

# Large-Scale Digital Rock Physics Simulations with LBPM

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Advanced Research Computing



HPCE WORKSHOP





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# Overview

- **Digital Rock Physics**
  - Direct numerical simulations performed on real rock geometry
  - Inform reservoir models (permeability, relative permeability)
- Simulation protocols derived from established special core analysis (SCAL) approaches
- LBPM software is available through the **Open Porous Media** initiative
- LBPM is one of eight OLCF CAAR applications for the Frontier supercomputer

## OPEN POROUS MEDIA

The Open Porous Media (OPM) initiative encourages open innovation and reproducible research for modeling and simulation of porous media processes.



Office of Science

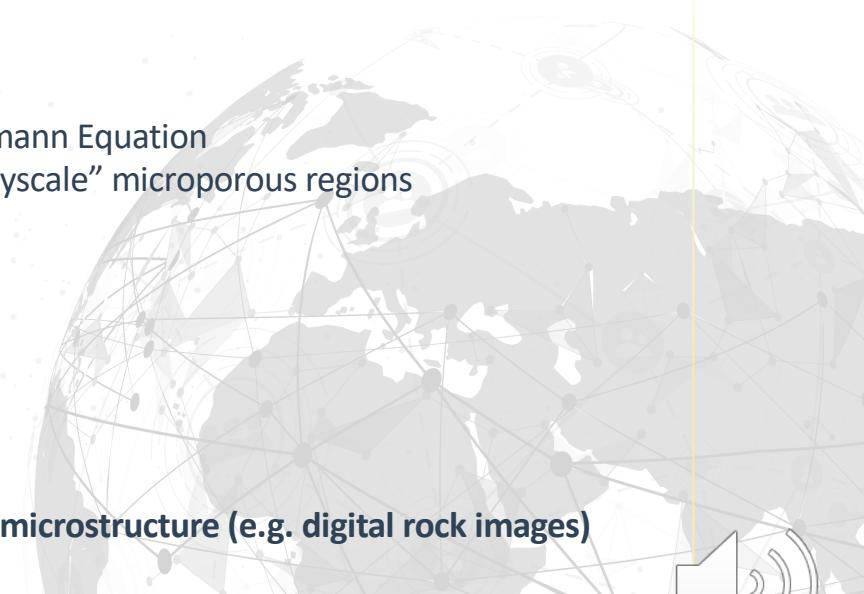


LEADERSHIP COMPUTING  
FACILITY



# Lattice Boltzmann Methods

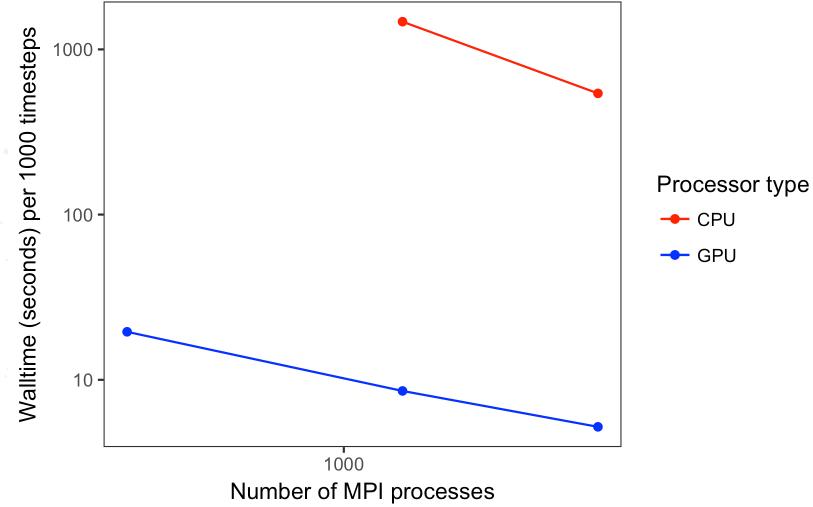
- General class of numerical methods that can be used to simulate wide range of physical phenomena
  - Navier-Stokes equations (single fluid flow)
  - Immiscible fluid flow (capillary dominated systems)
    - Capillary number:  $1e-6 < Ca < 1$
    - Viscosity ratio:  $0.01 < M < 100$
    - Static and dynamic aspects of wetting
  - Ion transport based on Nernst-Planck and Poisson Boltzmann Equation
  - Hybrid models coupling N-S with Darcy-Brinkman in “greyscale” microporous regions
- Relies primarily on mesoscopic closure relationships
  - Formulated from a kinetic theory perspective
  - Quasi-molecular interaction rules
- Familiar forms are recovered with 2<sup>nd</sup> order accuracy
- Well-suited toward simulation of flow processes in complex microstructure (e.g. digital rock images)



# Computational Performance

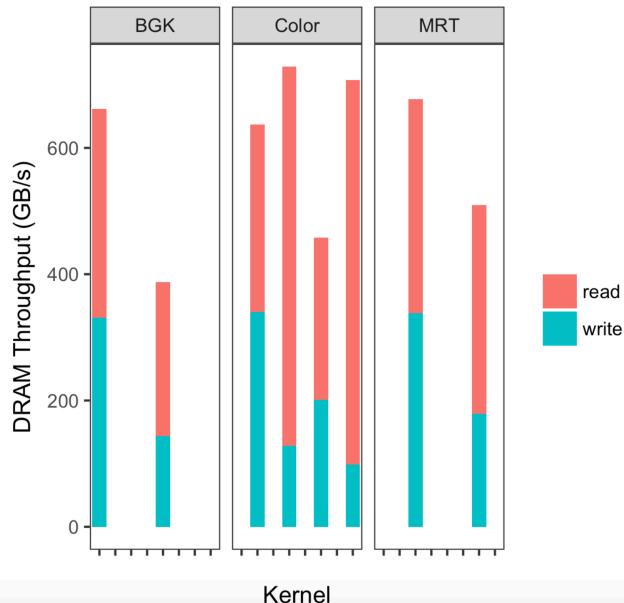
- Efficient computational implementation
  - Fully parallel (using MPI)
  - Support for multiple architectures
    - CPU implementation (C++)
    - NVIDIA GPU (CUDA)
    - AMD GPU (HIP)
- Performance on Summit (two-fluid flow)
  - Summit Node
    - 6 x NVIDIA V100 GPU
    - 2 x IBM Power9 CPU (20 SMC)
    - NVLINK connects GPU within a node
  - CPU comparison is one MPI process per core
  - GPU comparison is one MPI process per GPU

Strong Scaling on Summit

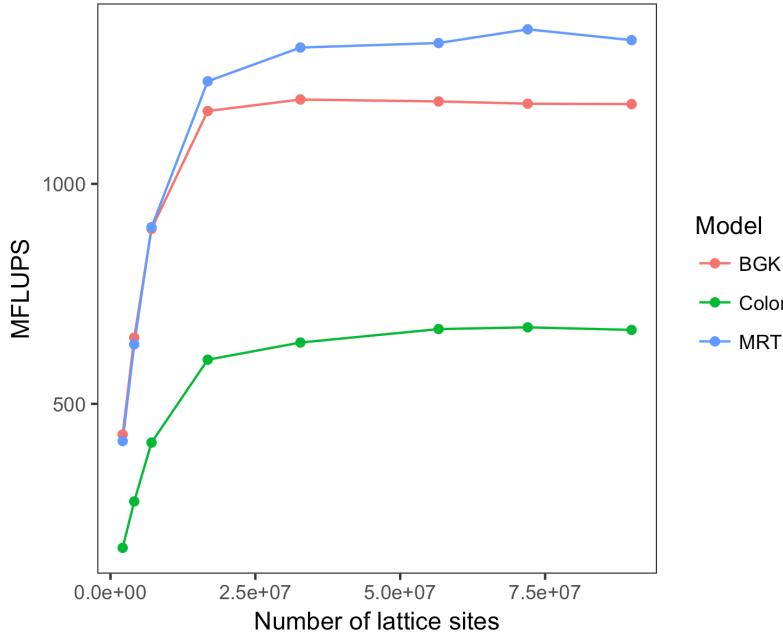


# Computational Performance

Bandwidth on V100 GPU

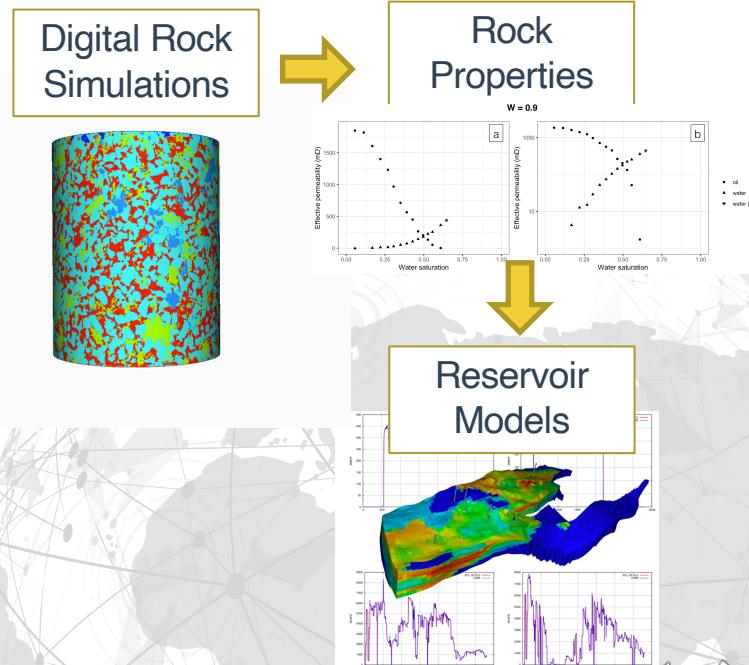


Performance for different physics models



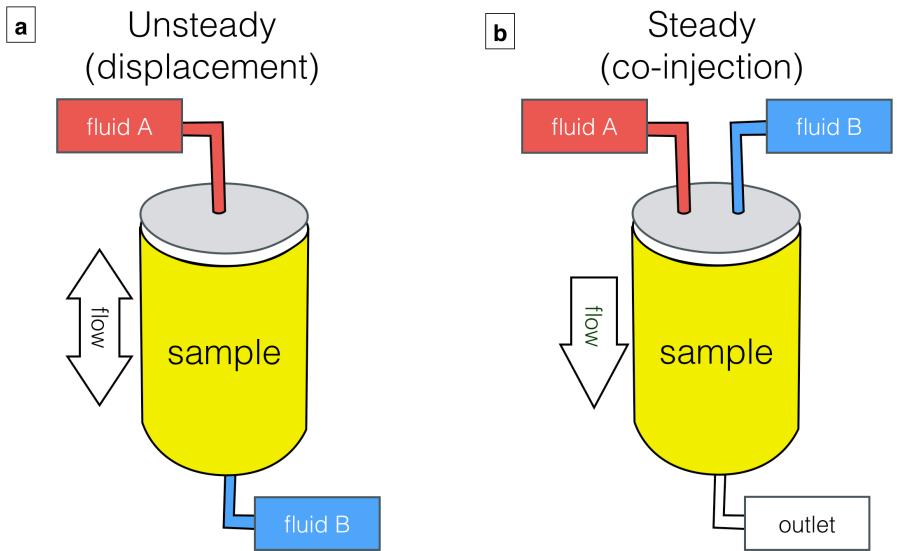
# Reservoir Model Parameters

- Reservoir models rely on information to characterize the rock properties
  - Absolute permeability – length scale heterogeneity
  - Relative permeability – accounts for effect of fluid and solid microstructure on flow behavior
- Direct imaging of rock micro-structure is becoming more effective and cheaper
  - 3D rock images can be used to perform direct numerical simulation
- Simulation approaches seek to provide
  - Deeper understanding for role of rock properties in determining fluid flow behavior
  - Computational analog of traditional experiments
  - Reduce uncertainties associated with parameter estimation
  - Generate information that is not accessible from experiments



# SCAL Experimental Protocols

- Established experimental protocols to measure rock properties from SCAL experiments
- Simulations designed as a computational analog of these experiments
- **Unsteady displacement**
  - Fluid injected into sample using a pump
  - Saturation changes due to displacement
- **Steady-state fractional flow**
  - Fluids are co-injected into the sample to cause simultaneous flow of both fluids
  - Goal is to infer steady-state relative permeability (constant saturation)
- **Centrifuge protocol**
  - Fluids mobilized based on centrifugal forces
  - Goal is to infer capillary pressure and endpoint behavior

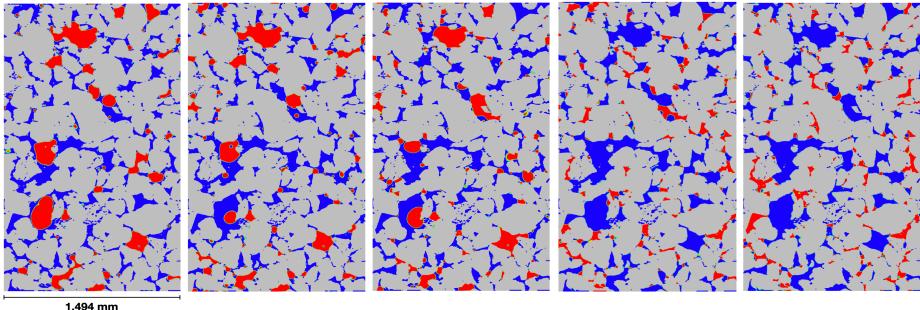


McClure, J.E., Li, Z., Berrill, M. Ramstad, T. The LBPM software package for simulating multiphase flow on digital images of porous rocks. *Comput Geosci* **25**, 871–895 (2021).  
<https://doi.org/10.1007/s10596-020-10028-9>

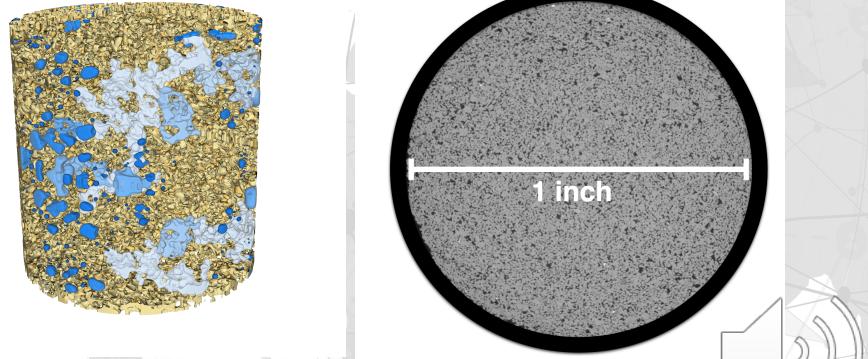
# Digital Rock Data

- Image data generated from micro-computed tomography (micro-CT)
  - Typical resolution: 0.5 – 15 micron
  - Image size:  $512^3$  – 2500 x 2500 x 7200
- Representation of the actual rock micro-structure
  - Mineral structure can be filled in from SEM
- Fluid flow occurs within the pore-structure within the rock
  - Fluid configurations within rock can be directly imaged

Fluid distributions in Bentheimer sandstone

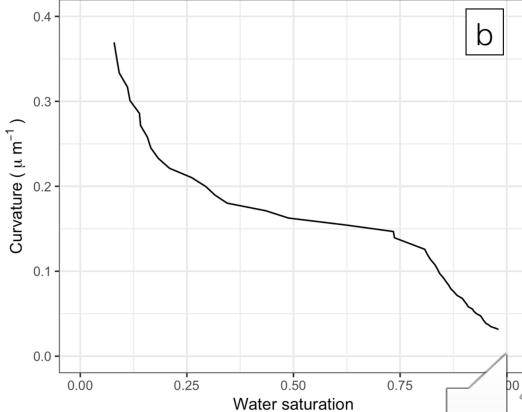
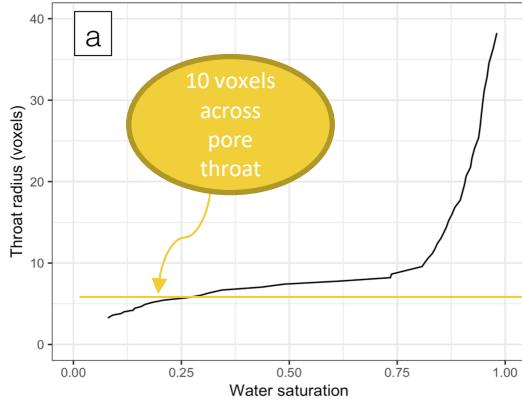


Berea Sandstone Core



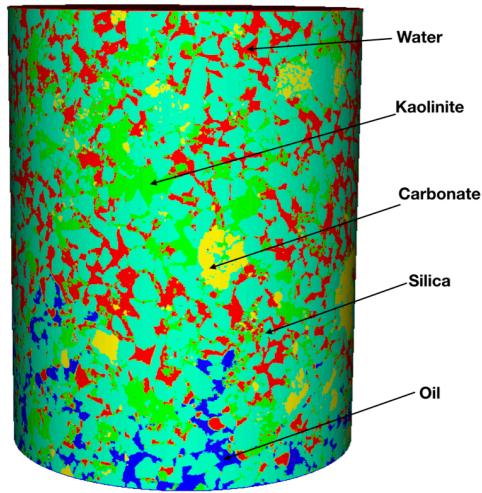
# Image Data Quality

- Rock micro-structure is heterogeneous at all length scales
- Direct numerical simulation can be quite sensitive to image resolution
- Resolving dominant flow pathways is critical to accurately simulate physics of multiphase flow
- LBPM includes **morphological analysis tools** that can be used to
  - Quickly assess resolution of digital rock images
  - Assess capillary pressure behavior and percolation criteria
  - Determine structure of dominant flow pathways under water-wet conditions
  - Generate initial conditions for flow simulation

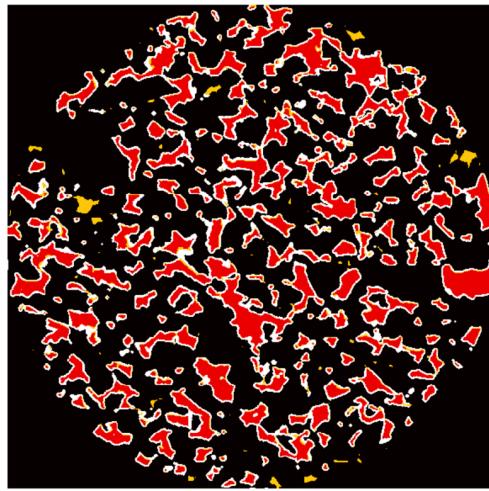


# Complex Wetting Conditions

A “Fractional wet” wetting condition controlled by local mineral type



B “Mixed wet” wetting condition controlled by history of grain contact with oil

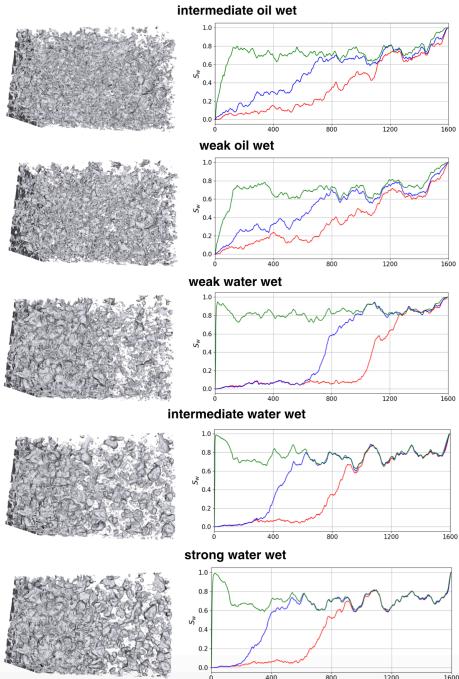


- Oil
- Water
- Solid (water wet)
- Solid (contact oil)

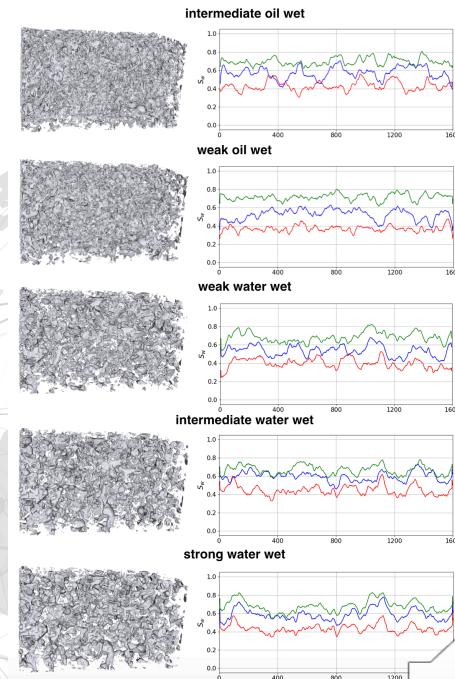
# SCAL Simulation Protocols

- **Unsteady displacement**
  - Displacement can be driven by constant pressure boundary conditions or fixed flow rate
- **Steady-state fractional flow**
  - Periodic boundary conditions
  - External body force drives flow
  - Customized mixing layers to minimize boundary effects
- **Centrifuge protocol**
  - Boundary condition setup is unsteady protocol
  - Enforce zero pressure drop with a body force

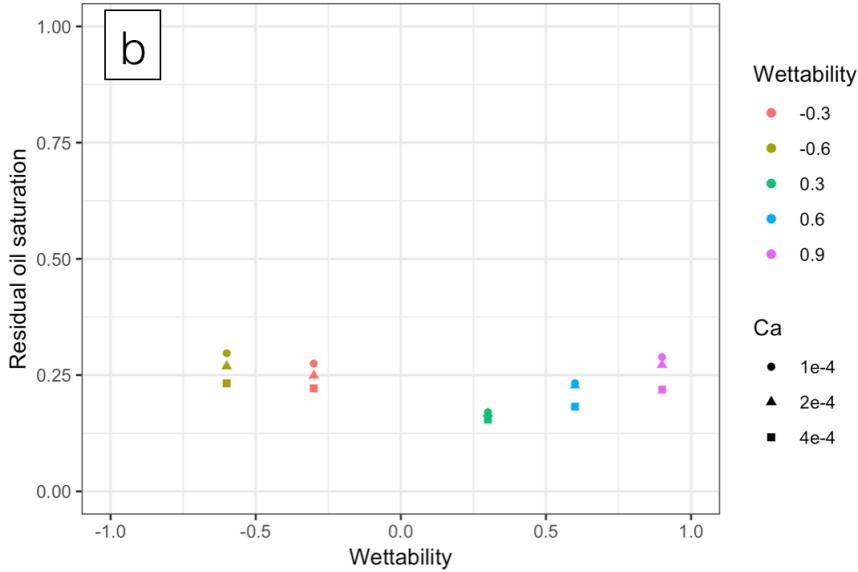
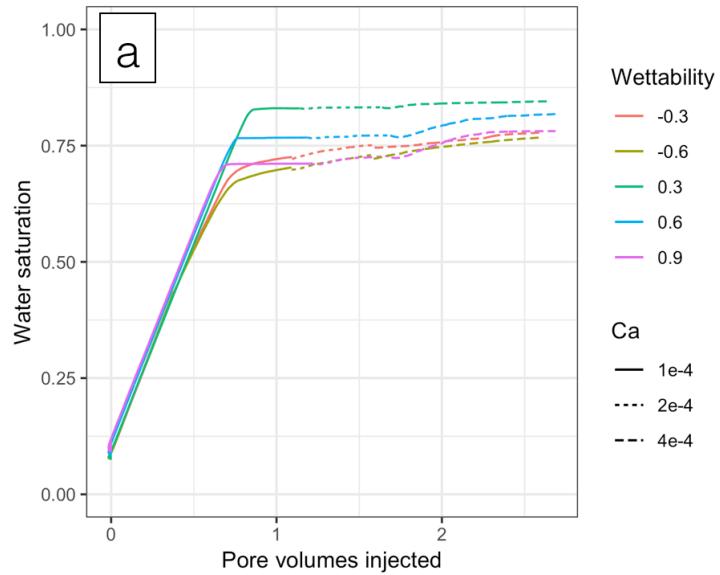
Unsteady core-flooding



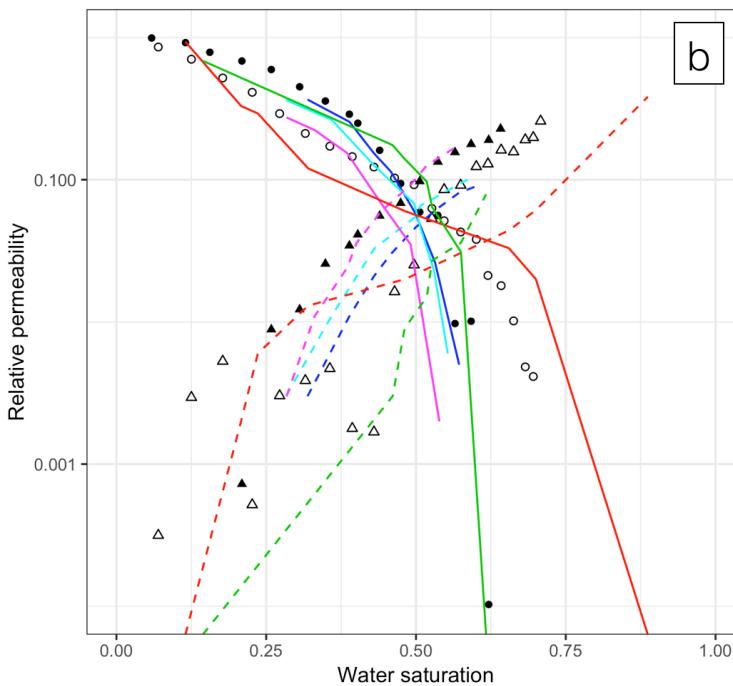
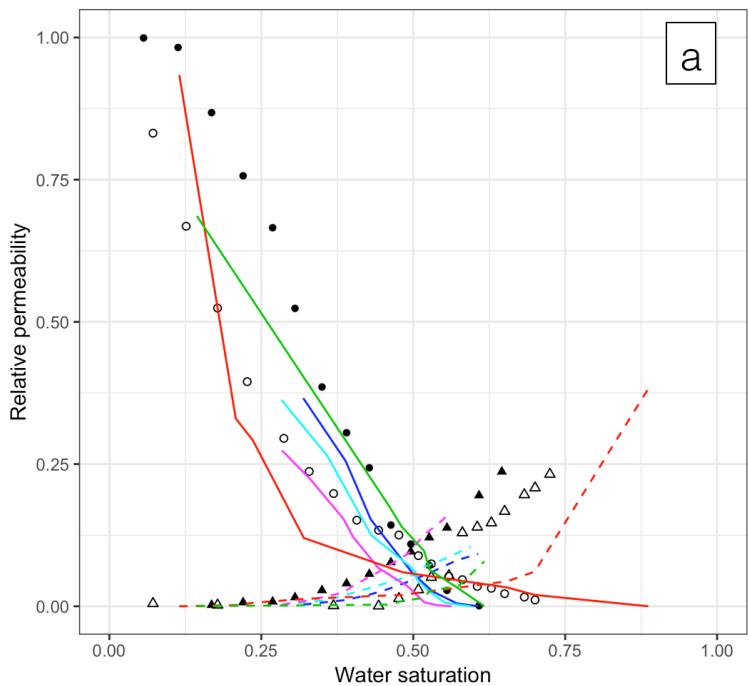
Steady-state flow



# Unsteady Water-flooding



# Steady-State Relative Permeability



Simulations

- oil ( $W=-0.3$ )
- oil ( $W=0.6$ )
- △ water ( $W=-0.3$ )
- ▲ water ( $W=0.6$ )

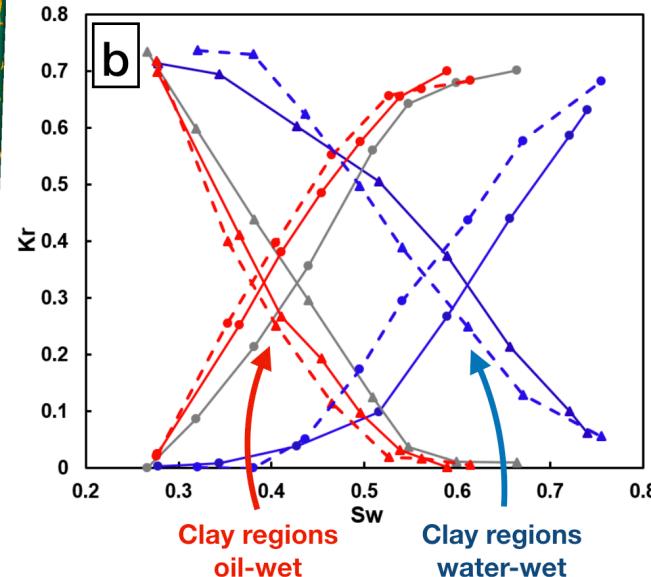
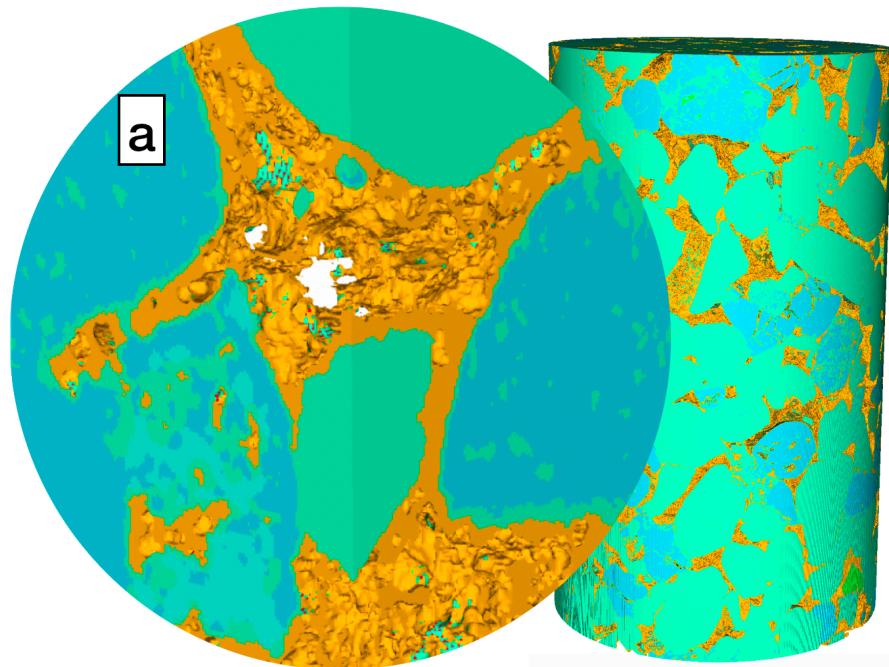
Experiments

- Lin et al. #1
- Lin et al. #2
- Ramstad et al. #1
- Ramstad et al. #2
- Ramstad et al. #3

Fluid

- oil
- - - water

# Mineral structure and wetting



Fan, M., McClure, J. E., Armstrong, R. T., Shabaninejad, M., Dalton, L. E., Crandall, D., & Chen, C. (2020). Influence of clay wettability alteration on relative permeability. *Geophysical Research Letters*, 47, e2020GL088545. <https://doi.org/10.1029/2020GL088545>

# Getting Started with LBPM

- **Source Code**
  - Available from Open Porous Media Initiative
  - <https://github.com/opm/lbpm>
- **NVIDIA GPU Container Registry**
  - Pre-configured container optimized for NVIDIA GPU
  - LBPM and dependencies already compiled
  - Suitable for cloud systems or HPC
  - <https://ngc.nvidia.com/catalog/containers/hpc:lbpm>
- **Documentation**
  - Basic documentation with step-by-step examples
  - Installation, Absolute Permeability, Multiphase Flow, Visualization, etc.
  - <https://lbpm-sim.org/>
- **Collaborators**
  - Steffen Berg (Shell)
  - Mark Berrill (Oak Ridge National Lab)
  - Cheng Chen (NJIT)
  - Ming Fan (Virginia Tech)
  - Alessandro Fanfarillo (AMD)
  - Remco Hartkamp (TU Delft)
  - Zhe Li (Virginia Tech)
  - Tim Mattox (HPE)
  - Johan Padding (TU Delft)
  - Maša Prodanović (University of Texas)
  - Ryan Armstrong (UNSW)
  - Thomas Ramstad (Equinor ASA)





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