Industry-proposed project:

Project Background:
OpenGoSim specialize in developing reservoir engineering software for subsurface carbon dioxide and hydrogen storage, with a view to making a substantial contribution to achieving the net-zero emissions target.
The company wishes to provide easy-to-use modelling tools to reservoir engineers who are working at the forefront of the carbon capture and storage industry.

Objective:
Physical parameters appearing in the models, such as the permeability and porosity of the sub-surface, are typically impossible to determine fully or accurately from observations, and are hence subject to significant uncertainty.

In practice, it is crucial to study the influence of this uncertainty on the outcome of the simulations, in order to correctly quantify risk and make decisions.
In this component of the project, we will look at improving the computational efficiency of Monte Carlo

Methods:
(i.e., sampling/ensemble based) approaches to uncertainty quantification using recent advances such as Multilevel Monte Carlo [5,6] and Quasi-Monte Carlo [7] methods.

Result:

Keywords:
PDEs, Monte-Carlo, carbon capture, earth and environment

Research Timeline

Prepare

3.4 Fortrain Training
Install Petsc &
Run Tutorial Analysis
Review Monte Carlo
Revisit Divide and Conquer
23 First meeting with OpenGo
understand industry need

Methods

Uncertainty Quantification
Experiments
Simulation
Optimize code

Evaluation

Performace Analysis
of parallel code
measure
Computational
Efficiecy through
different Monte Carlo
metrics: effective
sample size, CPU time

April | May | June | July | Aug | Sept

Proposal

17 Literature Review &
Project plan deadline

Compare UQ approaches
Review of relevent literature
Literature critically evaluated
Aims/ Purpose

Results

include strategies that helps
to achieve our goal

Conclusion

limitation and see what to
improve and revisit methods
and results

R&D Responsibilities

Research

Design UQ model
WIth Anne Reinarz

Analyse new use cases and work with an experienced computer scientist to **design**, **prototype**, and **implement solutions**

Monday

Prepare

Evalate UQ model
WIth Anne Reinarz

Prepare new data sources and methods to **evaluate** the **quality** of our solutions

Collaborate

Check Validity
WIth OpenGoSim Paolo Salinas

Work closely with internal Users to **ensure** our solutions **help** them work **more efficiently**

Involve industry expertise in Geo-physical parameter

Continously Improvement

Improve UQ model
WIth Anne Reinarz

Contribute to continously **improving** how Data Science team works with UQ methods

UM-Bridge
Weekly update with developer's meeting

Fortrain
Improve Existing Code

MPI
Optimize and Parallelize Code

Algorithm Design

Divide and Conquer

Numerical Problem

Voronoi Diagrams

Boost Library

Install Petsc and Pflotrain on Docker

Docker Data Storage

build on Hamilton

Read Tutorial 3, successfully run simulation

Visualization Tools

Implement 4 classes of monte Carlo in calcualting Pi to build up the initial prototype

Thoroughly understand Monte Carlo mechanism

Comparing Classical Monte Carlo with Multilevel Monte Carlo and Quasi Monte Carlo

Goal: reduce variance as well as computational cost, improving convergence rate

Sampling Approaches:
treat input data as random field
QMC: sample through clever deterministic choice of points {X}

function level
experiment with different sizes of grid
MLMC: sample not just from one approximation Q_M of Q but from several.{Ml: 1,...,L}

How Academia can further assist industry research in terms of prediction and estimation of **Quantity of Interest?**

Parametrization

$$E(g(x)) = \int g(x) f(x) dx = \frac{1}{n} \sum_{i=1}^{n} g(x_i)$$

Design Stage

Forward Problem
simulate
→analyse
→benchmark

x→ [ ] →**g(x)**

Outer Loop : QMC
UQ Framework
Monte Carlo Methods
for each parameter

Inner Loop : MLMC
PFlortran Function
Forward Model
for 1:N

Provide an easy-to-use modelling tool

Prototype Stage

generative

Data Smooth

GMM

Data Distribution

Coarse Grid

Surrogate Model

Gaussian Process

Refined Mesh

Model

Approach
Convergence and Accuracy

Experimentation VS. Theory
Error VS. number of samples
compare plots of convergence
Computational Time(Big O Time Complexity)
MC/QMC/MLMC/QMC+MLMC

Data:
Input: permeability, porosity
3D Output: saturation, pressure

3D output, construction of shape & location
structured Grid,

Q: Where is the Best location for CO_2 storage layer?

Recursion Algorithm

multigrid geometry recursion

https://arxiv.org/pdf/2010.00626

https://mlmc.readthedocs.io/en/latest/examples_quantity.html

https://en.wikipedia.org/wiki/Multigrid_method

https://como.ceb.cam.ac.uk/publications/CCE-96-103-114/