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Pore-scale modeling of moving contact line problems in immiscible two-phase flow

Alec Kucala, David Noble and Mario Martinez

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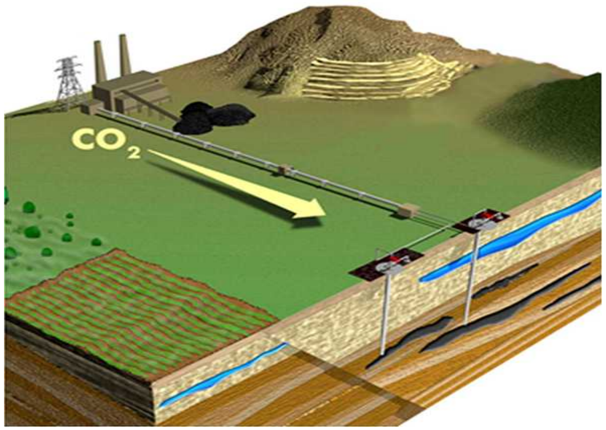
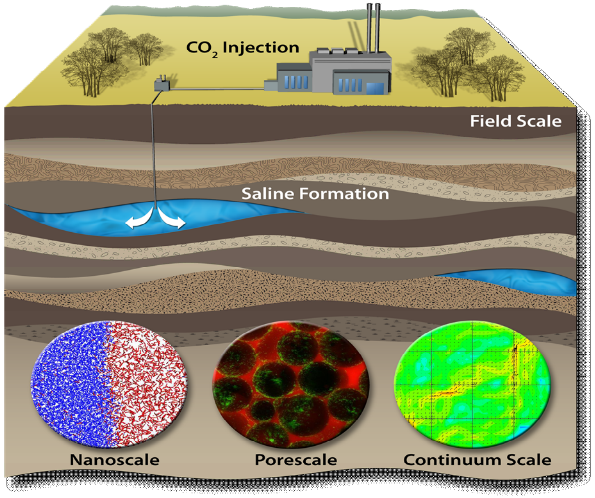
Introduction

- Injection of CO_2 into reservoir rocks is a strategy of reducing greenhouse gas emissions
- Modeling CO_2 migration and capillary trapping at the pore scale is important in predicting the permeability characteristics of reservoir rocks
  - Hydrophobicity or hydrophilicity of the reservoir rock can influence contact line dynamics
- Use computational fluid dynamics to model the multi-phase flow through heterogeneous reservoir rock pores
  - Conformal decomposition finite-element method (CDFEM)
  - Dynamic contact line modeling
- Can be applied to other surface tension dominated flows

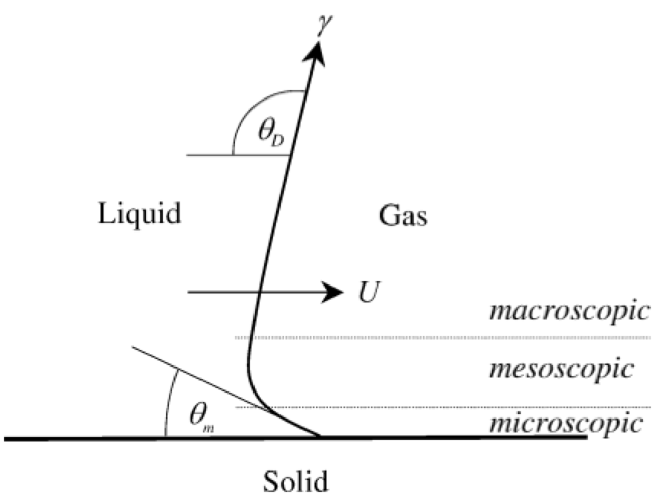




Overview of contact line models

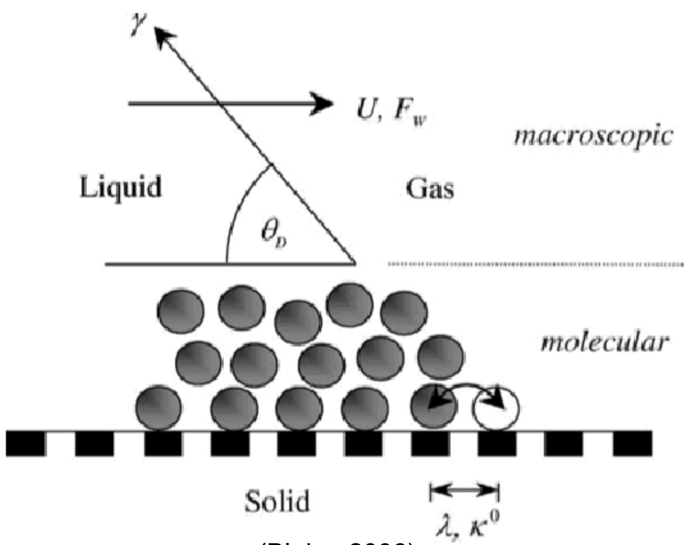
- Two immiscible fluids in contact with a solid surface in equilibrium form a static contact angle
- When this equilibrium is disturbed, the contact angle becomes dynamic and the contact line moves
- Must model relationship between contact angle and contact line velocity as the physics are poorly understood

Hydrodynamic Models



(Blake, 2006)

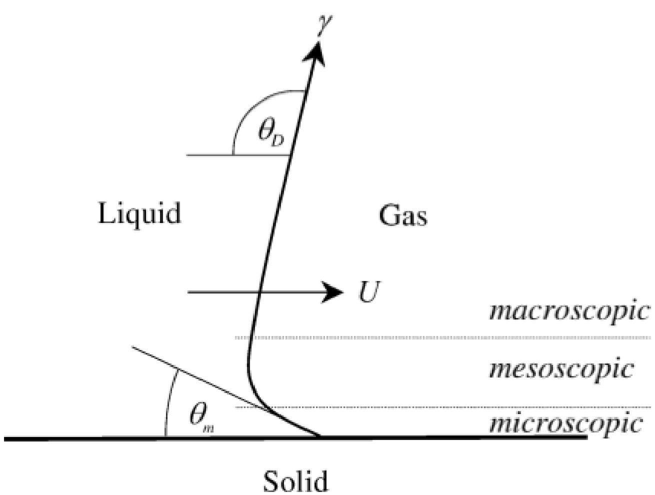
Molecular Models



(Blake, 2006)

Hydrodynamic and molecular models

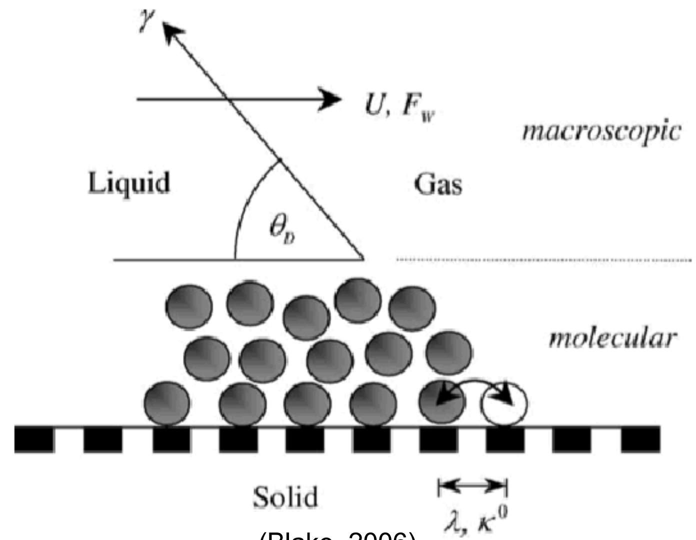
Hydrodynamic Models



(Blake, 2006)

- Three length scales near the contact line: macroscopic, mesoscopic, and microscopic
- Changes in experimentally observed macroscopic dynamic contact angle is attributed to viscous bending of the interface in the mesoscopic region
- Microscopic angle is usually assumed as the static angle and velocity independent
- Voinov, 1976; Cox, 1989; Huh & Scriven, 1971.

Molecular Models

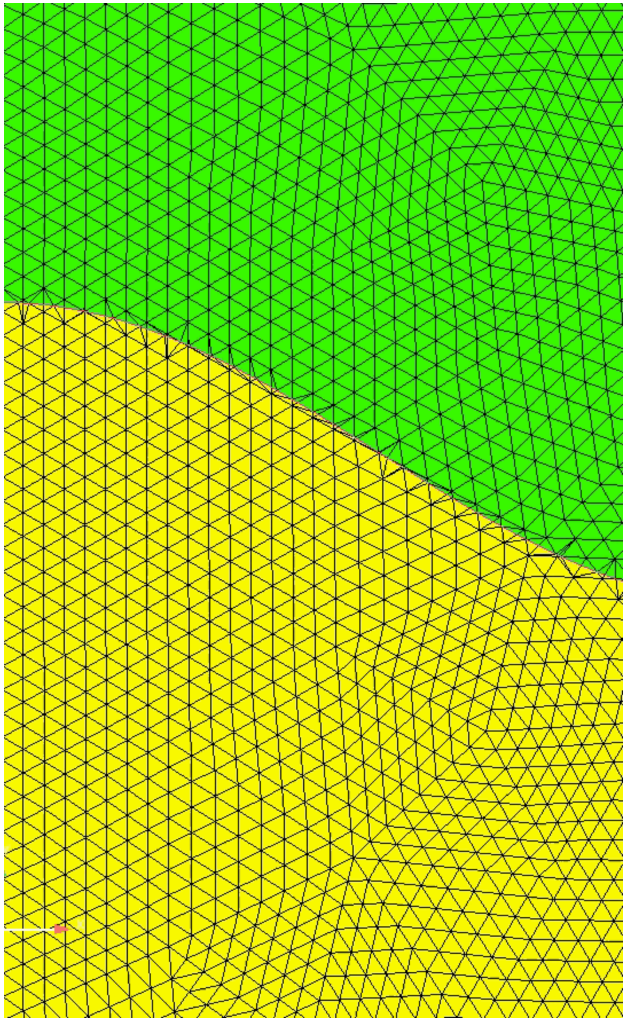


(Blake, 2006)

- Two length scales: macroscopic and molecular
- Contact line motion is determined by the statistical dynamics of the molecules at the molecular scale
- Driving force of contact line is proportional to the disturbed and equilibrium contact angles.
- Blake, 1969

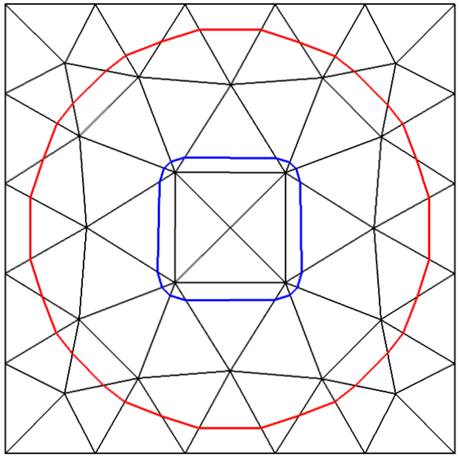
Conformal decomposition finite element analysis (CDFEM)

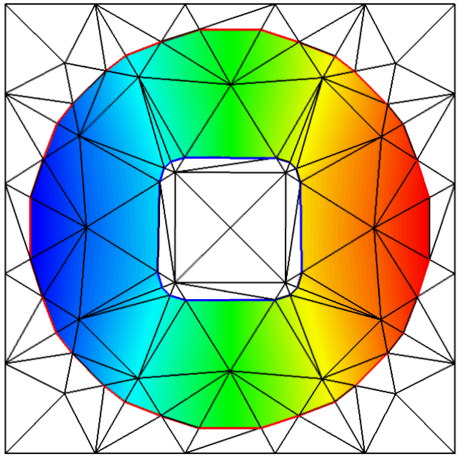
- Relatively new method (Noble et al., 2010) used to discretize moving interfaces that do not conform to static finite element meshes
- Used in conjunction with level sets to track interface motion
- Adds degrees of freedom by adding nodes to mesh which lie on the exact interface location
- Can apply boundary conditions directly at interface
  - Surface tension
  - Wetting line models
- Demonstrated to accurately model surface tension driven flows



CDFEM (cont.)

- Simple Concept (Noble, et al. 2010)
  - Use one or more level set fields to define materials or phases
  - Decompose non-conformal elements into conformal ones
  - Obtain solutions on conformal elements
- Related Work
  - Li et al. (2003) FEM on Cartesian Grid with Added Nodes
  - Ilinca and Hetu (2010) Finite Element Immersed Boundary
  - S. Soghrati and P.H. Geubelle (2012) Interface Enriched Finite Element
- Properties
  - Supports wide variety of interfacial conditions (identical to boundary fitted mesh)
  - Avoids manual generation of boundary fitted mesh
  - Supports general topological evolution (subject to mesh resolution)
- Similar to finite element adaptivity
  - Uses standard finite element assembly including data structures, interpolation, quadrature





Computational model

1. P. Notz, S. R. Subia, M. M. Hopkins, H. K. Moffat, and D. R. Noble, Aria 1.5: User Manual, SAND2007-2734 (Sandia National Laboratories, Albuquerque, NM, 2007)

Computational model

- Utilize Galerkin triangular finite elements to discretize Navier-Stokes equation

Navier-Stokes Equation

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho(\mathbf{x}) \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\, \mathbf{u} \right) = -\nabla p + \nabla \cdot \left(\mu(\mathbf{x}) \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}} \right) \right)$$

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Computational model

- Utilize Galerkin triangular finite elements to discretize Navier-Stokes equation
- Use level set equation to track two-phase interface

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Level Set Equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$$

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Computational model

- Utilize Galerkin triangular finite elements to discretize Navier-Stokes equation
- Use level set equation to track two-phase interface
- CDFEM used to discretize the interface boundary
- Solved using Sierra multi-physics suite at SNL[1]

Navier-Stokes Equation

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho(\mathbf{x}) \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla \cdot \left(\mu(\mathbf{x}) \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}} \right) \right)$$

Level Set Equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$$

Interface Boundary Conditions

$$[\mathbf{u}]_{\Delta} = 0, \qquad \mathbf{x} \in \Gamma$$ ***(impermeability)***

$$\left[-p\mathbf{I} + \mu(\mathbf{x}) \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}} \right) \right]_{\Delta} \cdot \hat{\mathbf{n}} = -\gamma \kappa \hat{\mathbf{n}}, \qquad \mathbf{x} \in \Gamma$$ ***(surface tension)***

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Time-discretization scheme (2nd Order)

Momentum Prediction

$$\int_{\Omega^n} (\nabla \cdot \tilde{\mathbf{u}})\, w_i \mathrm{d}\Omega = 0,$$

$$\int_{\Omega^n} \rho \left(\frac{\frac{3}{2}\tilde{\mathbf{u}} - 2\mathbf{u}^n + \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} + (\tilde{\mathbf{u}} \cdot \nabla)\, \tilde{\mathbf{u}} \right) \cdot \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Omega^n} -P\mathbf{I} + \mu \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^t \right) \cdot \nabla\mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Gamma_f^n} \sigma \left((\mathbf{I} - \mathbf{nn}) + \Delta t \underline{\nabla}\tilde{\mathbf{u}} \right) \cdot \nabla\mathbf{w}_i \mathrm{d}\Gamma = 0,$$

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Levelset Advection

Time-discretization scheme (2nd Order)

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Momentum Prediction

$$\int_{\Omega^n} (\nabla \cdot \tilde{\mathbf{u}})\, w_i \mathrm{d}\Omega = 0,$$

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Levelset Advection

Momentum Correction

$$\int_{\Omega^{n+1}} \left(\nabla \cdot \mathbf{u}^{n+1} \right) w_i \mathrm{d}\Omega = 0.$$

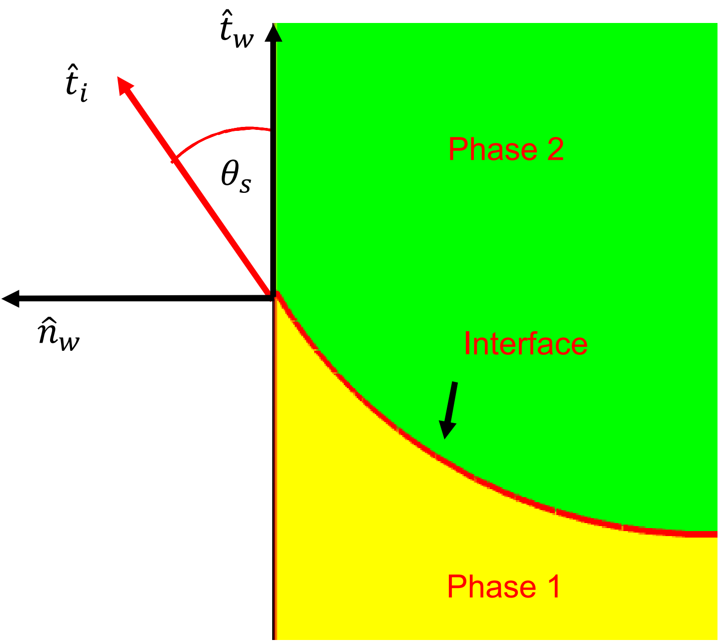
$$\int_{\Omega^{n+1}} \rho \left(\frac{\frac{3}{2}\mathbf{u}^{n+1} - 2\mathbf{u}^n + \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} + \left(\left(\mathbf{u}^{n+1} - \dot{\mathbf{x}} \right) \cdot \nabla \right) \mathbf{u}^{n+1} \right) \cdot \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Omega^{n+1}} -P\mathbf{I} + \mu \left(\nabla\mathbf{u} + \nabla\mathbf{u}^t \right)^{n+1} \cdot \nabla\mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Gamma_f^{n+1}} \sigma \left((\mathbf{I} - \mathbf{nn}) + \Delta t \underline{\nabla} \left(\mathbf{u}^{n+1} - \tilde{\mathbf{u}} \right) \right) \cdot \nabla\mathbf{w}_i \mathrm{d}\Gamma = 0,$$

Moving contact line model

Wetting Line Force

$$\vec{f} = \gamma \hat{\tau}_i$$

$$\hat{\tau}_i = \hat{\tau}_w \cos\theta_s + \hat{n}_w \sin\theta_s$$



- Assume microscopic (static) contact angle is a constant (θ_s) (hydrodynamic type method)
- For a given fluid pair, specify kinematic and physical properties, surface tension force (γ), and static contact angle (θ_s)
- Pull contact line with surface tension force at Young's equilibrium contact angle

Moving contact line model

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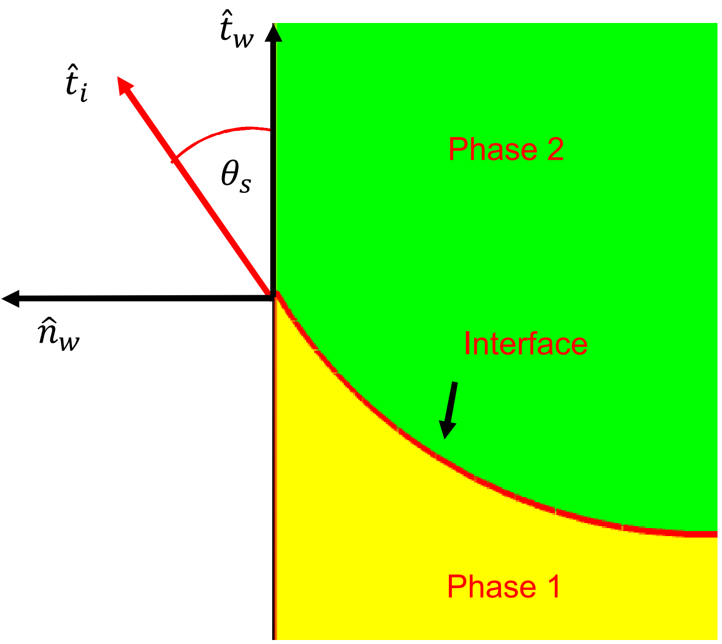
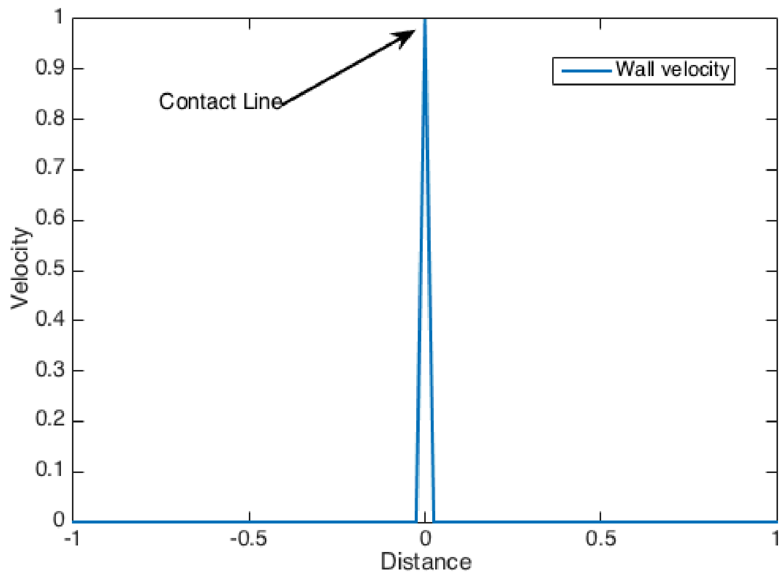


Navier-Slip Condition

$$\vec{f} = \frac{\mu}{\beta}(\vec{v}_w - \vec{v}_{CL})$$

$$Flux = \int \vec{n} \cdot \vec{f} \phi^i \mathrm{d}S$$



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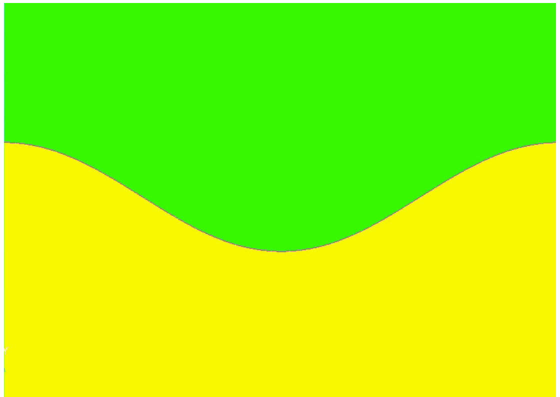
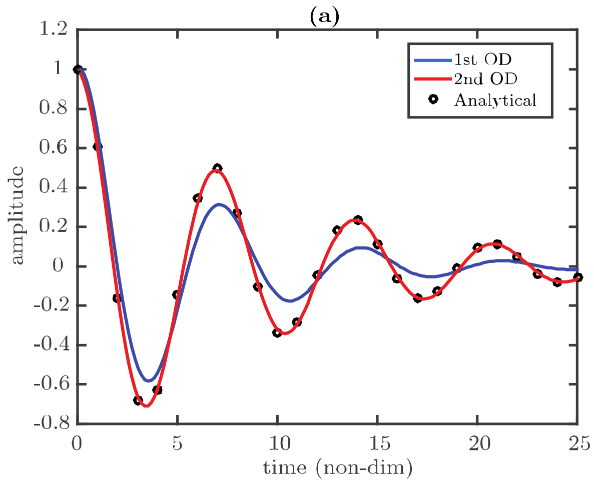
- For a given fluid pair, specify kinematic and physical properties, surface tension force (γ), and static contact angle (θ_s)
- Pull contact line with surface tension force at Young's equilibrium contact angle
- Select the Navier-Slip length (β) to fit to experimental data

Verification and validation (capillary wave decay)

- Perturb two-phase interface with sinusoidal disturbance
- Interface shape should decay with specific frequency and rate (Prosperetti, 1981) at small amplitudes
- Accurate prediction of capillary wave frequency and amplitude decay
- CDFEM discretization of interface accurately captures surface tension dynamics
- 2^{nd} order mesh convergence observed

Interface Dynamics





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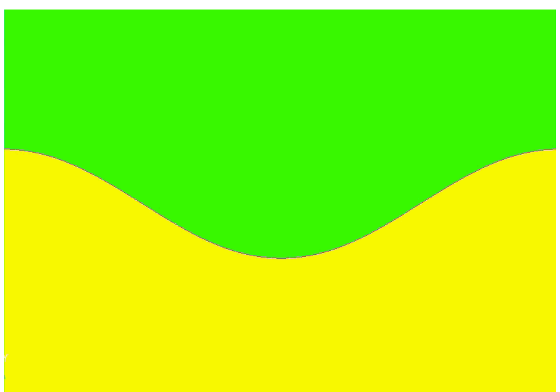
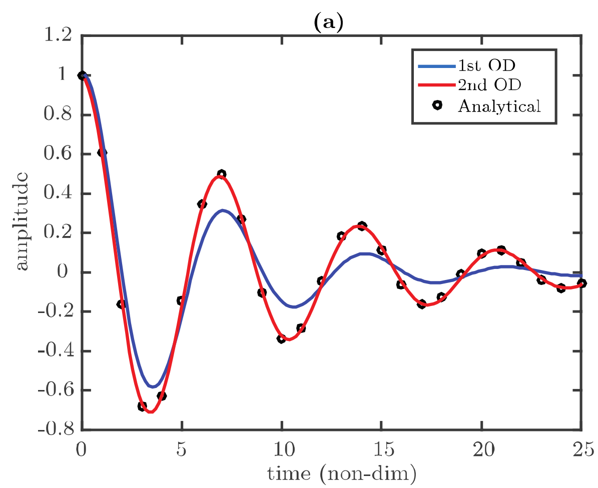
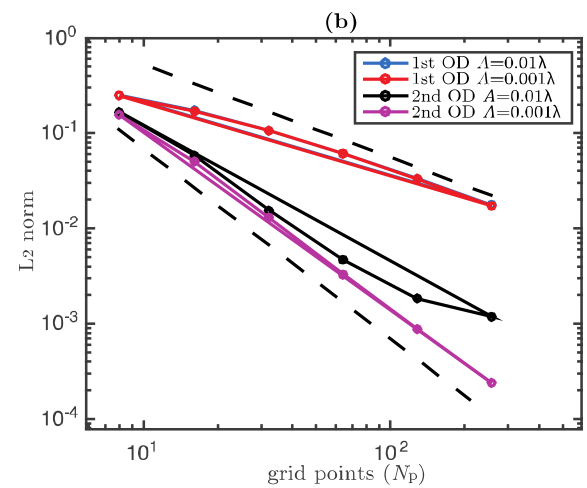




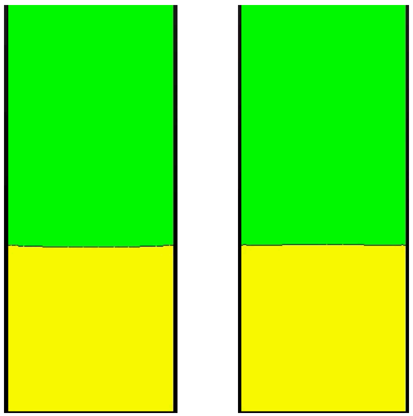
Convergence



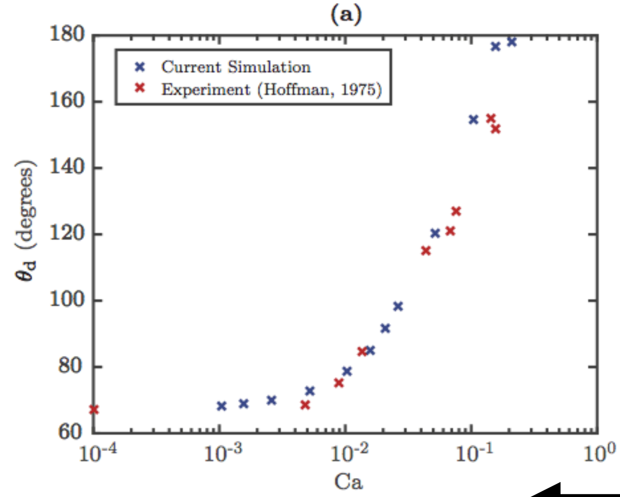
Verification and validation (capillary injection)

Interface Dynamics

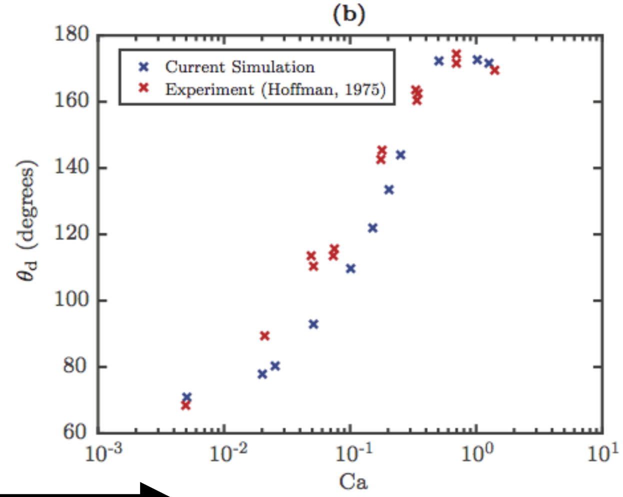
Ca = 5.2e-3 (low) | Ca = 4.4e-2 (high)



Sancitizer 405 ($\theta_s = 67°$)



Amdex 760 ($\theta_s = 69°$)



$$\beta = 4 \times 10^{-8}\ \text{m}$$

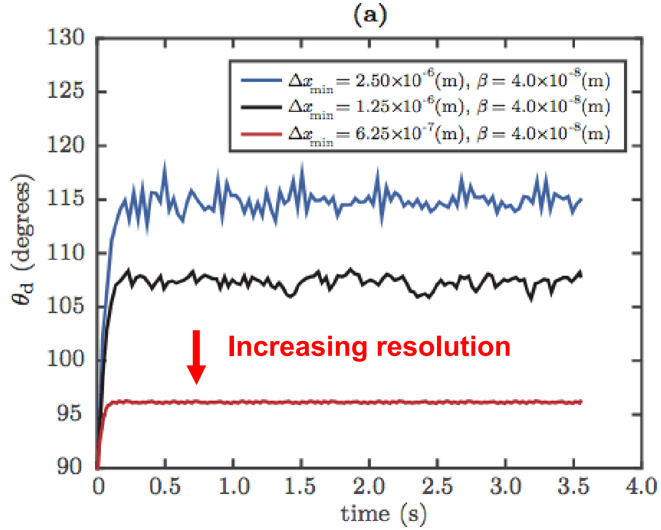
- Injection of fluid into capillary changes dynamic contact angle
- Demonstrate ability to capture dynamic contact angle dependency on capillary number
- Once data is fitted to experiment (one point), specified slip length β becomes independent of fluid type and capillary number

Verification and validation (capillary injection cont.)

Mesh Dependency

MESH DEPENDENT

$\beta = 4.0 \times 10^{-8} = \text{constant}$



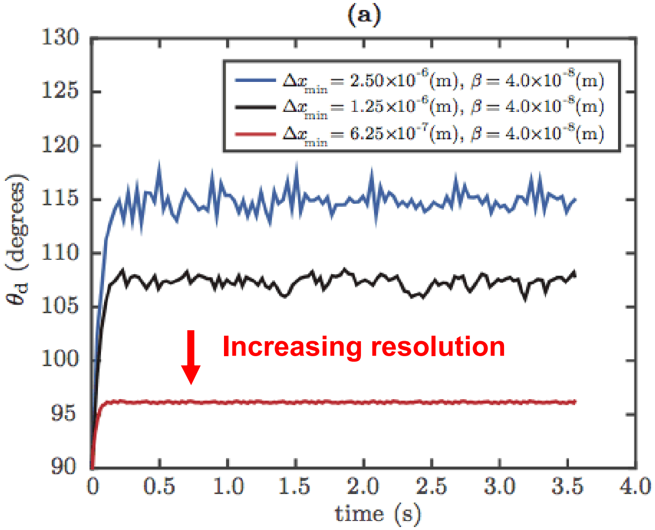
- Solution exhibits mesh dependency (slip length must be adjusted to accommodate resolution changes)

Verification and validation (capillary injection cont.)

Mesh Dependency

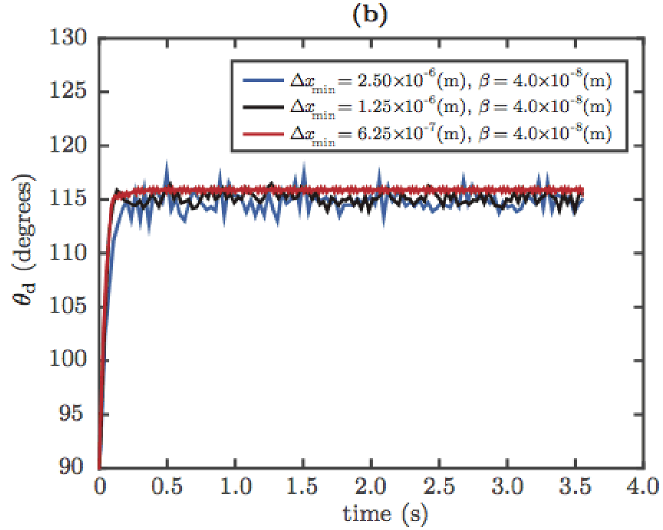
MESH DEPENDENT

$\beta = 4.0 \times 10^{-8} = \text{constant}$



MESH INDEPENDENT

$\Delta x/\beta = \text{constant}$

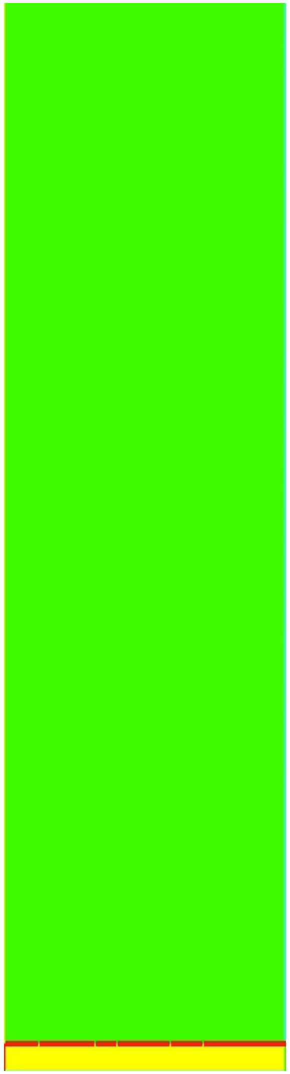


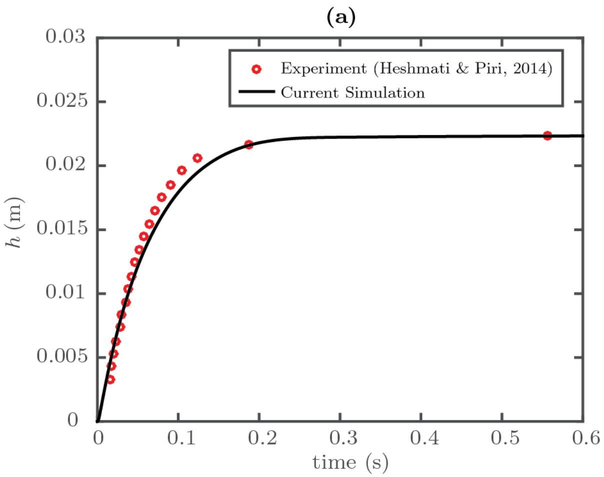
$$\text{Ca} = 4.4 \times 10^{-2}$$

- Solution exhibits mesh dependency (slip length must be adjusted to accommodate resolution changes)
- Mesh independency alleviated once ratio between grid resolution and slip length is held constant
- Allows the use of this model for other more complicated geometries where mesh size is not known *a priori* after slip coefficient is fitted to simple experimental data.

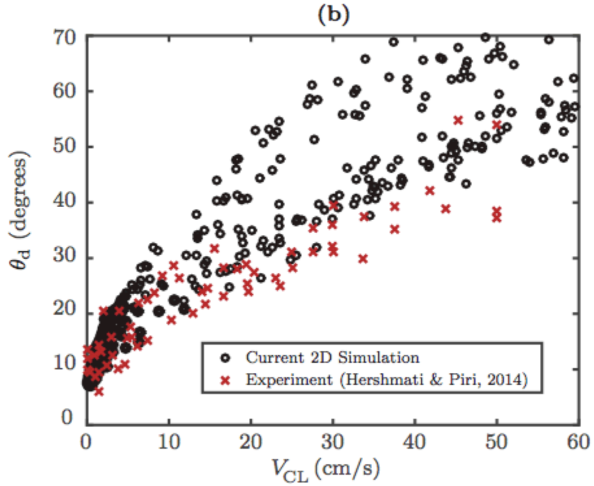
Verification and validation (capillary rise)

2D Capillary Rise



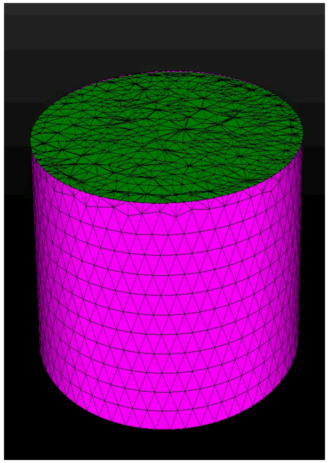


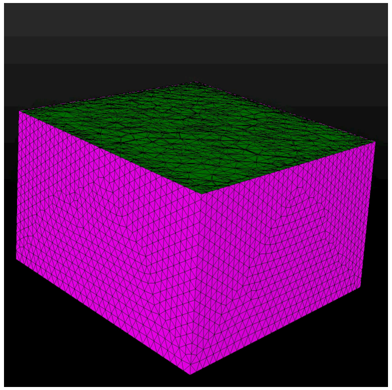
Rise height vs. time

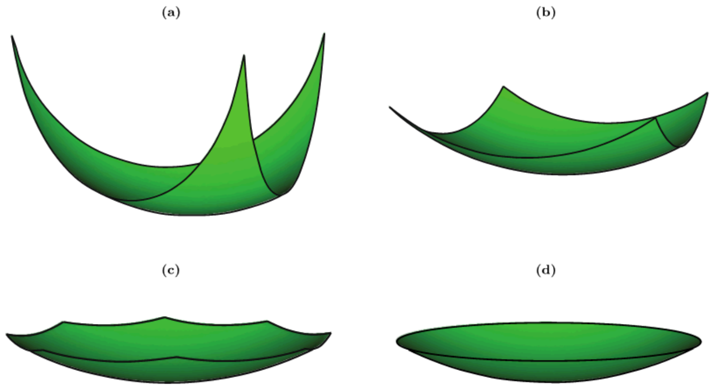


Dynamic angle vs. CL velocity

3D Interface Shapes

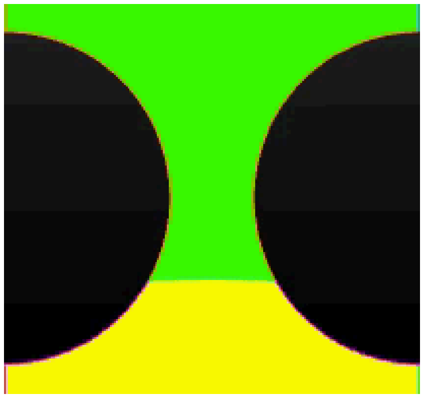




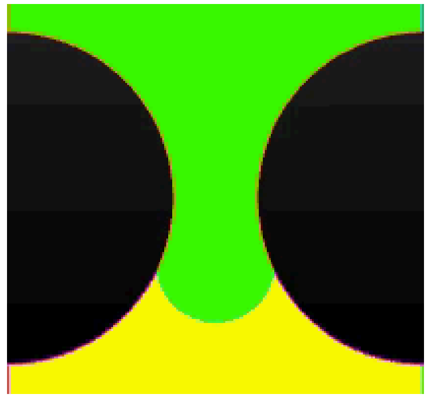


Verification and validation (pore throat)

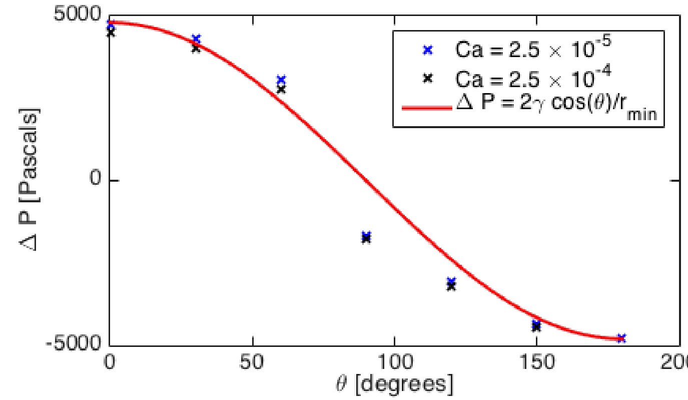
$\theta = 150^\circ$ (non-wetting)



$\theta = 30^\circ$ (wetting)



Capillary Pressure Curve

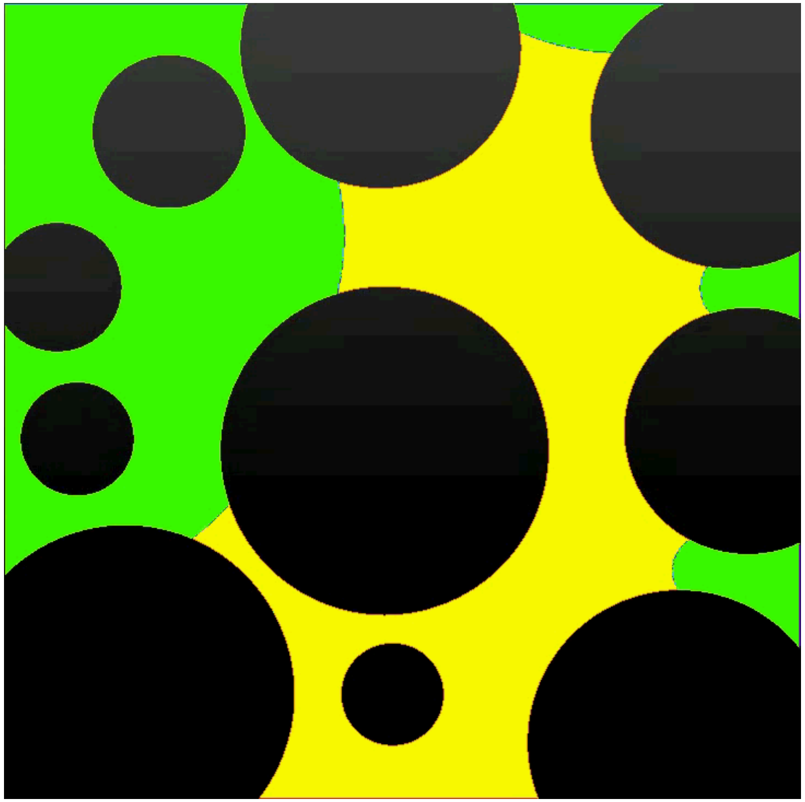


- Forced flow through a pore throat $(\mathrm{Ca} = 1 \times 10^{-5})$
- Important to capture the affect of wetting angle on capillary pressure as it can select preferential flow path in complicated pore lattices.
- Good agreement with predicted capillary pressure curve
  - Wetting line model is accurate
  - Surface tension is accurately represented
- Can be extended to more complicated geometries (2D, 3D)

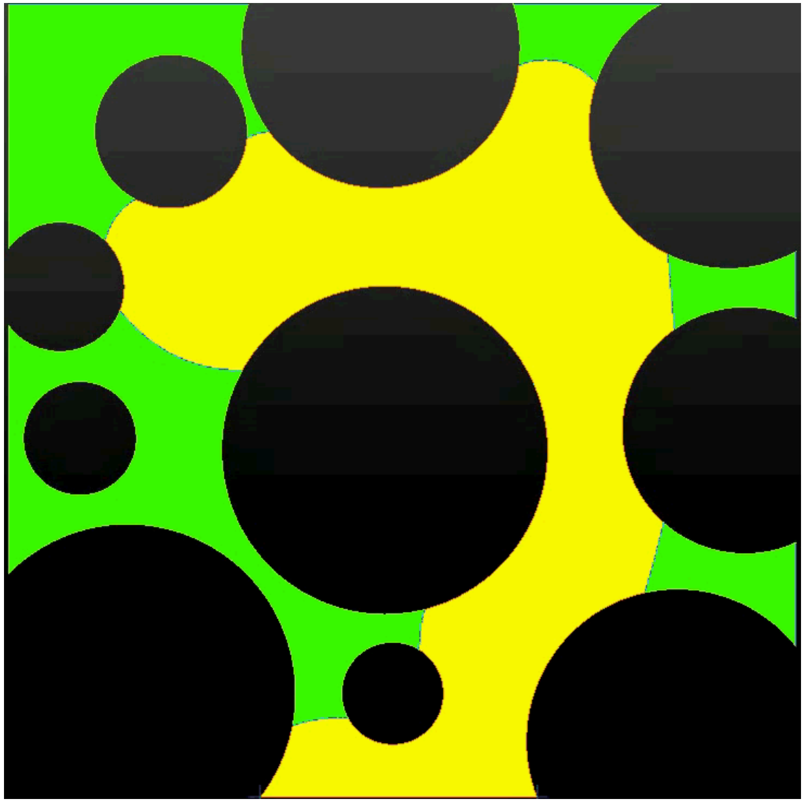
Flow through pore network

Flow Through a Pore Network

Imbibition

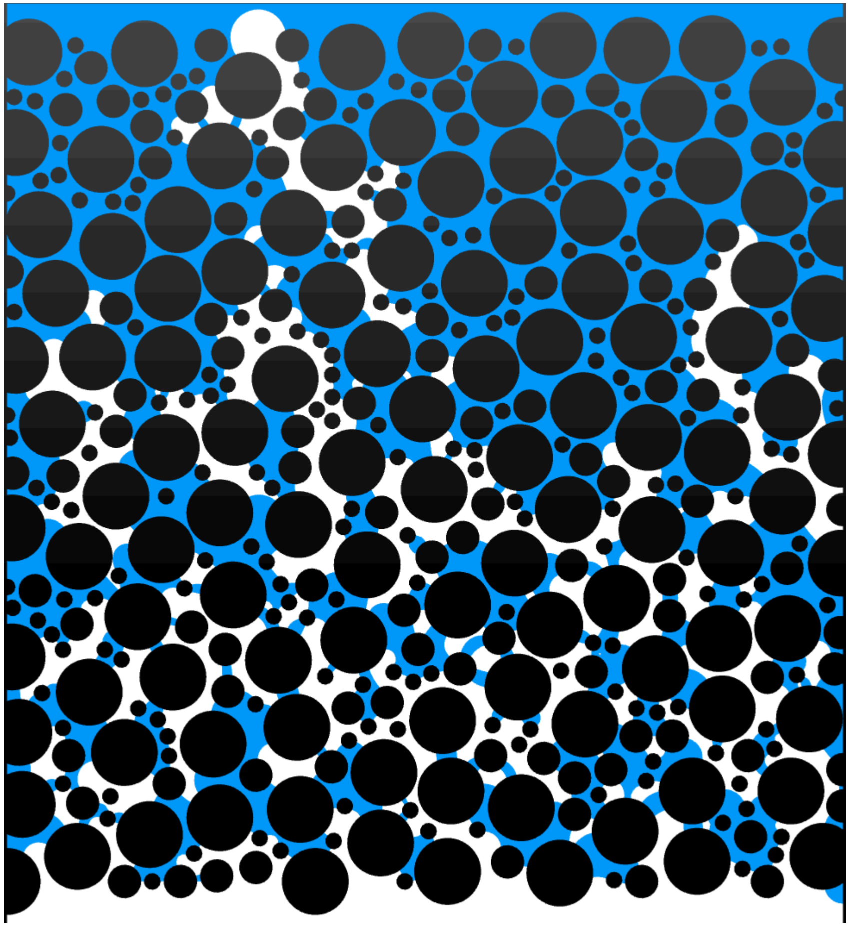


Drainage

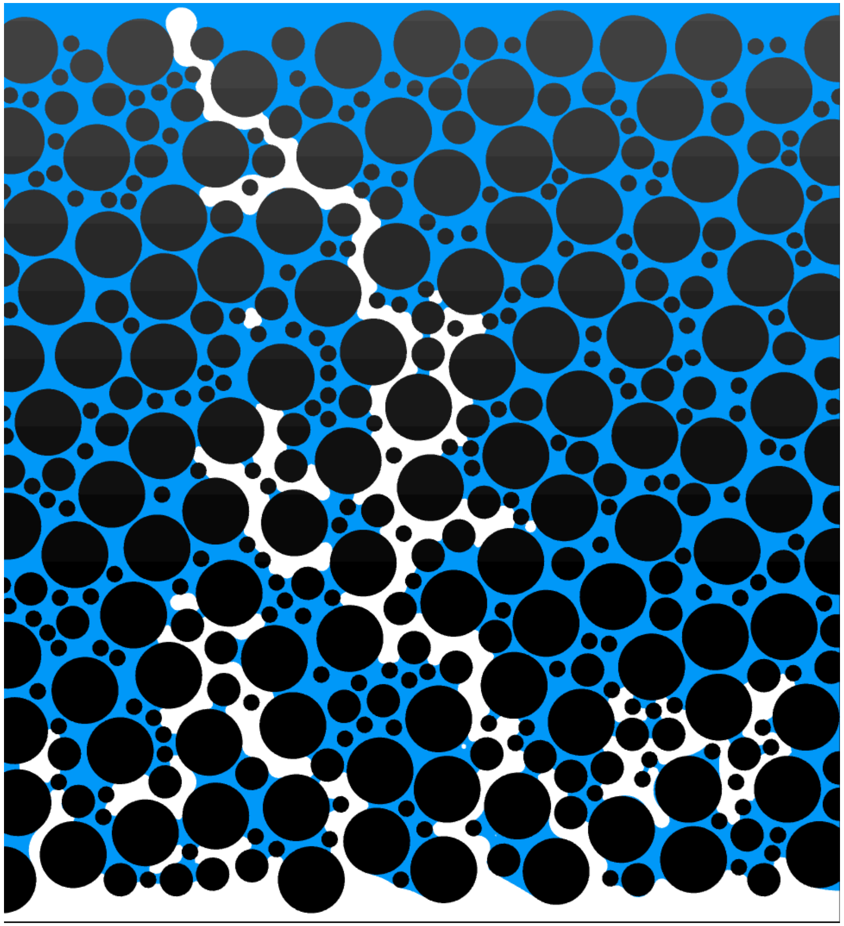


Drainage simulations through random pore network (2D)

Weakly Wetting

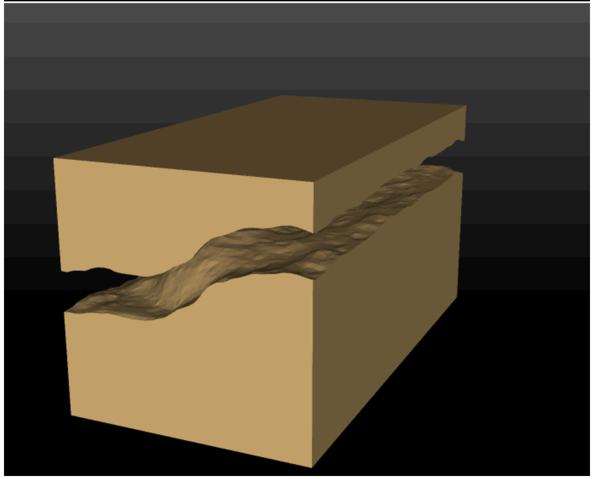


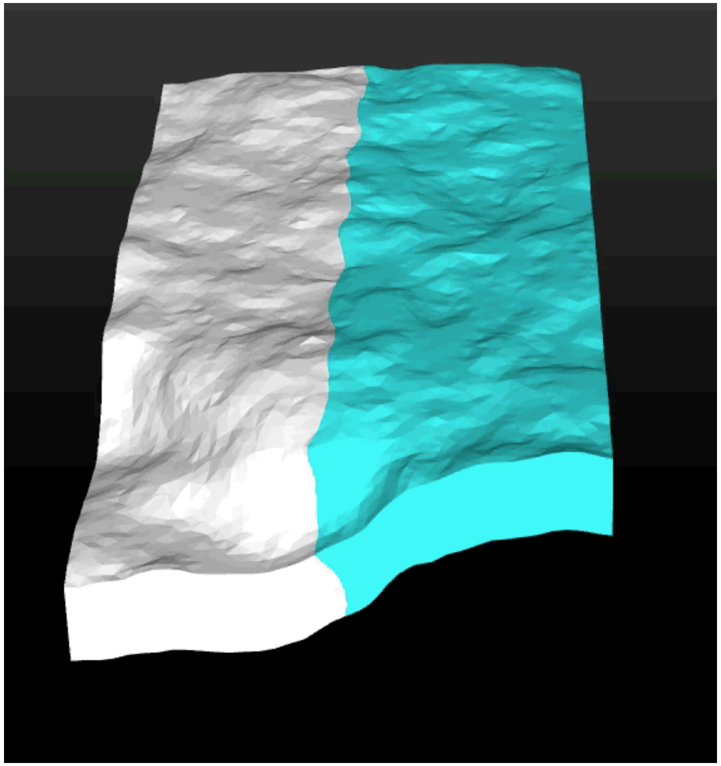
Strongly Wetting



Flow through a scan of a real 3D fracture

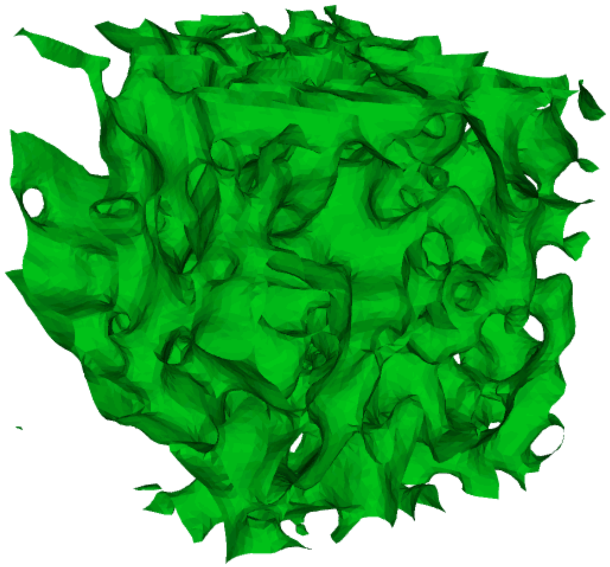
- Micro-CT scan of real sandstone fracture
- Mesh generation using CDFEM
- Run multiphase flow on mesh





Ongoing/Future Work

- Use recently developed CDFEM framework to simulate pore-scale two-phase flow
- Complex pore networks
  - Micro CT Scan data
- Compare with core-flood experiments
- Supplement IP model development
- Predict permeability through reservoir rock based on wettability



3D micro CT scan of sandstone sample

Questions & Acknowledgements

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- Questions?