Machine learning for physics-based modeling

The workshop is the second workshop organized in the context of the Indo-Dutch project, "Digital Twins for pipeline transport networks". The aim of the project is to develop a digital twin that connects sensor data and advanced fluid solvers in order to detect possible leakage of fluid from the pipeline in real-time. Of particular interest is then also to develop machine learning based solvers for physics-based models, as traditional solvers are typically much too slow for real-time applications. Next to the presentations discussing the progress in the project, we have also invited speakers from outside the project, presenting their work on physics-based modeling and efficient computation.We thank the NWO (the Netherlands), MeitY (India) and Shell (the Netherlands) for funding the project.
In the present workshop the following talks have been scheduled:

Speaker 1: Karen Veroy-Grepl

Dimension reduction: Recent advances towards combining models and data
Abstract: TBA
Bio: TBA

Speaker 2: Ankit Tyagi and Abhineet Gupta

Machine learning for multiphase flow modelling in pipelines
The design and analysis of multiphase flows in wells, pipelines, and risers, as used in energy industry, is typically based on either empirical correlations (e.g., Beggs and Brill, Mukherjee and Brill, Duns and Ross) or on first-principles mechanistic models (e.g., the Shell Flow Correlations, the TUFFP Unified model, the Leda Flow point model, or the OLGA flow correlations).
Over the last few decades, Shell has developed its own set of two-phase and three-phase flow models that calculate the flow characteristics in pipelines, such as the flow pattern, the pressure-drop, and the liquid hold-up. These characteristics depend on input variables, such as the superficial velocities, the pipe diameter, angle inclination, wall roughness, and fluid thermodynamic properties, like density, viscosity, and surface tension. These multiphase flow (sub)models are collectively known as the Shell Flow Correlations (SFC).
The present work considers the development of a machine learning model trained on synthetic and lab data for the steady-state multiphase pipe flow. We propose a new method for calculating the flow characteristics (such as the flow regime, pressure drop, and liquid holdup) in a pipe segment based on ANNs and transfer learning technique. The segment module consists of three sub-models, namely, for determining the flow regime, pressure drop, and liquid holdup, respectively. For the creation of such a sub-model, we use the transfer learning methodology. In the first stage, the ANNs are trained on synthetic data, which we generate by using SFC mechanistic model. In the second stage, we train meta-models additionally on the real data, which in our case consist of lab measurements. As a result, we create the new multiphase flow correlation, which includes the basics of the physics-based SFC model and is tuned for real data.

Bio: Ankit Tyagi is working as an AI Resident in Systems Modelling group at Shell. He finished his B.E. in Chemical Engineering from Thapar university. He completed his Master's and PhD from Indian Institute of Science, Bangalore in Computational Fluid Dynamics. After completing his PhD, he joined HPCL RD center as a Research Associate in the modelling group of hydro-processing. During the tenure at HPCL, he developed a deep interest in AI and machine learning and he worked in a couple of startups. He worked on NLP, Computer vision, Predictive maintenance and other time series projects in his professional career. His research interests are to combine the data driven models with CFD to solve the industrial fluid flow problems. He has an extensive experience with simulations using DNS, RANS and LES based methods and used computational languages like C++, Python and R along with machine learning and deep learning libraries.

Abhineet is working as a researcher in Systems Modelling team at Shell. He obtained his undergraduate degree from Indian Institute of Technology, Kanpur in aerospace engineering. He graduated with honors from the aerospace engineering department of TU Delft. He has a PhD in applied physics with specialization in computational fluid dynamics and turbulence modelling from TU Eindhoven with several publications in internationally renowned journal and conference proceedings. His areas of interest are multiphase flows, turbulent flows, systems modelling and use of machine learning for fluid flow modelling.

Speaker 3: Vineet Tyagi

Digital twin for real-time detection of leakages in water pipeline networks
We discuss a machine learning based method to identify and localize leaks in a Water Distribution Network (WDN). In urban water distribution networks, it is difficult to obtain realtime demand data, which is a necessary input for a hydrological model. Using the pressure and flow data at few locations in WDN (obtained using ideally an IoT network of sensors), we develop an interpretable classification model to predict occurrence of an incremental leak and also locate its occurrence in the network. Using hydrological simulations we demonstrate the efficacy of the model.

Bio: Vineet Tyagi has been working at IISc for the last 2 years on a project aimed at identifying leaks in large Water Distribution Networks using Machine Learning. Prior to that, he has been working in analytical profiles in wealth management, business consultancy and business operations space. Vineet completed his BTech and MTech studies in Metallurgical Engineering and Materials Science from IIT Bombay. During his Masters program, he worked on simulating viscous flow using CFD equations which could help in understanding workings of a blast furnace.

Speaker 4: Nikolaj T. Mücke

Markov Chain Generative-Adversarial Neural Networks for Solving Bayesian Inverse Problems
Abstract: Inverse problems are important in the area of computational fluid flow dynamics. Prominent examples of inverse problems are state and parameter estimation which are difficult to deal with because of the expensive computational models and the lack of accurate measurement data. An elegant approach to solve this inverse problem is with a Bayesian framework, which provides regularization as well as uncertainty estimates. However, the computational costs of sampling from the posterior are typically prohibitive in practical cases.
We present a new approach, Markov Chain Generative Adversarial Neural networks (MCGANs), to alleviate the computational costs associated with solving the Bayesian inference problem. GANs are an excellent framework to aid in the solving of Bayesian inference problems, as they are designed

to generate samples from high-dimensional complicated distributions. By training a GAN to sample from a low-dimensional latent space and then embedding it in a Markov Chain method, we can highly efficiently sample the posterior, by replacing both the high-dimensional prior and the expensive forward map.
The approach is shown in several test cases, including the important engineering setting of detecting leaks in pipelines that transport water.

Bio: Nikolaj T. Mücke is a Ph.D. student in the Scientific Computing group at Centrum Wiskunde & Informatica (CWI) and at Utrecht University. His research is in the area of physics-informed machine learning and digital twins with applications primarily in fluid dynamics and engineering.

Speaker 5: Deepak Subramani

Machine Learning in the Geosciences
The growth of data science, machine learning and deep learning has opened several new research avenues in the Geosciences, which abounds with rich spatiotemporal datasets and physics-based models. We focus on recent applications of machine learning in satellite oceanography, and habitat suitability estimation in human-wildlife conflict. First, we show a novel W-Net architecture that we developed for extracting synoptic ocean features from concurrent satellite images. Second, we develop a random forest algorithm for studying the habitat suitability of Asian elephants in India.

Bio: Dr. Deepak Subramani is an Assistant Professor in the Dept. of Computational and Data Sciences at the Indian Institute of Science (IISc) in Bangalore. He obtained his Ph.D. in Mechanical Engineering and Computation from the Massachusetts Institute of Technology (MIT), USA, and B.Tech in Mechanical Engineering from IIT Madras. He works in using ML/AI for geoscience applications, aerospace systems, uncertainty quantification, and optimal routing of autonomous vehicles. He is an expert in data-driven modeling, numerical optimization, and scientific computing. Website: http://cds.iisc.ac.in/faculty/deepakns/