

PhD Position Multiscale AI-Assisted Modelling of CO₂ Sequestration

Multi-scale Multi-physics Modelling (M3) Laboratory · Hangzhou, China

The opportunity

The M3 Laboratory at Westlake University invites expressions of interest from highly motivated prospective PhD researchers to investigate geological CO₂ storage through coupled multiscale simulations and AI-assisted scientific discovery. The goal is to connect pore-scale mechanisms with larger-scale behavior, identifying the governing physical relationships for reliable sequestration assessment.

Research directions

- Pore-scale CO₂-brine physics: Study multiphase displacement, dissolution and capillary trapping, interfacial dynamics, wettability and pore-throat effects under geologically relevant conditions.
- Multiscale numerical modelling: Use Lattice Boltzmann (LBM), Discrete Element (DEM) and, where appropriate, molecular-scale and continuum methods to connect fluid-solid interactions across scales.
- AI-guided dimensionless analysis: Apply symbolic regression to discover interpretable governing relationships and identify key dimensionless groups controlling CO₂ transport, trapping and dissolution.
- Agent-assisted multiscale research: Investigate AI agents that help plan, coordinate and interpret simulation campaigns across scales, including parameter selection, cross-scale information exchange and hypothesis testing.
- Scientific computing: Develop and validate reproducible numerical workflows, drawing on the group's high-performance parallel C++/CUDA multiphase simulation expertise.

Why the M3 Lab?

The group combines computational and physical modelling across scales, with expertise in LBM, DEM, molecular dynamics and related numerical methods. Its research includes supercritical CO₂ dissolution trapping in nanoporous media and the effects of pore geometry and wettability. This project extends those strengths through interpretable AI-based discovery and coordinated multiscale investigation.

Candidate profile

Applicants from engineering, geosciences, applied mathematics, computational physics or related fields are welcome. Experience in porous-media flow, numerical methods, scientific programming (Python/C++), high-performance computing, symbolic regression or AI agents is advantageous. Strong physical intuition and mathematical rigor are valued.

How to express interest

Prepare a CV, academic transcripts, a brief research statement and relevant publications or code samples (if available). Application contact and deadline: to be confirmed by the M3 Lab. Formal eligibility and application procedures should be checked through Westlake University graduate admissions.

M3 Lab: <https://m3.westlake.edu.cn/> | Graduate admissions: <https://en.westlake.edu.cn/admissions/graduate/>

Draft advertisement — confirm position availability, funding and application instructions before publication.