

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:

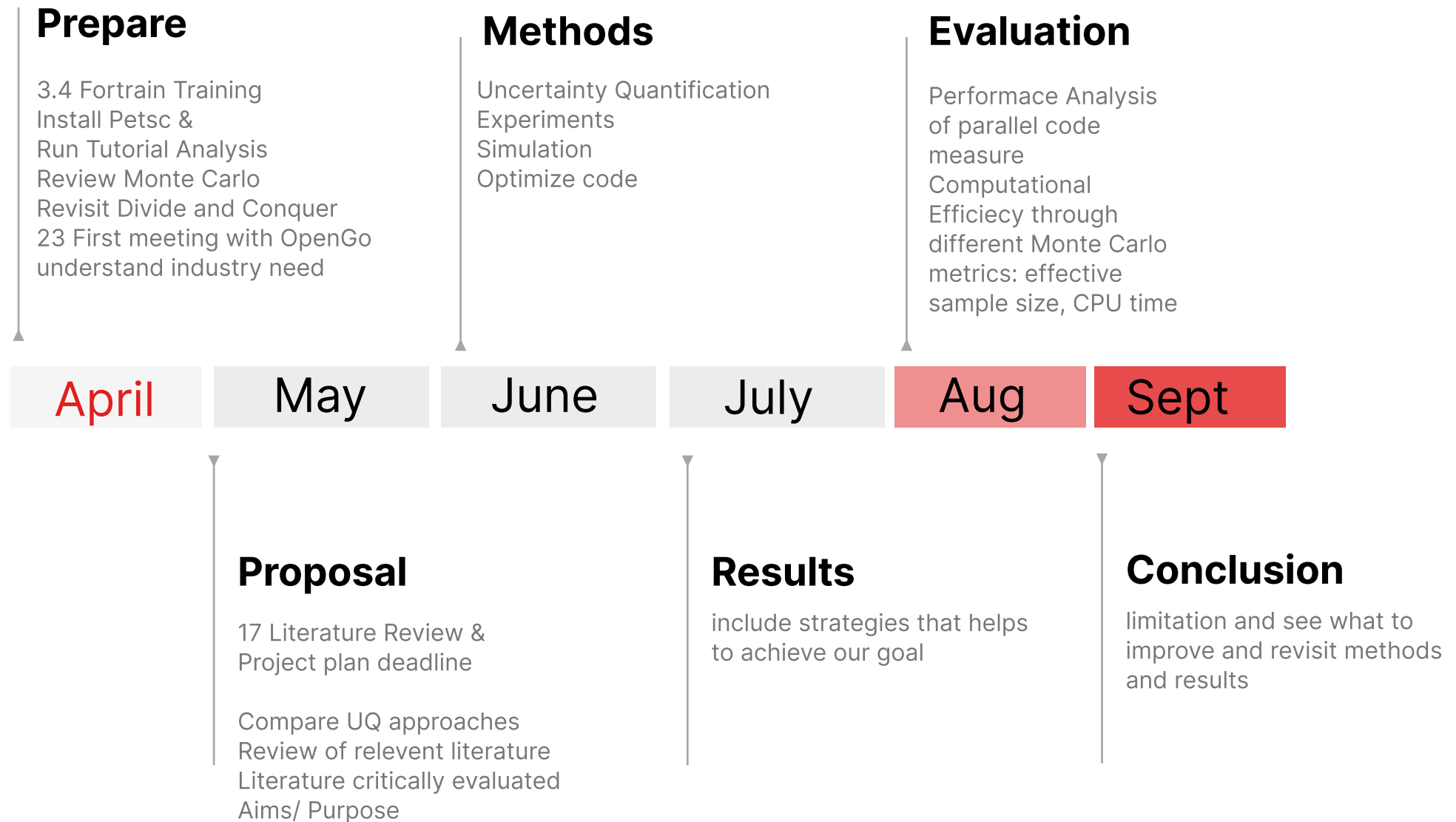
(i.e., sampling/ensemble based) approaches to uncertainty quantification using recent advances such as Multilevel Monte Carlo [5,6] and Quasi-Monte Carlo [7] methods.

Result:

Keywords:

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

Research Timeline



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

Evaluate 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

Continuously Improvement

Improve UQ model
With Anne Reinarz

Contribute to continuously
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 calculating 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

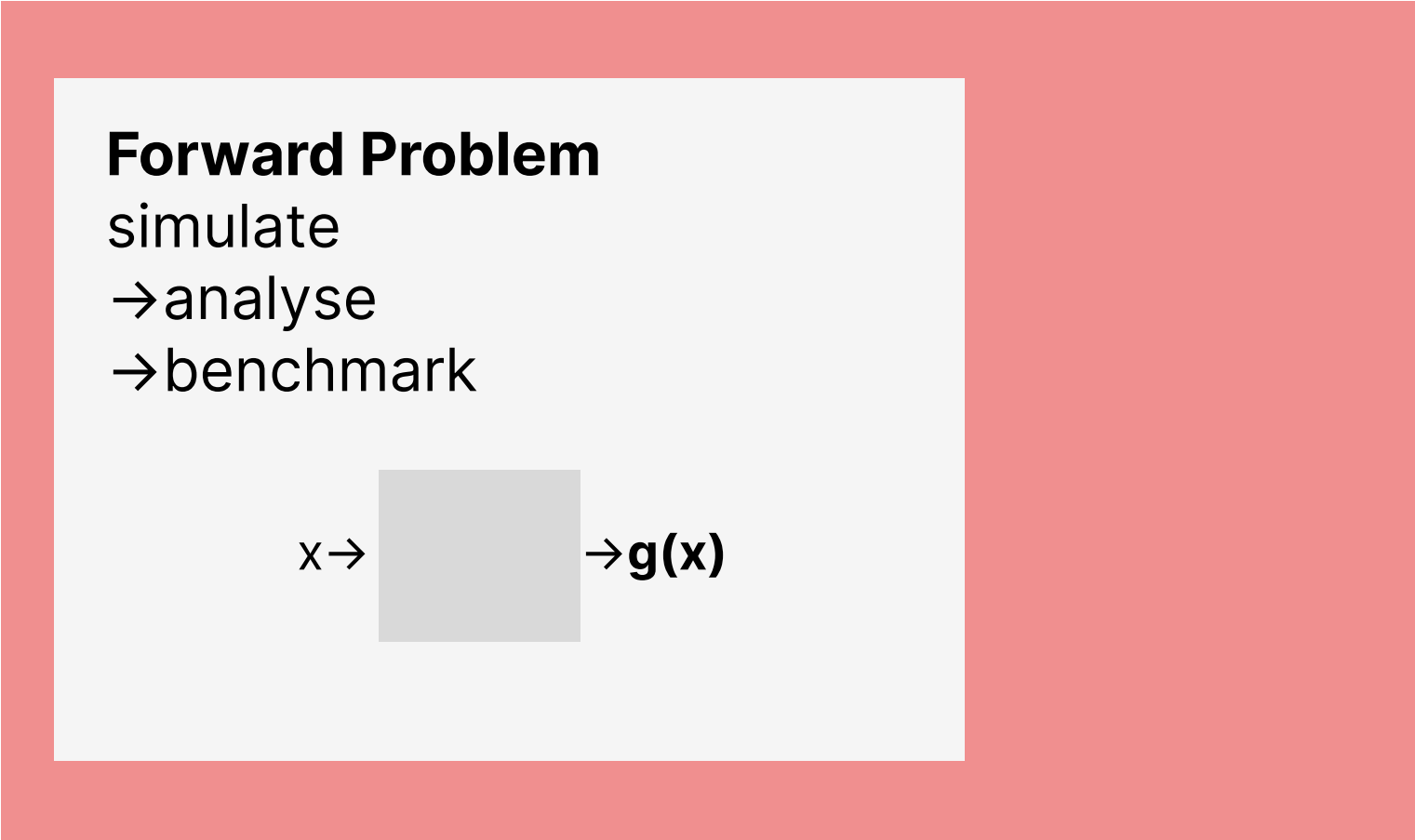
MLMC: sample not just from one approximation QM of Q but from several. $\{M_l: 1, \dots, L\}$

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



Outer Loop : QMC

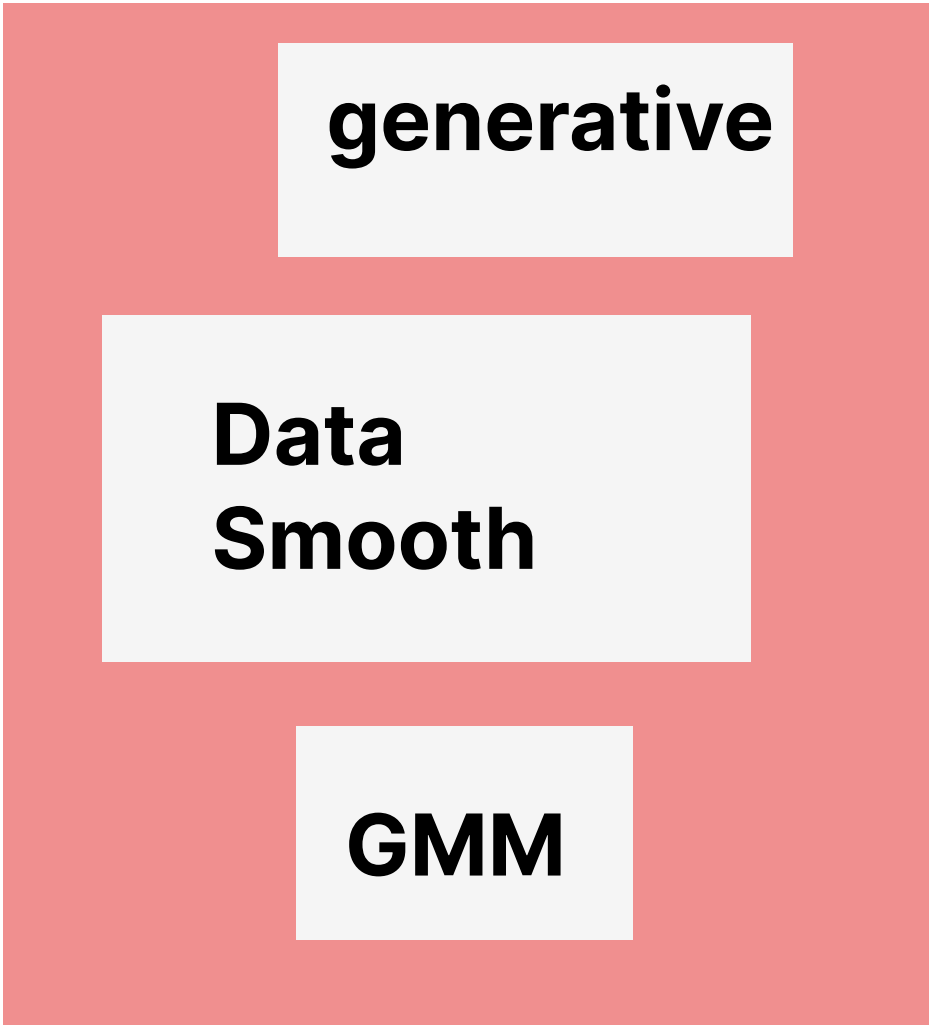
UQ Framework
Monte Carlo Methods
for each parameter

Inner Loop : MLMC

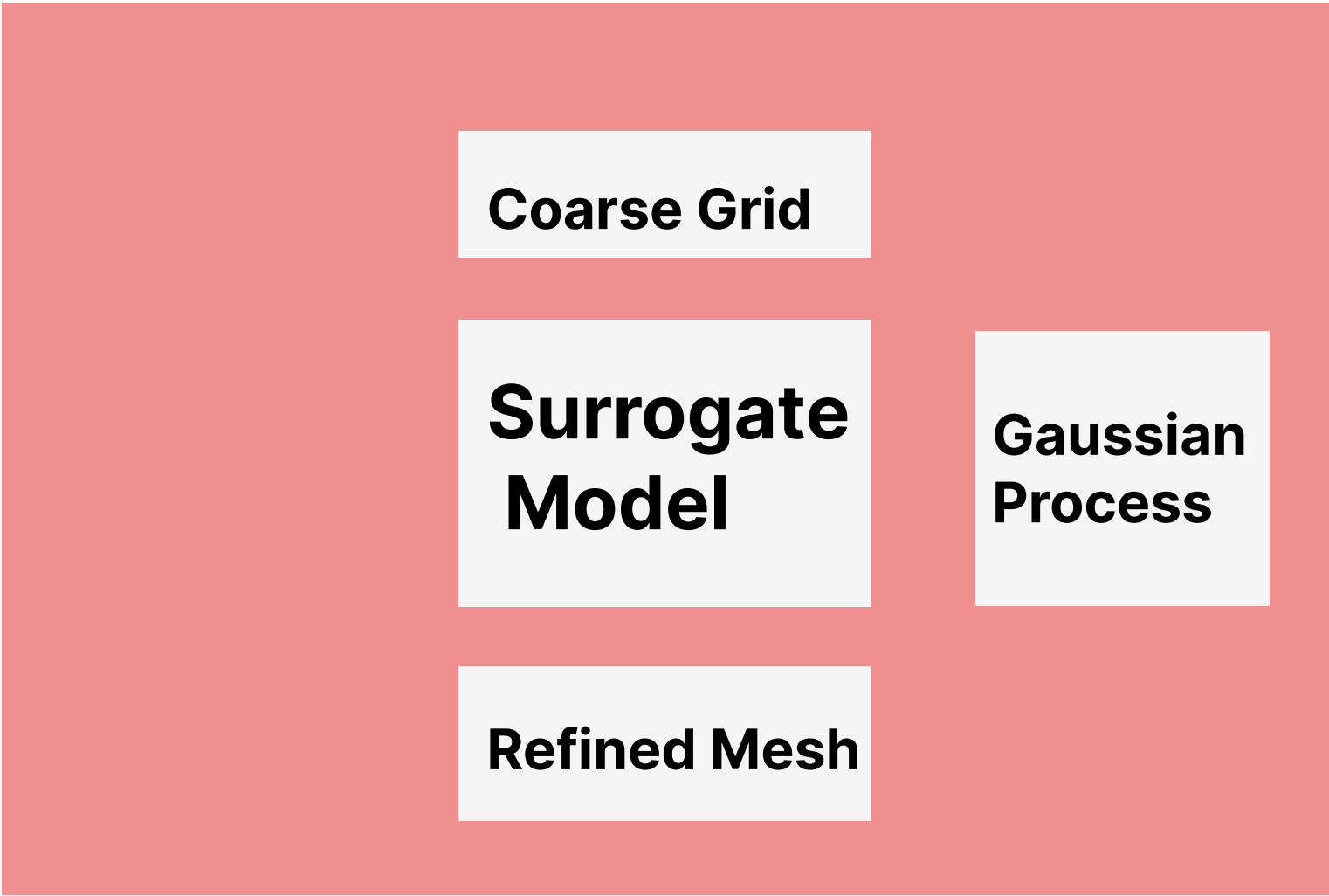
PFlortran Function
Forward Model
for 1:N

Provide an
easy-to-use
modelling
tool

Prototype
Stage



Data Distribution



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 CO2 storage layer?

Recursion Algorithm

multigrid geometry recursion

<https://arxiv.org/pdf/2010.00626>

**[https://mlmc.readthedocs.io/en/latest/
examples_quantity.html](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/](https://como.ceb.cam.ac.uk/publications/CCE-96-103-114/)**