PIRE ARM: Modeling & Simulation Thrust

Continuum Modeling by Lattice Boltzmann Method

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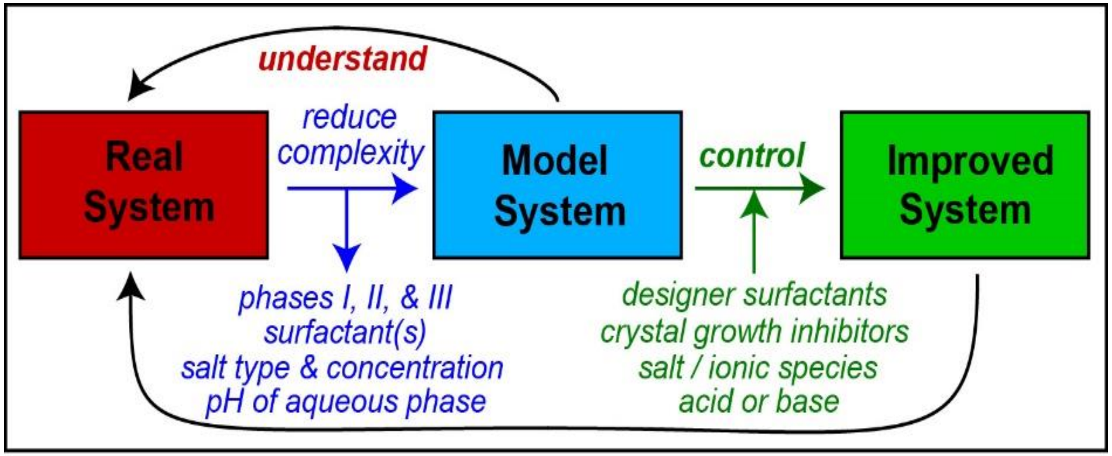
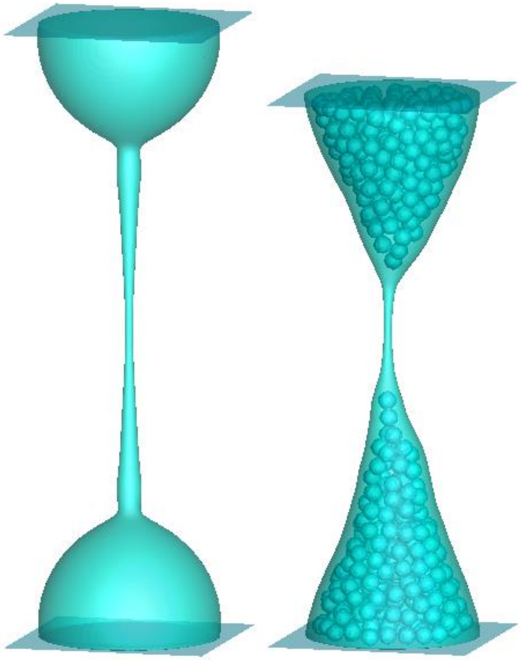
Overview of Modeling & Simulation Thrust



- Support other thrust areas by providing better and deeper understanding of model systems: Gas Hydrate, Drilling Fluids, PCM Nanoemulsion, Asphaltene
- Previous thrust meeting (June 7, 2018): Identification of short term Modeling & Benchmark cases in PCM Nanoemulsion, drilling fluids, and gas hydrates thrusts
- Modeling tools
  - Continuum based models: Lattice Boltzmann Method (LBM) & Boundary Element Method (BEM)
  - Molecular Dynamics (MD)
  - Density Functional Theory (DFT)
- Multiscale modeling strategy

Triple Contact Line Dynamics on Non-colloidal Particles

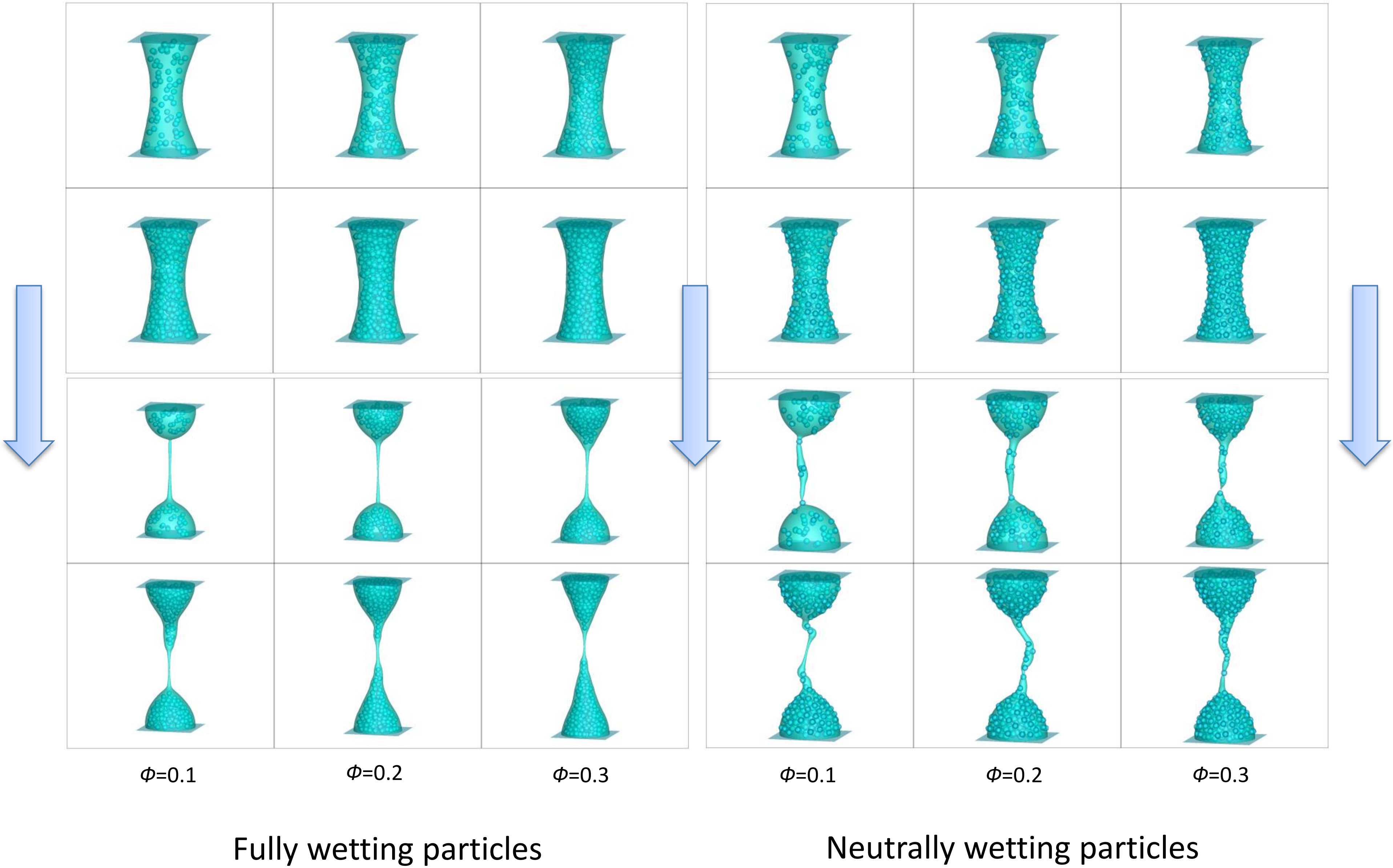


Pinch-off structure for a pure fluid with viscosity equal to the effective viscosity of a $\phi \approx 0.30$ (particle volume fraction) suspension (left) and corresponding suspension (right)

- Particles resist deformation in bulk fluid regions, leading to effective suspension properties different from the properties of the interstitial fluid
- Suspension flows that involve a free surface can also exhibit capillary forces due to particles which cause deformation of the interface
- Wetting properties of the particles and local deformation of the interface can result in surface tension forces that transport particles along the interface

Due to finite size and wetting properties of particles, particles deform an interface locally, which can lead to capillary interactions

Connington, **Lee**, **Morris**, JCP 2015; Connington, Miskin, **Lee**, **Morris**, Jaeger, IJMF 2015



Φ=0.1
Φ=0.2
Φ=0.3
Φ=0.1
Φ=0.2
Φ=0.3
Fully wetting particles
Neutrally wetting particles

Incompressible Navier-Stokes Equations

$$\nabla \cdot \boldsymbol{u} = 0 \qquad or\ \ \boldsymbol{PPE}: \quad \nabla \cdot \left(\frac{1}{\rho}\nabla P\right) = -\nabla \cdot \left(\boldsymbol{u} \cdot \nabla \boldsymbol{u} - \frac{1}{\rho}\nabla \cdot \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) + \frac{\partial \boldsymbol{u}}{\partial t}\right)$$

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla P + \nabla \cdot \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$$

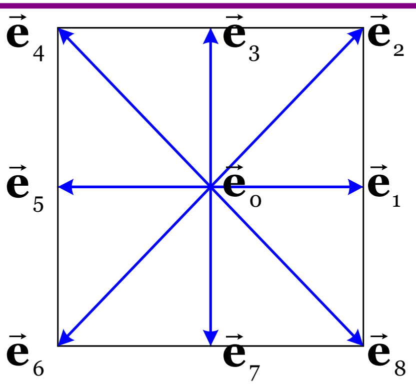
Lattice Boltzmann (Discrete Boltzmann) Equations

$$\frac{1}{\rho c_s^2}\frac{\partial P}{\partial t} + \nabla \cdot \boldsymbol{u} = 0 \qquad for\ \ small\ Ma = \frac{|\boldsymbol{u}|}{c_s^2}$$

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla P + \nabla \cdot \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) + O(Ma^3)$$

$$\underbrace{+\boldsymbol{F}}_{surface\ tension}$$

Lee & Fischer, PRE 2006



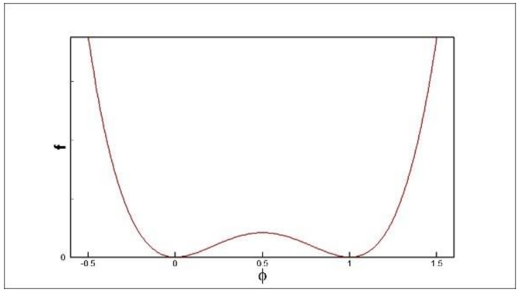
9 velocity model (2D)

Interface tracking equation:

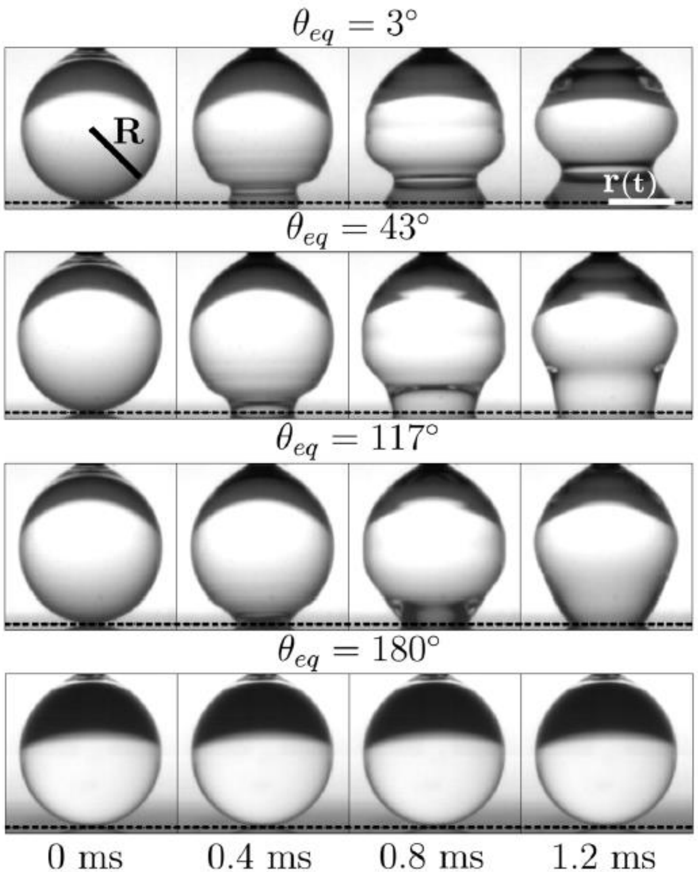
$$\frac{\partial \rho}{\partial t} + \boldsymbol{u} \cdot \nabla \rho = \rho \nabla \cdot \boldsymbol{u}$$

or

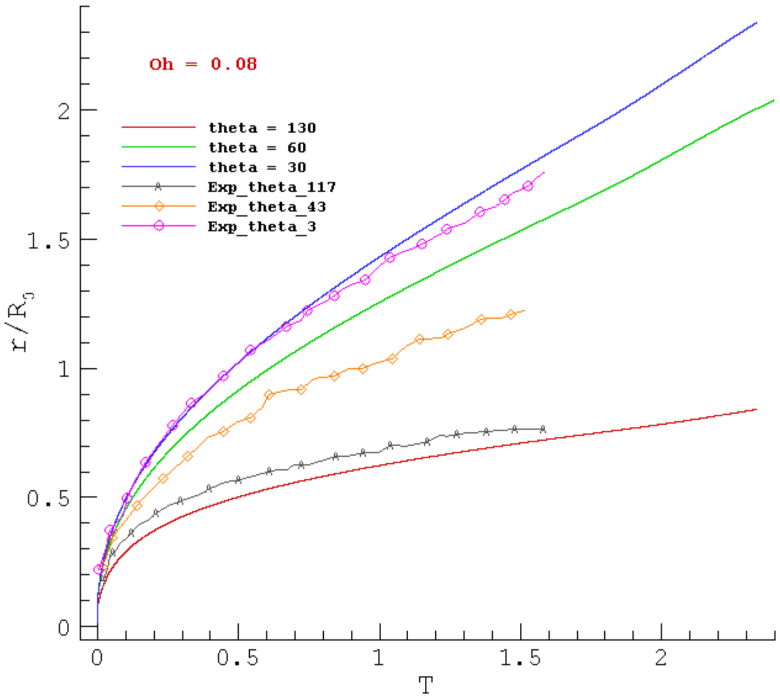
$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \nabla \cdot M \nabla \mu = \nabla \cdot \left[M \nabla \left(\frac{\partial^2 f}{\partial \phi^2} - \nabla^2 \phi\right)\right]$$



Modeling Partial Wetting by LBM (parameter free)



Bird, Mandre, Stone, PRL 2008



Comparison of LBM with experiment (Lee, Fischer, PRE, 2006; Baroudi & Lee, DSFD 2018)

Kinetic nature of LBM allows local slip at contact line under stress

Current Status & Research Issues

- Multiphase LBM code with O(100) non-colloidal particles
  - Parallelization via Message Passing Interface (MPI)
  - Interface tracking by Phase-Field approach on fixed grid → partial wetting of liquids on solid particles

- Scientific/Technical Issues:
  - Mass conservation at liquid phase interface
  - Mass conservation at solid-liquid interface of moving particles → Diffuse Bounce Back (Geng Liu)
  - Wetting at 3-phase interfaces (Fanny Thomas)
  - Surfactant adsorption at (phase changing) three-phase contact line: requires input from MD
  - OpenLB implementation (Marc Haussman & Max Gaedtke)