Introducing GeoChemFoam to ARCHER2

https://github.com/GeoChemFoam/

The GeoChemFoam Project

The goal of The GeoChemFoam Project is to provide a collaborative open-source platform where all OpenFOAM development made by the porous media community is made accessible to non-OpenFOAM specialists. The development of GeoChemFoam (Geochemistry for OpenFOAM) started in 2015 at Heriot-Watt University and the code became open-source in 2019. It includes a range of numerical methods that are summarised below. However, OpenFOAM's meshing strategies are not optimised for a High Performance Computing environment. The goal of this project is to parallelise and upgrade the meshing and the pre-, and post-processing modules so that they are optimised for HPC environments and to create an on-demand multiscale adaptive meshing module to improve the scientific applicability of our solvers to highly heterogenous porous systems. **As part of the project, we have also released a new module 'GCFv5.0' which is now centrally available to all Archer2 users, along with user documentation and installation guide.** Visit our github → for links to the source code, precompiled dockers, a users' wiki with tutorials, publications, a discussion forum and more!

Motivation

Current meshing strategies are not parallelised and dominate the total simulation time in HPC environments with many CPUs [Fig 1].

Remeshing is required during the simulation for many dynamic processes such as reactive and multiphase flow leading to further slow-downs.

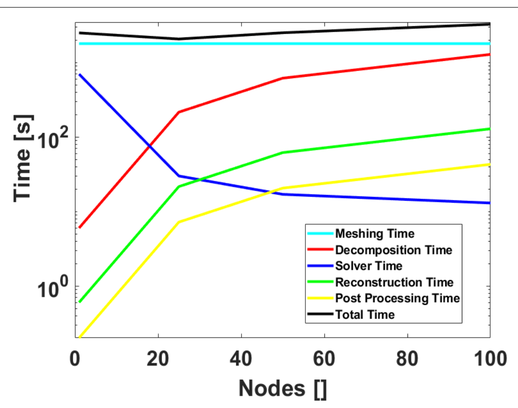


Fig 1: GeoChemFoam runtimes on ARCHER2.

Goal of the Project

Develop a parallel on-demand multiscale adaptive meshing module for fast meshing and remeshing of the multi-scale domain.

This will enable efficient multi-scale model runs for a range of dynamic processes applied to the Energy Transition (e.g. CO_2 capture & storage, hydrogen generation, geothermal, & radionuclide transport) [Fig 2].

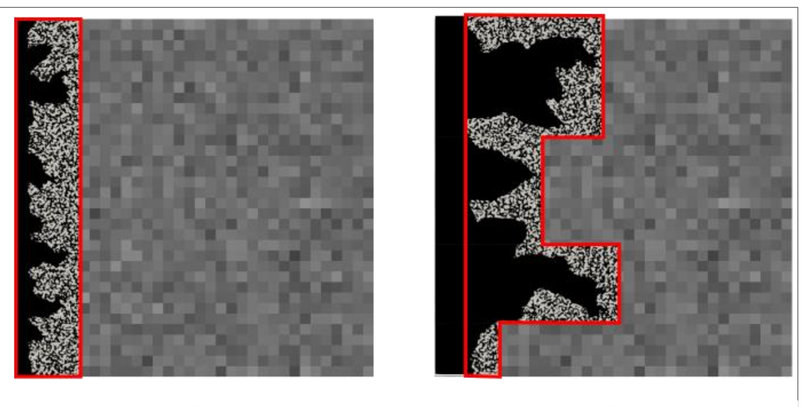
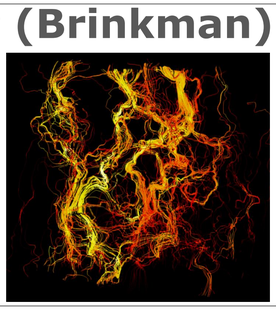


Figure 2 (left) domain at early time, with refinement shown in red. (right) domain at later time.

Single-phase Flow (Brinkman)

- Uses the Brinkman equation to simulate flow in micro-CT images including solid phase (no-flow) and unresolved porosity (Darcy flow)
- Example: Estaillades carbonate

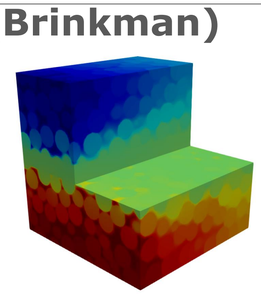


Formation Factor

- Solves a Laplacian equation in micro-CT images and calculates its formation factor
- Example: Fontainebleau sandstone

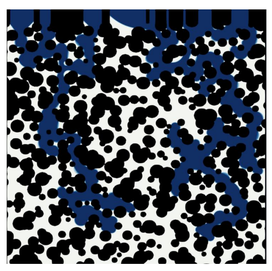
Heat Transport (Brinkman)

- Solves the heat transport equation in micro-CT images using the Brinkman equation for the flow and heat conduction in both fluid and solid
- Example: Porous heat exchanger



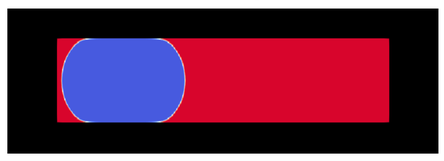
Multiphase Flow (VOF)

- Solves multiphase flow using the Volume-Of-Fluid method
- Improved calculation of interface curvature
- Example: drainage in 2D micromodel



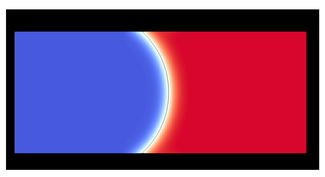
Multiphase Flow (VOFOS)

- Operator-splitting time-step strategy for efficient simulation at low capillary number
- Separates capillary force and viscous injection
- Example: Bubble in a channel at $Ca=10^{-9}$



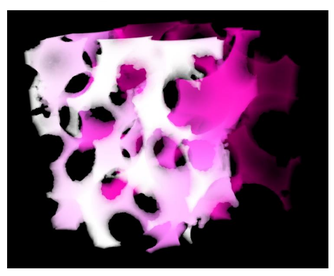
Multiphase Flow (Phase-Field)

- Diffuse interface model for multiphase flow
- Couples Navier-Stokes with Cahn-Hilliard
- Example: Drainage in 2D channel at $Ca=10^{-5}$ (no parasitic currents)



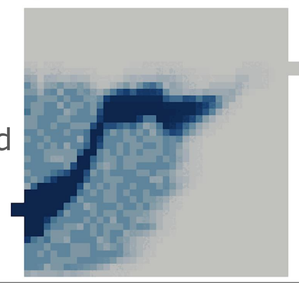
Species transport

- Solve an advection diffusion equation for an unrestricted number of species
- Example: Flow and transport in Ketton Carbonate



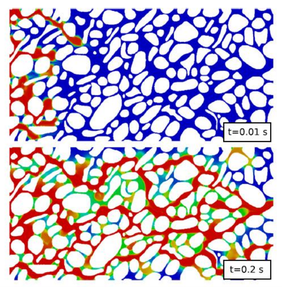
Species transport (Brinkman)

- Solve an advection diffusion equation for a species including flow and diffusion in unresolved porosity
- Example: transport in fracture/matrix system



Multiphase Transport

- Multiphase flow with transport equations for a diluted species
- Boundary conditions at the interface modelled using the CST method
- Example: multiphase transport in a micromodel

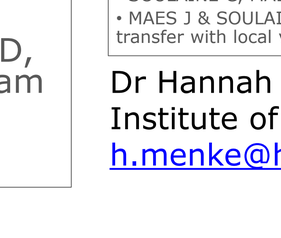


Reactive transport

- Single-phase transport with equilibrium reactions in the fluid (speciation) and at the solid surface (surface complexation)
- Couples OpenFOAM and PHREEQC
- Example: Bimolecular reaction in micromodel

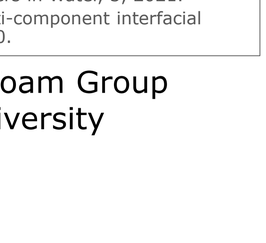
Reactive transport with ALE

- Single-phase transport with dissolution reactions at solid surfaces
- Pore geometry updated using the ALE method
- Example: channelling in a micromodel



Reactive transport with VoS

- Single-phase transport with dissolution reactions at solid surfaces
- Pore geometry updated using the VoS method
- Example: Wormhole formation in Ketton Limestone



Multiphase transfer

- Extension of the CST method when a species is diluted in the liquid phase but pure in the gas
- Example: dissolution of a rising bubble of gas in liquid

Multiphase reactive transport

- Multiphase transport with equilibrium reactions in fluid or at solid surfaces
- Reactions solved using PHREEQC
- Example: low-salinity injection in Bentheimer sandstone

Multiphase reactive transfer

- Multiphase transport with equilibrium reactions (PHREEQC) and dissolution of pure gas
- Example: dissolution of a CO_2 bubble in cavity

The GeoChemFoam Project team

Dr Hannah Menke is a Research Fellow at Heriot-Watt University and an expert in pore-scale imaging and data-driven upscaling of flow processes.

Dr Julien Maes is an Assistant Professor at Heriot-Watt University and an expert in pore-scale modelling of reactive transport, heat transfer and multiphase flow. In 2019, Dr Maes and Dr Menke founded The GeoChemFoam Project. The GeoChemFoam Research Team currently includes six PhD students and two PDRAs who develop and use the code.

Dr Gavin Pringle is a Research Software Engineer at EPCC specialising in CFD, and optimising HPC applications in general. Dr Pringle joined the GeoChemFoam project in 2023 and leads the development of parallel architectures for GeoChemFoam.

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