Imperial College London
Department of Earth Science and Engineering
MSc in Geo-energy with Machine Learning and Data Science

Independent Research Project
Project Plan

Rapid modelling of ATES using Machine Learning

by

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Abstract

The project aims at developing machine learning models to increase the efficiency of ATES simulation while retaining its accuracy from current numerical simulations. With a wide range of simulation results obtained from different parameters and aquifer configuration by in-house numerical model of IC-FERST, the study will focus on the implementation of machine learning models from multiple architecture including Graph Neural Network (GNN), transformer (attention mechanism), Fourier Neural Operator (FNO) or Convolutional Neural Network (CNN) on predicting the output of numerical simulation in adaptive time steps and irregular spatial mesh (dynamically deformed across time steps). The evaluation on performance will shed light on the capability of capturing the physics behind and its accuracy of replicating the results from numerical simulations. The final model is expected to unleash the potential of machine learning models accelerate current numerical simulations and to provide instant insights on ATES installation. As a pioneering model in the field, the project may ultimately discover the possibility of creating a digital twinning to replicate the complicated physics under various conditions.

1 Introduction

1.1 Background and Problem Description

ATES provides a low carbon technology solution to regional heating and cooling at the heart of energy transition. The design of ATES installation involves numerical simulations on subsurface fluid flow and heat transfer within the aquifer, which the numerical simulations are often computationally expensive with its fine spatial grid and closely spaced time steps to ensure accuracy.
To facilitate fast ATES simulation for providing instant insights on installation, the study proposes deploying machine learning models to increase the efficiency from numerical simulations while retaining the accuracy. As the numerical simulation by in-house model of IC-FERST is implemented on adaptive mesh and irregular time steps, this project will evaluate the capability of proposed models to capture the physics of subsurface fluid flow and the thermodynamics under unstructured mesh (graph). Models including Graph Neural Network (GNN) or Fourier Neural Operator (FNO) will allow extra flexibility in deforming the mesh adaptively in each time steps, while conventional Convolutional Neural Networks (CNN) which takes in a regular mesh grid may require extra steps in pre-processing including casting an unstructured graph to a structured grid before training the model.

The difference in architecture between the models may result in a difference in the physics captured, which the project may discover further upon compilation of those architecture. The final model is expected to deliver simulations of 240 timesteps and record the change of physical quantity across irregular timesteps throughout simulation.

1.2 Review of Existing Work

As the project involves dealing with unstructured graph data for spatial-temporal modelling, review of existing work will focus mainly on the implementation of machine learning models including GNNs, FNOs, CNNs and their variations in other applications.

1.2.1 Graph Neural Network (GNN)

Previous work demonstrated a representation of unstructured mesh graph data by deploying GNNs to capture the time evolution of subsurface CO_2 plume migration (Ju et al., 2023). GNNs capture the spatial-temporal relation in the subsurface even with complex geometry involving faults, in which CNNs in regular cartesian mesh grid may not be able to handle such heterogeneity accordingly (Ju et al., 2023). The outstanding generalisation capability leveraged by GNN can potentially be incorporated into different model architecture to enhance efficiency but retaining certain accuracy.

1.2.2 Fourier Neural Operator (FNO)

FNOs are introduced in existing work to deal with complex PDEs, leveraging it generalisation capabilities upon higher dimension problems. Previous work incorporated FNO into U-net structure in which FNO successfully capture spatial pattern globally in an efficient way with its fast Fourier transform (FFT), combining it with the capability of capturing local features with convolutions to enhance the representation power (Wen et al., 2021). With its robust generalisation power, the U-FNO model is faster and more data efficient comparing with conventional CNN while retaining accuracy (Wen et al., 2021).

1.3 Objectives

With all the existing work successfully model the subsurface multi-phase fluid flow in CCS project, the project aims at developing a machine learning model that captures spatial-temporal features in unstructured graph data, providing a fast simulation for ATES installations. If time allows, multiple models with a range of architecture will be trained and evaluated to compare its capability to capture the physics, computational or data efficiency, and accuracy.

1.4 Significance

As a pioneering model in the field, significance of the project sheds light on providing insight for accelerating numerical simulations with machine learning approach at sufficiently low time complexity or simulation runtime, speeding up the development of technology solution and ultimately contributing to a faster yet reliable transition to our low carbon future.

The model architecture may serve as a key component in creating surrogate models and digital twinning of a complicated system to encapsulate the physics behind not only in the field of subsurface engineering at the heart of energy transition, but transferable to other similar systems with physical quantities coupled together in a complicated way.

2 Methodology

2.1 Data acquisition

As the model will be trained on simulation input parameters, mesh, and simulation results, 840 sets of numerical simulations from in-house code IC-FERST are prepared as training dataset. The figure below outlines the data involved in each simulation scenario:

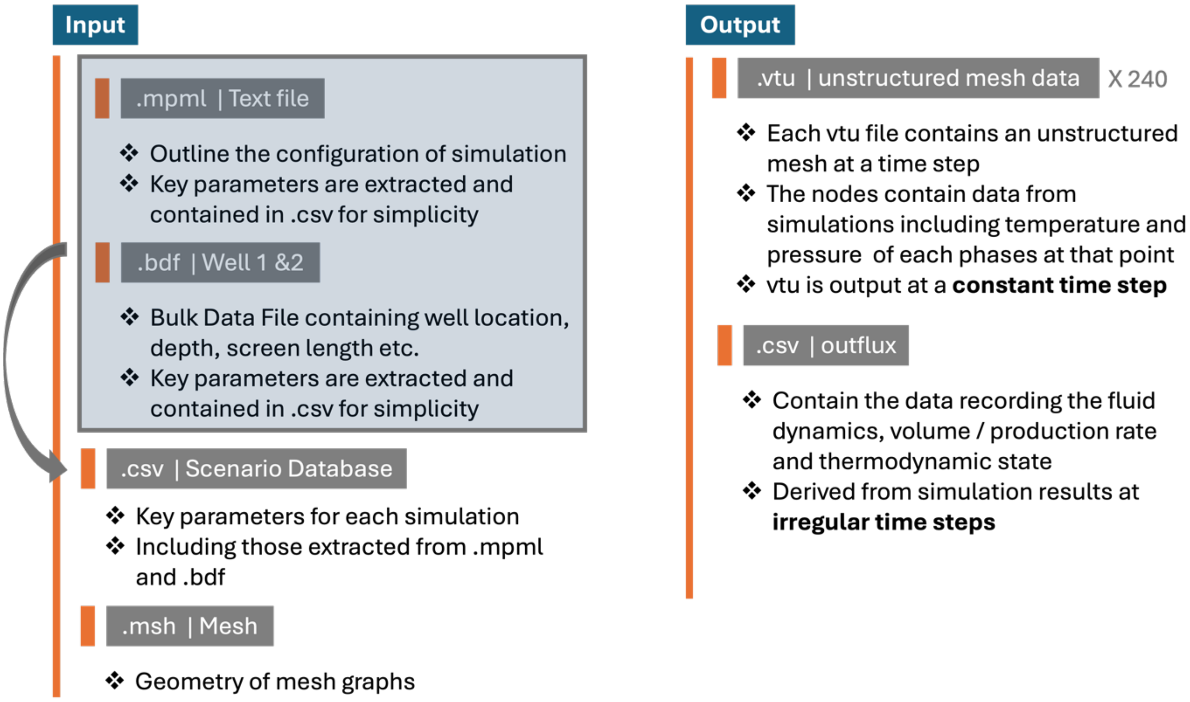

Figure 1 | Input and output of the model from simulation data

The figure outlines the required data from IC-FERST simulation for each simulation, which the model will be trained on (1) parameters from scenario database, and (2) mesh to predict 240 timesteps of simulation results and the data as in the outflux.csv.

2.2 Pre-processing

As different model architecture may require slightly different data pre-processing pipeline, 2 pathways of data pre-processing are proposed.

2.2.1 Unstructured graph data for GNNs

Input data pre-processing

1. Read the nodes in mesh and store it as a graph data.
2. Create a one-hot encoded attributes to nodes informing the location of wells.
3. Incorporate thermodynamical parameters (density, heat capacity, thermal conductivity, initial temperature) from the scenario database.csv into nodes representing overburden, aquifer and underburden accordingly.
4. Create another graph in which the nodes are located at the barycentre of the existing thermodynamics graph, containing information regarding the dynamics of fluid flow in the subsurface (velocity, porosity, and permeability). The new staggered graph is created to allow message passing for the flux of controlled volume of nodes in previous graph throughout training.

Output data pre-processing

1. Read the mesh from .vtu and store as graph
2. Incorporate the simulation results (stored as nodes in.vtu) into the graph.

2.2.2 Structured grid data for CNNs

Input data pre-processing

1. Follow all the steps as for unstructured graph data, attaining 2 staggered graphs containing thermodynamics and fluid flow parameter respectively.
2. Cast the 2 unstructured graphs into a single mesh grid of structured cartesian grids (may also consider store as staggered grid as of Arakawa C grid).
3. Perform interpolation whereas necessary.

Output data pre-processing

1. Follow all the steps as for unstructured graph data, attaining a graph
2. Cast the graph into a single mesh grid of structured cartesian grids.
3. Perform interpolation whereas necessary.

2.3 Model Architecture

2.3.1 Graph Neural Networks (GNNs)

The project will focus mainly on GNNS and may consider its variants including the incorporation of attention layer and U-net architecture. As the inputs of the project involves staggered unstructured graphs, the message passing within (horizontal pass) and across (vertical pass) the 2 graphs are considered in the design of architecture.

GraphCast model by Lam et al. (2023) from Google Deepmind suggested an auto-regressive way to cast multiple graphs of different resolutions to allow vertical message pass after horizontal message pass. It is computationally efficient to perform all horizontal message pass simultaneously at different resolution level, with the capability to capture features from different scales. The project may take reference from the way it casts graph and facilitates horizontal and vertical message passing.

2.3.2 Convolutional Neural Networks (CNNs)

CNNs serves as an alternative to work on structured spatial mesh grid, in which U-net structure may facilitate the feature extraction and reconstruction of simulation results at different time steps with skip connections. In this project, it is proposed to incorporate: (1) self-attention layer on the encoder after each convolution layer, (2) Residual connections vertically as suggested in Resnet for deeper network, (3) LSTM cell at the bottleneck (optional).

3 Expected Outcomes/Deliverables

The project is expected to yield a model for rapid simulation of ATES, and to develop a metric to evaluate (1) the capability of models to capture the physics (as compared with the ground truth of output at each timesteps and the outflux data), and (2) the accuracy in reconstruction of simulation results at each timesteps. If time allows, multiple models will be compared laterally.

4 Project plan

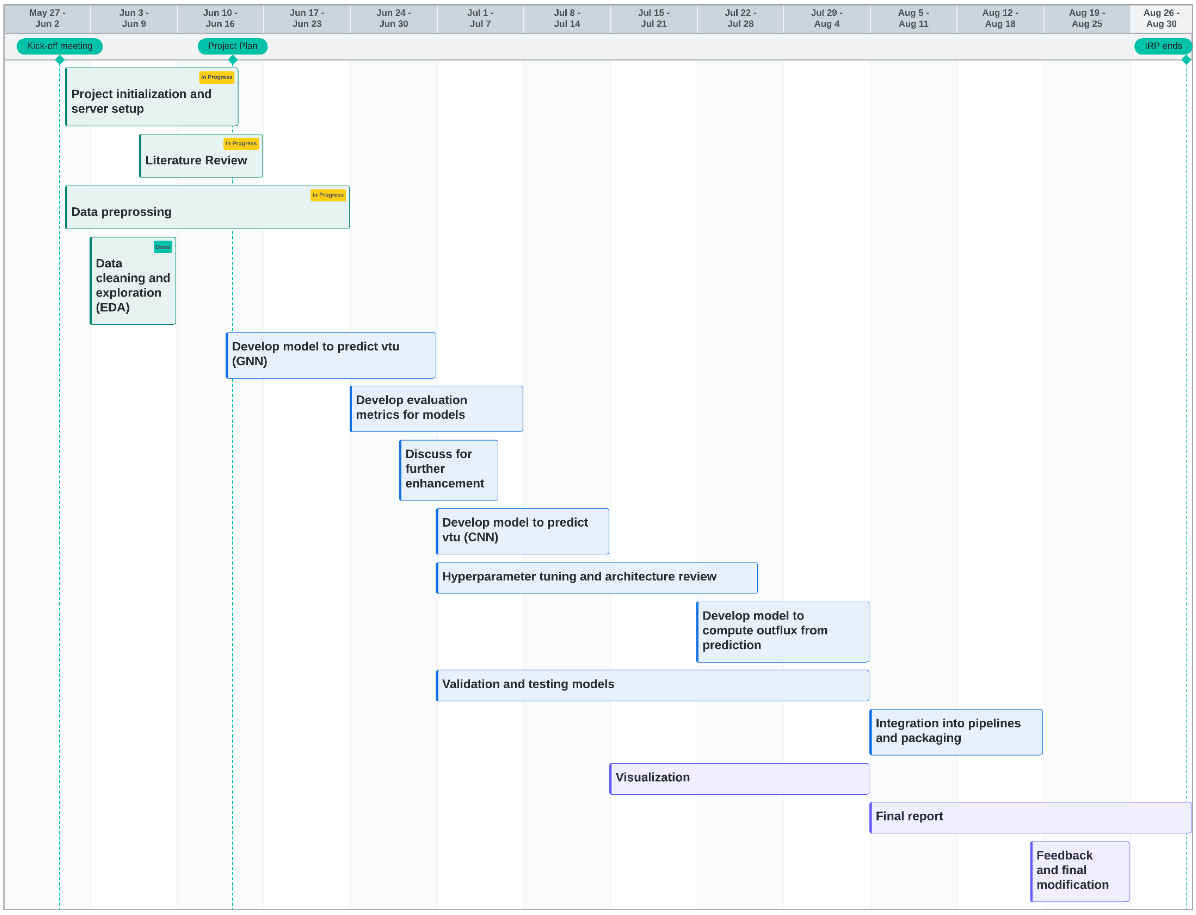

Figure 2 | Gantt Chart showing the rough schedule for project plan at each stage.

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