CNN in a wide variety of porous structures with a computational cost of several orders of magnitude smaller. The CNN results improves the prediction by conventional Bruggeman equation by almost 2 orders of magnitude, especially for those samples with small porosities and strong heterogeneity.

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