Rapid modelling of reactive flow using machine learning and dynamic mesh optimisation

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Reactive flows in porous media are important in many natural and engineered systems; examples include carbon dioxide, hydrogen and heat storage in underground aquifers, geothermal energy production, and magma reservoirs that feed volcanic eruptions. Numerical models for flow and transport that include chemical reactions and their impact on solid and fluid compositions and porous media properties, are important to understand and predict the complex coupled behaviour of these systems. However, chemical reaction calculations are typically computationally expensive, and are required in every mesh element and at every timestep in non-iteratively coupled reactive transport models, so millions to tens of millions of chemical reaction calculations are required in a typical simulation. This number is further increased in iteratively coupled approaches, because the chemical reaction calculations are repeated several times at a given timestep to ensure the transport and chemical models have converged to a consistent solution. Chemical reaction calculations typically occupy c. 75 to 99% of the total simulation cost.

The aim of this project is to develop and apply a rapid framework for reactive flow simulations by combining two approaches. In the first approach, the chemical reaction calculations will be replaced by a proxy model developed using machine learning (ML), that is orders of magnitude faster to execute. Several different ML approaches, including purely data-driven methods and physics-informed approaches, will be tested for different reactive flow problems. The project will also test offline training, in which the ML model is trained prior to simulation, and online training in which the ML model is trained during a simulation.

In the second approach, the ML model will be implemented in flow and transport calculations that use unstructured dynamic mesh optimisation (DMO) within the open-source Imperial College Finite Element Reservoir Simulator (IC-FERST). IC-FERST incorporates state-of-the-art technology for porous media flow simulation, including DMO, high order element methods and surface-based representation of complex reservoir architecture. When chemical reaction changes (dissolves, cements or replaces) the porous media properties, the heterogeneity distribution changes, and thus the surface-based representation needs to be updated dynamically. Once the functionality is implemented, it will be used to study a variety of subsurface systems.

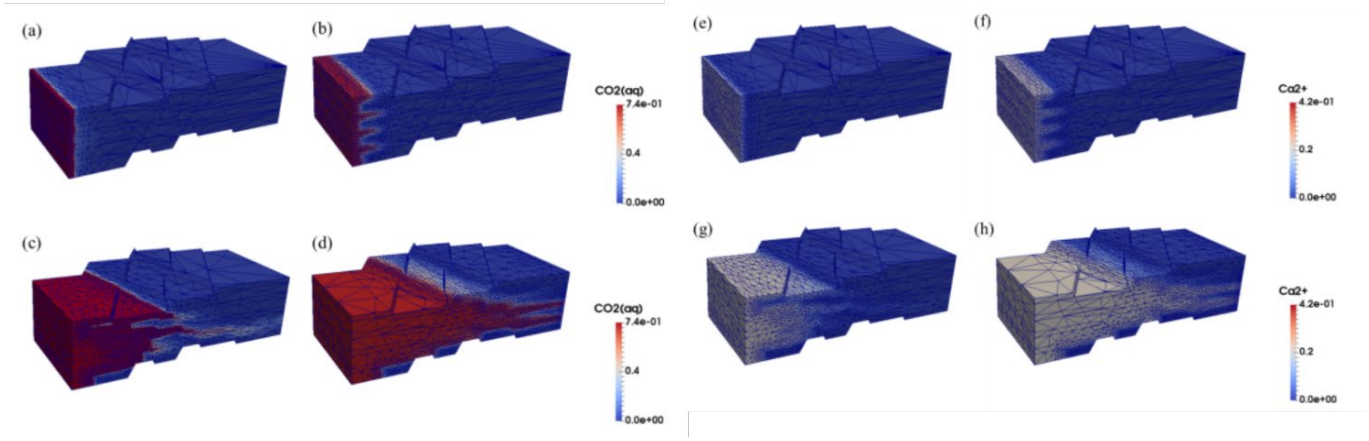

Fig. 1: Flow simulation results of a reactive fluid dissolving a faulted carbonate succession. (a-d) Dissolved CO_2 concentration (mol/Kg), and (e-h) Ca_{2+} concentration (mmol/Kg) with mesh adaptivity at 1, 2, 4, and 6 PV injection.

Applicants should have a good degree in an appropriate subject (e.g. earth science, physics, mathematics, or engineering) and a strong interest in computational modelling. The project is hosted by the NOvel Reservoir Modelling and Simulation (NORMS) group within the Department of Earth Science and Engineering and will involve extensive interactions with other research groups within the department and internationally. Skills developed during this project will include machine learning methods, high performance computing, advanced computational fluid dynamics for reactive flow simulations, computer aided design for geological modelling, linear and non-linear solvers, dynamic mesh optimisation techniques and unstructured meshing technologies. The successful candidate will be encouraged and supported to develop their career and profile, including presenting at conferences and publishing journal articles.

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