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Project 1: Fluid Connectivity in Porous Media

Project Lead: Nitish Nair

Background:

Reservoir rocks are complex porous structures composed of tortuous pathways and variable porosities. The complexity of the pore geometry influences the displacement and distribution of fluids (e.g., oil and water) in the medium. Certain zones are more likely to be wetted by water (hydrophilic) while others are preferentially wetted by oil (oleophilic). Given a porous medium with specific wetting characteristics, the equilibrium distribution and interconnectivity of oil-water domains determine its hydraulic and electrical conductances. This problem is not limited to flow in rocks alone but can be translated to various other porous media – e.g., battery electrodes, catalyst pellets etc.

Objective:

The intern will develop codes that compute the distribution of fluids in 3-D digital representations of porous media. Capillary flow governs the displacement of fluids in the rock. The computational challenge is twin-fold: (i) tracking the progress of multiple oil-water interfaces across pores of different diameters; (ii) detecting the presence of disconnected water or oil clusters. These aspects are crucial in determining the ultimate fluid configuration. Both problems have solutions drawn from the image processing domain, specifically, cluster identification and tracking. An additional complication is the design/choice of data structures used to store/update the cluster information. The overall goal is to build an efficient algorithm to track interfaces in porous media. The intern's task is to: (a) survey the state-of-the-art in cluster identification methods, (ii) choose or build optimal data structures for cluster storage, (iii) assimilate algorithms of choice in the existing flow code, and (iv) verify the results against simple 2-D and 3-D structures.

Qualifications:

Candidates majoring in Computer Science, Chemistry, Physics, Math, Mechanical Engineering or Earth Science are welcome apply. The candidate should be willing to learn new algorithms, simulation techniques and apply it to challenging problems. Familiarity with the Linux programming environment, C/C++/Fortran is essential.

Helpful references:

1. http://www.slb.com/~/media/Files/core_pvt_lab/industry_articles/201406_wo_core_flow_simulations_evaluate_recovery.pdf
2. http://www.ingrainrocks.com/media/files/user/FBSept08.pdf
3. http://www.physics.purdue.edu/flow/MMproject/Wilkinson1983.pdf

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Project 2: QSAR Approach to Predict Solubility of Hydrocarbons and Their Mixtures with Computational Chemistry Team

Project Lead: Ravi Agrawal

Background:

Liquid fuels (petroleum products) are primarily constituted of hydrocarbons. These are usually a mixture of long chain aliphatic and alicyclic hydrocarbons ranging from a few carbon atoms to few 10s of carbon atoms. From an environmental perspective, their behavior in water is of prime relevance. To that end, we are involved in development of models which can predict the solubility behavior of these products in water. The solubility of these liquid fuels is dependent on the composition and the solubilities of individual components. In this work, a theoretical framework needs to be evaluated to correlate various physiochemical descriptors with the solubility behavior of individual components. The calculations of descriptors will require use of *ab initio* (density functional theory based) or semi-empirical molecular modelling methods. In the later part, an attempt to predict solubilities of mixtures will also be looked at.

Objective:

The aim is to establish a method for calculation of physiochemical descriptors and then automating the process for a few hundred of molecules. The data generated will be analyzed for correlations with solubility values available from experiments/external literature.

Qualifications:

The candidate should have a strong background in Chemistry, Physics, Material Science and/or Mechanical Engineering with basic knowledge of statistical tools for data analytics. Familiarity with Linux environment is required. Previous experience with Density Functional theory or other semi empirical methods like AM1, PM6, etc. would be helpful. The candidate should be willing to learn new simulations techniques and be able to apply it to challenging problems. The candidate should have good communication skills, report writing skills and the ability to work in a multidisciplinary diverse team.

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Project 3: Smoothed Particle Hydrodynamics: Multiphase flows inside complex packed bed geometry

Project Lead: Aarthi Thyagarajan

Background:

Smoothed-particle hydrodynamics (SPH) is a computational method used for simulating fluid flows and solid mechanics. SPH is a mesh-free, particles based, fully Lagrangian method. SPH is being applied in Shell for reactor designs in complex situations involving multi-physics (e.g. multi-phase, heat and mass transfer coupled with reaction), multi-scale (e.g. mesoscale and macroscale effects) and problems that involve irregular/complex solid geometry (e.g. Packed bed reactor for complex shapes of the catalyst).

Objective:

We have extended the in-house SPH code to multi-phase system and thermal effects, and have also implemented multiphase physics with surface tension effects tuned to capture the wettability effects. In 2015, an intern successfully implemented the adaptive particle resolution in SPH framework. This work was published in SPHERIC conference this year (Ref -6). In 2016, an intern implemented new inflow outflow framework to study multiphase flows. For 2017, we would like the intern to address the following subtopics:

1. The effect of surface tension on the multi-phase heat transfer for flow through a porous medium. In principle, radial mixing is expected to increase the heat transport, and that higher surface tension would in fact decrease radial mixing, especially in the liquid phase, so we expect it would negatively affect the heat transfer, but this is also related to the liquid viscosity. We would like to study the interplay between wettability on the solid surface, surface tension between phases and viscosity on the heat transfer characteristics.
2. The prediction of overall heat transfer coefficients in packed beds of different pellet shapes with co-current down flow of gas and liquid for different flow conditions.

Qualifications:

Candidates majoring in Engineering, Chemistry, Physics, Math, Mechanical Engineering or Earth & Climate Science are welcome to apply. The candidate should be willing to learn new simulation techniques and be able to apply it to challenging problems. Minimal experience in C++ and C programming is expected.

Helpful references:

1. Liu and Liu, Arch Comput Methods Eng 2010; 17: 25
2. Szewc et al., Int. J. Nonlinear Sci. Numer. Simul. 2012; 13(6): 383
3. Tartakovsky et al., Journal of Computational Physics 2007; 222: 654
4. Hu and Adams, Journal of Computational Physics 2006; 213: 844
5. http://geonumerics.mit.edu/
6. https://www.events.tum.de/frontend/index.php?folder_id=265

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Project 4: Dynamics of particles in droplets in complex fluids

Project Leads: Rutger IJzermans, Prashant Sinha, Kuochen Tsai

Background:
Shell's operations often involve complex fluids. Examples are oil droplets in water and sand particles in drilling mud. In order to gain a greater understanding of the practical behavior of complex fluids, we propose to numerically study the dynamics of particles and droplets in viscous fluids. Relevant parameters are the approach time between two particles and the effective restitution coefficient during the collision of two particles in a viscous liquid. The results will be useful for the design of separators and the optimization of operations with dense slurries.

Objective:
The numerical simulations can be carried out with Shell's in-house Smoothed Particle Hydrodynamics (SPH) code, which includes a Discrete Element Method (DEM) to predict rigid body motion. This code can be used to predict the dynamics of arbitrarily shaped particles and droplets in viscous fluids. For better physical accuracy for the motion of two nearby particles, it is planned to implement the lubrication force model from [1]. Ultimately, the goal is to perform a systematic analysis of approach time and coefficient of restitution for a range of relevant particle/droplet properties (e.g., Stokes number, Reynolds number), approach angles and particle geometries, using three-dimensional SPH simulations.

Qualifications:
Candidates majoring in Chemistry, Physics, Math, Mechanical Engineering or Earth & Climate Science are welcome apply. The candidate should be willing to learn new simulations techniques and apply it to challenging problems. Familiarity with C++ and the Linux programming environment is desirable.

Helpful References:

1. A. Vazquez-Quesada & M. Ellero (2016), "Three-dimensional simulations of dilute and concentrated suspensions using smoothed particle hydrodynamics", Computational Particle Mechanics, Volume 3, Issue 2, pp. 167–178.
2. A.M. Ardekani & R.H. Rangel (2008)," Numerical investigation of particle–particle and particle–wall collisions in a viscous fluid", Journal of Fluid Mechanics, Volume 596, pp. 437

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Project 5: Developing a General Fuel Property Screening Tool using Machine Learning

Project Leads: Indranil Rudra, Abhinav Verma

Background:

Exploring new additive chemistries allows the development of higher performing fuel products, such as Shell FuelSave Diesel and Shell V-Power Diesel. The differentiated fuels market has existed for approximately 20 years and in this time, diesel engine technology has rapidly evolved. Due to the need to reduce emissions and improve fuel economy and power simultaneously, modern injection strategies and other engine developments will trigger innovation in the traditional fuel additive technology space. The implication of this is that R&D fuels must rapidly start exploring new additive options, testing as many additive candidates as possible, and as fast as possible. This is best achieved through a joint high throughput computational and experimental process. The computational process shall extract data from chemical databases and experimental databases via data mining and statistical analysis to develop a quantitative structural activity relationship (QSAR) model, which will be used to identify suitable additive chemistries. The experimental section involves performing a series of benchtop tests (this is already an ongoing program in Fuels R&D) based on modelling recommendations.

Objective:

We aim to develop a general-purpose fuel property tool using machine learning, with the intent of screening molecules for desirable fuel properties (e.g. ignition delay, burn period). Given a list of training compounds (with identifiers and measured values) and a list of testing compounds (with identifiers) as input, the tool should incorporate user-provided features, impute missing values, perform feature reduction, build a classifier, and cluster compounds. The tool should then collect data for the testing compounds and predict class membership. It should then determine whether test compounds are found in the range of variability of the training data set.

Qualifications:

Candidates majoring in engineering or science are welcome to apply, with special interest in data analytics, machine learning and cheminformatics. The candidate must be fluent in programming in at least one of these languages: C, R, Python, MATLAB.

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Project 6: Modelling of Advanced Energy Storage Systems

Project Lead: Shashi Adiga

Background:
Physical, chemical and thermal processes in batteries occur in complex geometries over a wide range of time and length scales. The combination of materials (electrode, electrolyte and membrane) as well as architecture (thicknesses, porosity, particle size) and highly dynamic environmental conditions significantly influence the electrical, thermal, electrochemical, and mechanical responses of a battery system. Fundamental knowledge of the interplay different phenomena is critical to the design and optimization of affordable, high-performing, and long cycle life battery systems. To this end, computational and modelling and simulations using techniques ranging from atomistic simulations to continuum device scale simulations are proving to be very useful in providing understanding of fundamental processes as well as in design and optimization of materials and battery geometries.

Objective:
The main objective of the work is to use available computational tools to analyze electrochemical performance of electrode materials and full electrochemical cells. This would involve, for example, deriving electrochemical potentials and ionic diffusivity of materials from first-principles simulations and calculating current-voltage behavior of electrochemical cells using continuum methods. The goal of the project is to develop a workflow that will take in information from both first-principles simulations and experimental measurements of battery materials and use them in cell-scale continuum simulations to perform optimization of different parameters for improved battery performance.

Qualifications:
Candidates majoring in Chemistry, Mechanical Engineering and/or Physics are welcome to apply. The candidate should be willing to learn new simulations techniques and apply it to challenging problems. Familiarity with the Linux programming environment is desirable.

Helpful References:

1. https://www.electrochem.org/dl/interface/wtr/wtr05/wtr05_p39-42.pdf
2. http://web.mit.edu/braatzgroup/Modeling_and_simulation_of_lithium_ion_batteries_from_a_systems_engineering_perspective.pdf
3. http://www.nrel.gov/transportation/energystorage/model_simulation.html

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Project 7: Explosion Modeling: Validation of explosion modeling against small/large scale experiments

Project Leads: Pratap Sathiah, Debapriya Chakraborty

Background:
Ability to predict the consequences of gas explosions in petrochemical plant is important to assess risk and to provide control or recovery measures to mitigate the risk. Computational Fluid Dynamics (CFD) tool is used for prediction of gas explosions in a complex petrochemical plant. The tool allows prediction of flow, turbulence and combustion on a three-dimensional mesh comprising many thousands or even millions of computational cells. It is developed in an open source framework - OpenFoam (Opensource Field Operation and Manipulation, OpenCFD Ltd., 2005). The tool solves flow, turbulence and progress variable equations to track the turbulent and flame propagation.

Objective:
The goal of this project is to validate the existing in-house CFD tool against large sets of experimental data available in open literature. The results a) flame position, b) overpressure and c) impulse from the simulation will be compared against experiments. In addition, effects of grid size and Courant Number on explosion overpressure and turbulent flame speed will be investigated. Possibility of using adaptive mesh refinement for explosion modeling will also be explored.

Qualifications:
Candidates majoring in Mechanical or Chemical Engineering are welcome to apply; in particular fluid dynamics, with special interest in computational fluid dynamics and combustion science. The candidate must be fluent in programming in at least one of these languages: C++.

Helpful References:
For a quick understanding of CFD tool we are using, please see:
https://en.wikipedia.org/wiki/OpenFOAM

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Project 8: Blast Wave: Validation of prediction of decay of blast waves against large/small scale experiments

Project Lead: Pratap Sathiah, Debapriya Chakraborty

Background:
Ability to predict the consequences of gas explosions in petrochemical plant is important to assess risk and to provide control or recovery measures to mitigate the risk. Computational Fluid Dynamics (CFD) tool is used for prediction of gas explosions in a complex petrochemical plant. The tool allows prediction of flow, turbulence and combustion on a three-dimensional mesh comprising many thousands or even millions of computational cells. It is developed in an open source framework - OpenFoam (Opensource Field Operation and Manipulation, OpenCFD Ltd., 2005). The tool solves flow, turbulence and progress variable equations to track the turbulent and flame propagation.

Objective:
The goal of this project is to validate the existing in-house tool against large sets of experimental data available in open literature. The results a) overpressure and b) impulse at far field location from the simulation will be compared against experiments. In addition, effects of grid size and Courant Number on decay of overpressure will be investigated. Possibility of using adaptive mesh refinement for capturing the blast waves will be explored.

Qualifications:
Candidates majoring in Mechanical or Chemical Engineering are welcome to apply; in particular fluid dynamics, with special interest in computational fluid dynamics and combustion science. The candidate must be fluent in programming in at least one of these languages: C++.

Helpful References:
For a quick understanding of CFD tool we are using, please see:
https://en.wikipedia.org/wiki/OpenFOAM

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Project 9: Change-point models for GPS data

Project Lead: Saptarshi Das, Stijn Bierman

Background:
Data from permanent Global Positioning System (GPS) stations can be used to monitor surface displacements due to reservoir compaction. Sudden changes in the way the field is produced may be reflected in sudden changes in reservoir compaction and consequently surface displacement rates.

Objective:
High frequency (hourly) data from 12 permanent GPS stations above the Groningen gas field are available. Statistical methodology for the analysis of GPS data needs to be developed to infer, possibly delayed, trend changes which would evidence that sudden changes in gas production at 01-01-2014 have resulted in changes in reservoir compaction. The aim of this project is to apply a number of published statistical "change-point" methods from the scientific literature to the GPS data, and to discuss the relative merits and suitability of these methods to answer the question at hand.

Qualifications:
Expertise in data analytics, statistics and machine learning. Candidates majoring in Mathematics, Applied Math, Computer Science and Mechanical Engineering are encouraged to apply. Minimum requirements: knowledge of statistics, machine learning algorithms, programming in R/MATLAB, and experience/interest in data analytics.

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Project 10: Usage of open street map data in the analysis of Interferometric Synthetic Aperture (InSAR) data analysis

Project Lead: Saptarshi Das, Stijn Bierman

Background:
Interferometric Synthetic Aperture (InSAR) data can be used to monitor surface displacements due to reservoir compaction. Sudden changes in the way the field is produced may be reflected in sudden changes in reservoir compaction and consequently surface displacement rates.

Objective:
Low frequency (monthly) data from millions of Persistent Scatterers above the Groningen gas field are available. Statistical methodology for the analysis of InSAR data needs to be developed to infer, possibly delayed, trend changes which would evidence that sudden changes in gas production at 01-01-2014 have resulted in changes in reservoir compaction. The variability in InSAR signals is likely partly due to the object at the surface which is creating the back-scatter, such as a house, road, or woodland. The aim of this project is to assess the potential to use publicly available data, in particular Open Street Map (OSM) tiles to better explain the variability in InSAR signals.

Qualifications:
Expertise in data analytics, statistics and machine learning. Candidates majoring in Mathematics, Applied Math, Computer Science and Mechanical Engineering are encouraged to apply. Minimum requirements: knowledge of statistics, machine learning algorithms, programming in R/MATLAB, and experience/interest in data analytics.

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Project 11: Develop Advanced Analytics Insights for Lubricants Supply Chain

Project Lead: Laks Raghupathy

Background:
Shell runs world-class supply chains for its various businesses which among others includes its lubricant products. We are #1 in the world lubricants market consistently for many years in a row. Our business excellence is driven by product innovations developed with cutting edge R&D and a supply-chain underpinned by industry-best information technology backbone capturing large amounts of business data. Using this global data layer, we aim to unlock integrated business value by developing advanced analytical insights

Objective:
In this project, we will develop a data-driven approach using machine learning and data mining technologies, which will be developed on real-world data collected from Shell's business operations.

The goal of this project is to mine large sets of data in order to predict trends or spot patterns which may include demand forecasting, product lifecycle management among others. The intern will encouraged to explore and exploit state of the art tools especially in the areas of machine learning and artificial neural networks (read Deep Learning) using and building on tools such as Keras/Theanos on Google TensorFlow or equivalent. They will be involved in all aspects of the project, from data preparation to building robust and scalable models.

Qualifications:
Candidates majoring in Computer Science/Statistics/Applied Math with special interest in data analytics, machine learning and data visualization are welcome to apply. The preferred candidate must be fluent in programming in at least one of these languages: R, Python, MATLAB. Experience in visualization tools such Spotfire will be an added plus.

Helpful References:
For a quick understanding of some machine learning methods:
http://robotics.stanford.edu/~nilsson/MLBOOK.pdf

Check Wikipedia for basic ideas:
https://en.wikipedia.org/wiki/Deep_learning

Google's TensorFlow:
https://www.tensorflow.org/

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Project 12: Machine Learning and Data Science for Novel Materials Screening and Design

Project Lead: Praveen Pankajakshan

Background:
These are quite exciting times for Materials Sciences with new materials discovery propelling applications in Clean Energy, Space, National Security and Human Welfare [1]. However, the typical time frame of a material from the initial research and discovery to its incorporation in applications for first-use is remarkably long, of about 10 to 15 years. This is partly due to lack of an integrated approach that considers all aspects of materials development and the continued reliance of research on scientific intuition and trial-and-error kind of exploratory experimentation.

Objective:
Design of materials from first-principles simulations using advanced High Performance Computing (HPC) infrastructure (see [2]) is an attractive avenue to move away from pure empiricism, although the process is still lengthy and time-consuming. The next stage of innovation is on automating the process of intuition that is involved during materials synthesis: taking it from idea to the desired material. This project would be part of the toolkit to develop semi-automated workflows or 'recipes' that can help a Material Scientist to start from datasets of materials with their properties and descriptors and to learn models that can predict these properties accurately and reliably. The recipe will employ Machine Learning and Statistical Analysis through application to a case study leading to identification of descriptors relevant to the Material Science, starting from database of Materials and their properties. We expect that the methodology and algorithms developed to be versatile in obtaining chemical insights into complex phenomena, and extension of these models to designing next generation of materials [3].

Qualifications:
Candidates majoring in Applied Mathematics, Electrical Engineering, Computer Science, Statistics or others with background in Data Analytics/Machine Learning/Signal Processing are welcome to apply for this position. The candidate must be familiar with one of the two programming languages Matlab or Python.

Helpful References:

1. White House Genome Initiative: https://www.whitehouse.gov/mgi
2. Materials Project: https://materialsproject.org/
3. Can artificial intelligence create the next wonder material? http://www.nature.com/news/can-artificial-intelligence-create-the-next-wonder-material-1.19850