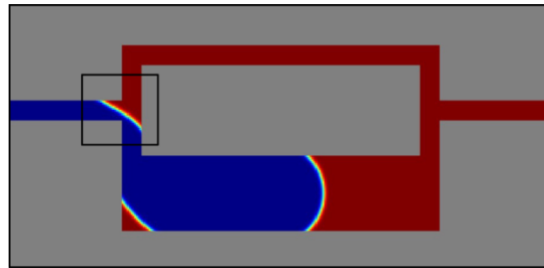
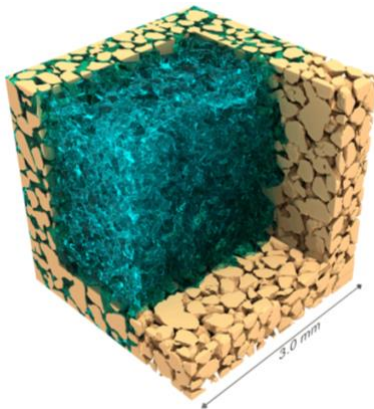


Computational Fluid Dynamics

Finite Element Simulation of Multiphase Flow in Porous Media



van Rooijen, W. A. et al. (2025). Dynamic simulation of hydrogen trapping in bifurcating water-wet microchannels using the lattice Boltzmann method. *International Journal of Hydrogen Energy*, 177, 151274.

Preface

Multiphase flow at the microscale is at the core of enabling new subsurface energy technologies, from CO₂ sequestration to Underground Hydrogen Storage, which are supporting the global energy transition. In porous rocks, the distribution and dynamics of immiscible fluids (such as water and gas) depend strongly on pore geometry and wettability (affinity to adhere to a solid surface). Microfluidic experiments have highlighted complex behaviours like the trapping of one fluid by another, but translating all these observations into predictive numerical models remains challenging. Developing robust microscale simulation tools would enable quantitative insight into fluid distribution, storage efficiency, and leakage risks, filling a critical research gap in the feasibility of those technologies.

Problem definition / Research question

This project aims to study how multiphase dynamics can be coupled with the Navier–Stokes equations. We propose to explore the capabilities of a phase-field formulation to model multiphase flow and evolving interfaces. The implementation will be carried out within the open-source finite element framework MOOSE^[1] (<https://mooseframework.inl.gov>), a C++ framework developed at Idaho National Laboratory (INL) that supports large-scale parallel simulations on more than 30,000 cores. A main part of the project will focus on algorithmic developments related to the phase-field formulation and interface tracking. This includes the analysis of convergence, stability, and numerical robustness. Given the diffuse representation of interfaces in phase-field methods, this work will investigate how well the approach can reproduce realistic interfacial phenomena, in particular contact angles. It will also quantify the sensitivity of the results with respect to interface thickness and mesh resolution. If feasible, we will additionally investigate parallel scalability on DelftBlue.

Student-profile

The project, with a strong focus on numerical analysis, is suitable for a student with a background in computational fluid dynamics, numerical analysis, and/or geoscience. It will be jointly supervised by Dr. Heinlein (numerical analysis) and Dr. Lesueur (geoscience), covering both numerical aspects and physical modeling accuracy. Applicants with a stronger background in one area should show clear interest in the other. Basic knowledge of C++ is an advantage. Training and guidance on the user- and developer-friendly software framework MOOSE will be provided by Dr. Lesueur.

Recommended literature:

[1] Mostafavi, A. et al. (2025). MOOSE-based finite element framework for mass-conserving two-phase flow simulations on adaptive grids using the diffuse interface approach and a Lagrange multiplier. *Journal of Computational Physics*, 527, 113755.

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