
An Arbitrary Lagrangian-Eulerian Method for the Direct Numerical Simulation of Particle-Bubble Interactions

Pengtao Yue (Mathematics, Virginia Tech)

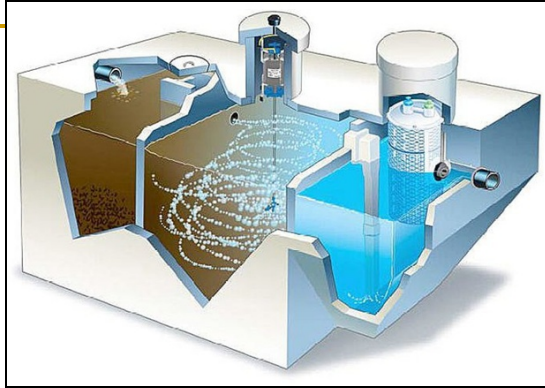
Collaborators:

Tong Qin, Saad Ragab (ESM, VT)

NETL Workshop on Multiphase Flow Science

August 6-7, 2013

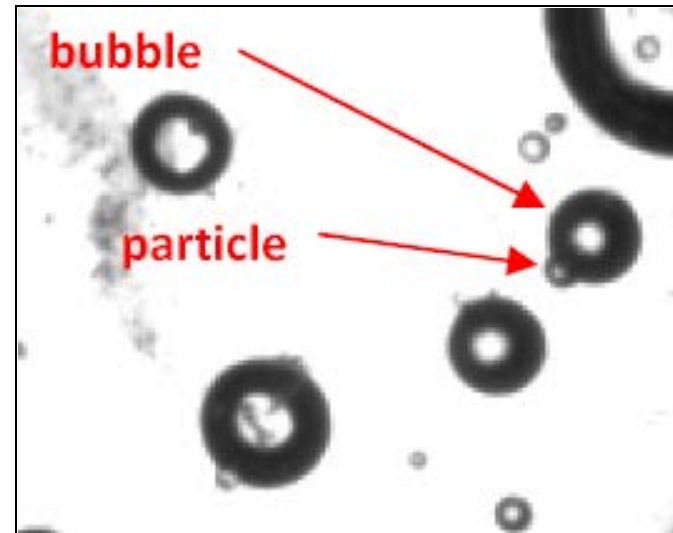
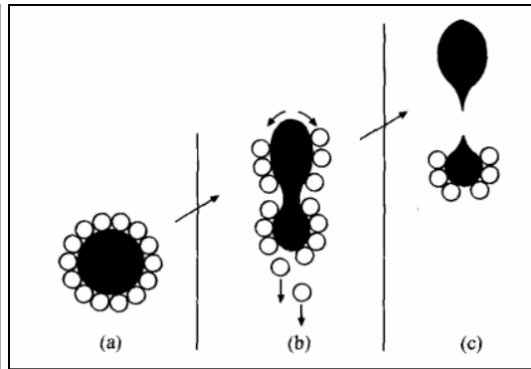
Motivation



← Wastewater treatment

Oil sands extraction

↓ Minerals processing

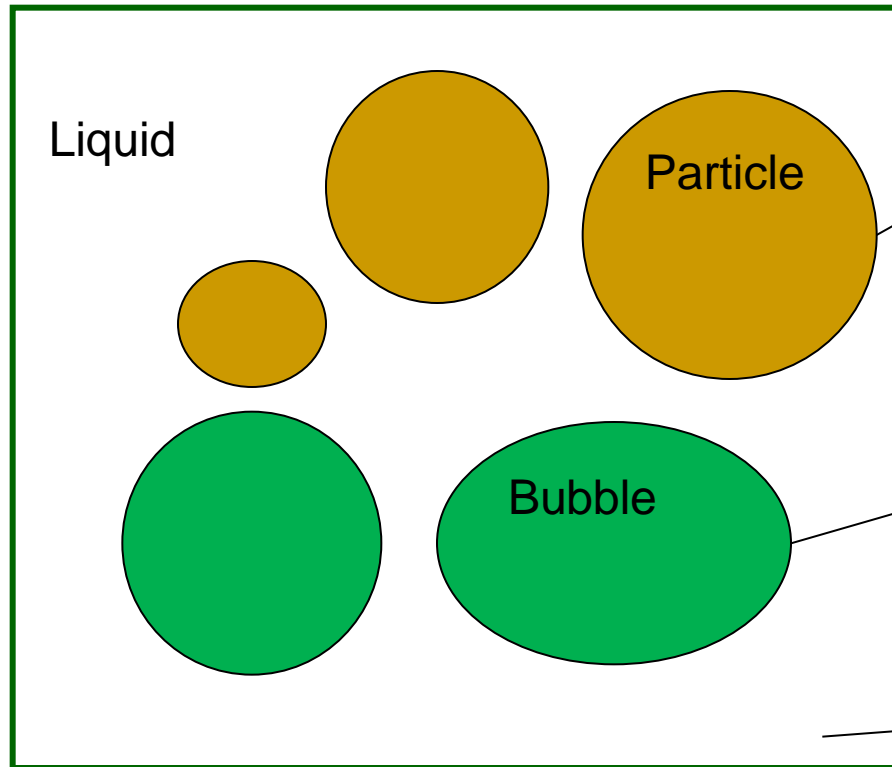


Upper left: <http://www.archiexpo.com/prod/norweco/domestic-wastewater-treatment-plants-59372-139048.html>

Lower left: <http://greenfriend.summerhost.info/activities/new%20file/29.pdf>

Right: experiment of Y. Yang

Problem description



- Immersed Boundary
- Fictitious Domain
- Extended Finite Element
- **ALE**
- ...

- Front tracking
- Interface capturing (VoF, level set...)
- **ALE**
- ...

- Non-Newtonian fluid rheology

Arbitrary Lagrangian-Eulerian (ALE) method

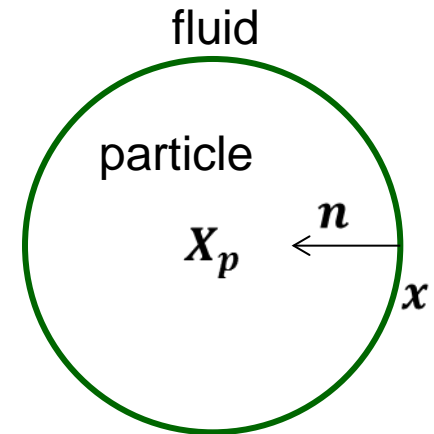
Governing equations

Fluid

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f}$$

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

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$$



Particle

$$m_p \frac{d\mathbf{U}_p}{dt} = - \int_{\partial\Omega_p} \boldsymbol{\sigma} \cdot \mathbf{n} dS + \mathbf{G}_p$$

Hydrodynamic force (internal)

$$\mathbf{I}_p \cdot \frac{d\boldsymbol{\omega}_p}{dt} = - \int_{\partial\Omega_p} (\mathbf{x} - \mathbf{X}_p) \times \boldsymbol{\sigma} \cdot \mathbf{n} dS$$

\mathbf{f} : body force on fluid
Particle:

m_p : mass

\mathbf{I}_p : inertia tensor

\mathbf{X}_p : centroid

\mathbf{G}_p : body force

\mathbf{U}_p : translational vel.

$\boldsymbol{\omega}_p$: angular vel.

Bubble

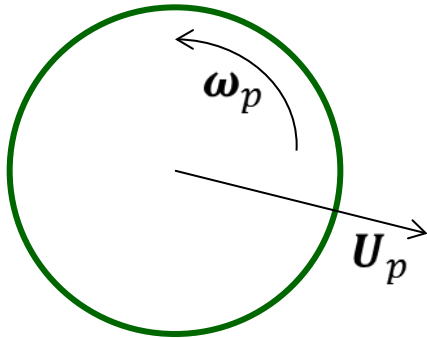
$$p_b V_b = \text{const}$$

Boundary conditions

Particle surface

- No-slip condition

$$\mathbf{u} = \mathbf{U}_p + \boldsymbol{\omega}_p \times (\mathbf{x} - \mathbf{X}_p)$$

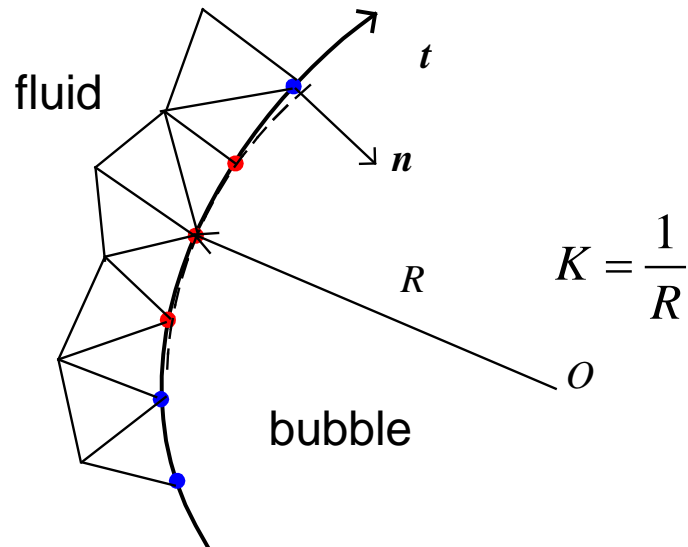


Bubble surface

- Young-Laplace eqn.

$$\mathbf{n} \cdot (-p\mathbf{I} + \boldsymbol{\tau}) = (-p_b + K\gamma)\mathbf{n}$$

curvature Surface tension



Non-Newtonian Rheology

■ Viscoelastic fluid (Oldroyd-B)

$$\boldsymbol{\tau} = \boldsymbol{\tau}_v + \boldsymbol{\tau}_p$$

$$\boldsymbol{\tau}_v = \mu_s [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$$

$$\boldsymbol{\tau}_p + \lambda_H \left[\frac{\partial \boldsymbol{\tau}_p}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\tau}_p - \boldsymbol{\tau}_p \cdot \nabla \mathbf{u} - (\nabla \mathbf{u})^T \cdot \boldsymbol{\tau}_p \right] = \mu_p [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$$

τ_v : viscous stress; τ_p : polymer stress; λ_H : relaxation time
 μ_s : solvent viscosity; μ_p : polymer viscosity

■ Generalized Newtonian fluid

$$\boldsymbol{\tau} = \boldsymbol{\tau}(\dot{\boldsymbol{\gamma}})$$

- Power-law fluid (shear-thinning, shear-thickening)
- Bingham fluid (yield stress)
- ...

Moving Mesh Scheme

Mesh velocity

$$\nabla \cdot (k^e \nabla \mathbf{u}_m) = 0$$

Boundary conditions

$$\mathbf{u}_m = \mathbf{u} \quad \text{on bubble surface}$$

$$\mathbf{u}_m = \mathbf{U}_p \quad \text{on particle surface}$$

Mesh position (Crank-Nicolson)

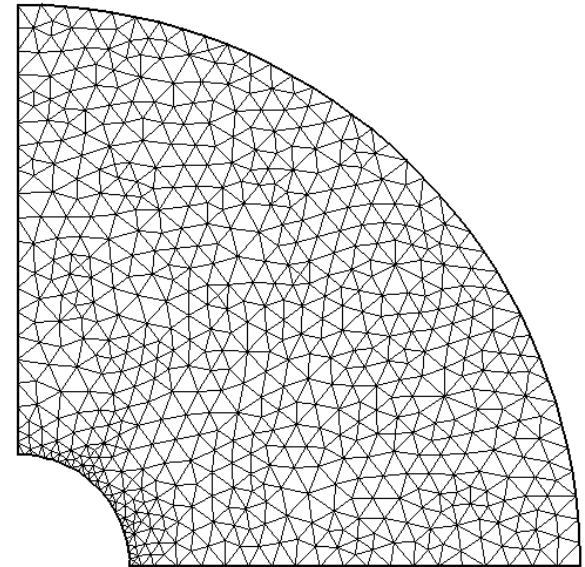
$$\mathbf{X}^{n+1} = \mathbf{X}^n + (\mathbf{u}_m^{n+1} + \mathbf{u}_m^n) \frac{\Delta t}{2}$$

\mathbf{u}_m : mesh velocity

\mathbf{u} : fluid velocity

k^e : inverse of element volume

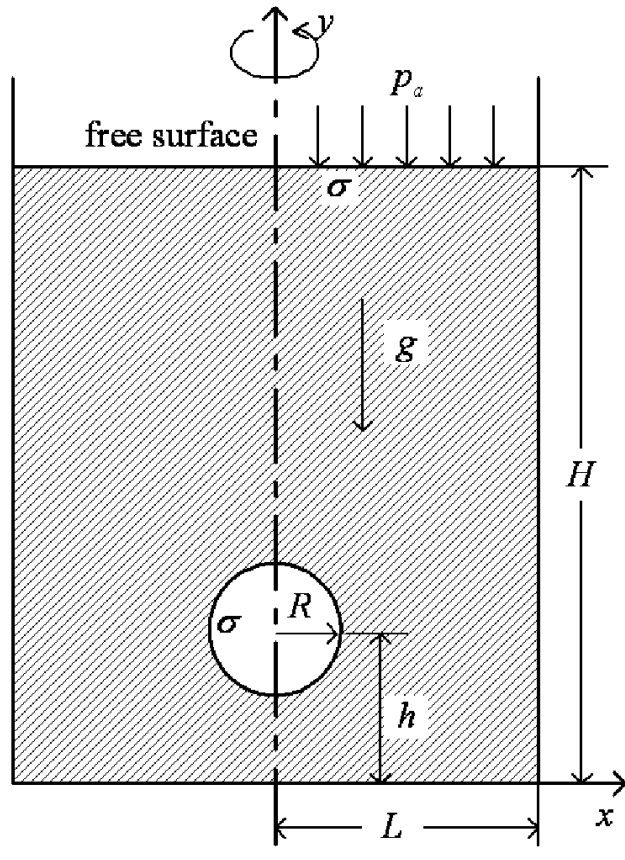
\mathbf{X} : mesh nodal position



Moving mesh around an oscillating bubble (1/4 shown)

Numerical Results

Bubble Rising

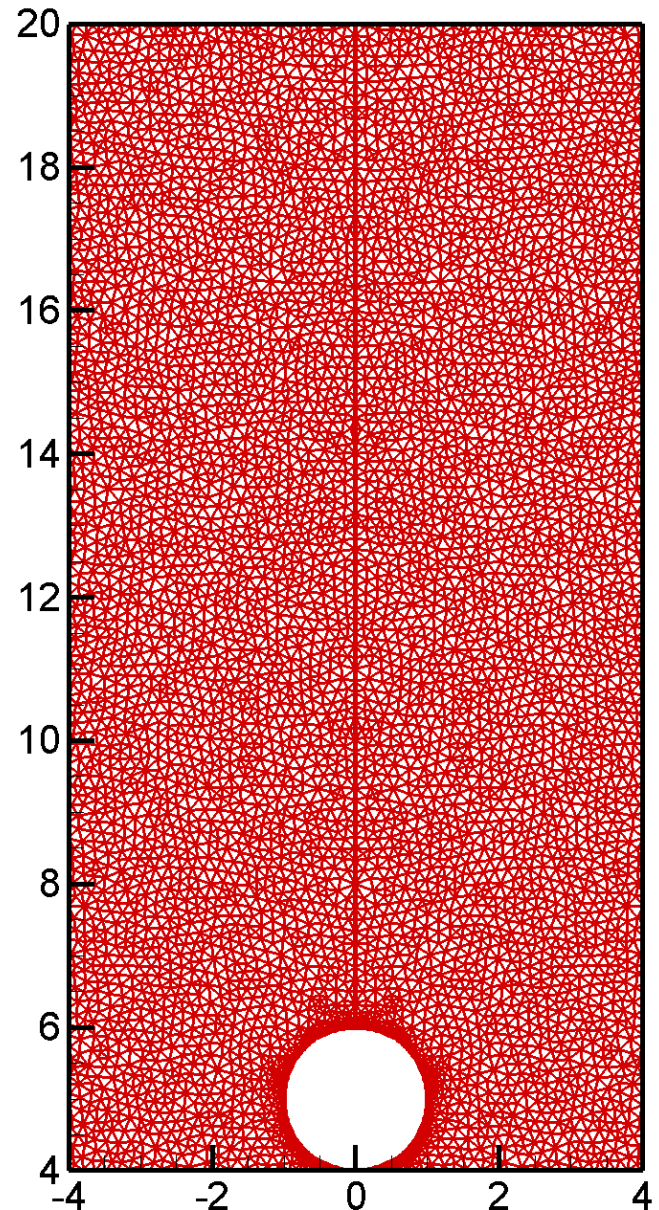


$$L=10R, H=30R$$

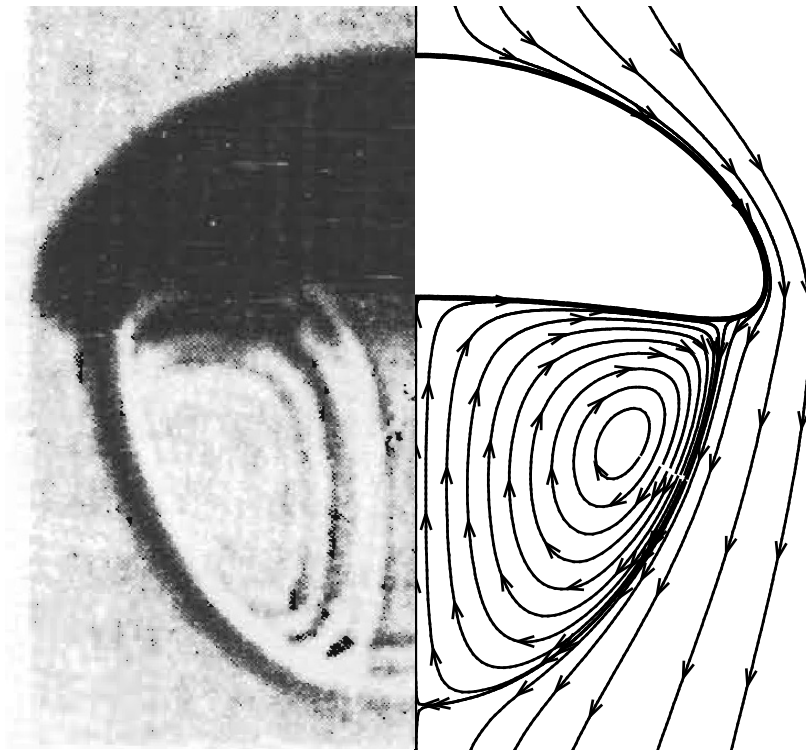
$$\rho = 0.8755 \times 10^3 \text{ Kg/m}^3 \quad \sigma = 32.2 \times 10^{-3} \text{ J/m}^2$$

$$R = 0.608 \text{ cm} \quad \mu = 0.118 \text{ Pa s}$$

Experiment by Hnat & Buckmaster, *Phys. Fluids* 1976

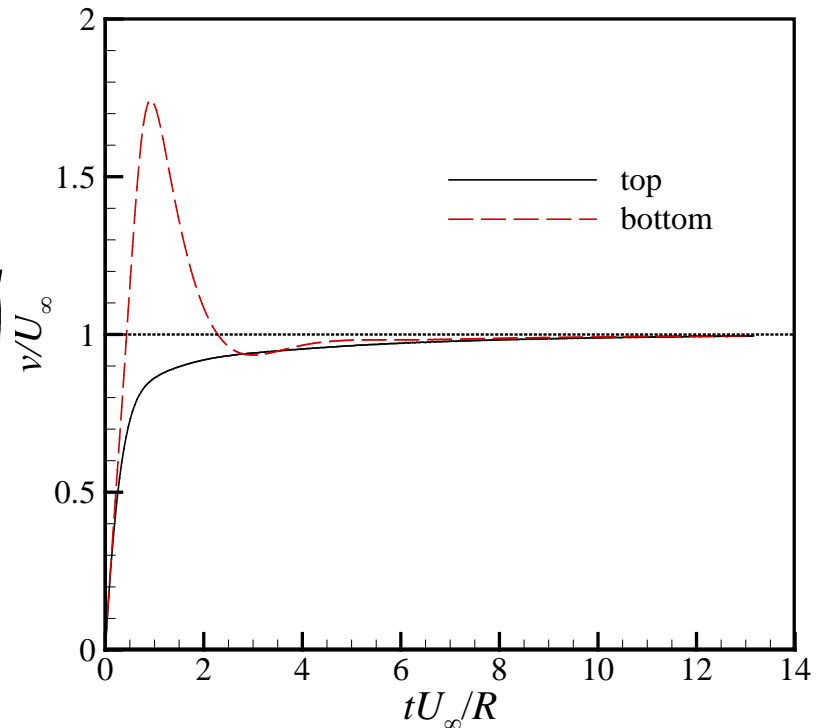


Comparisons with Experiment



Bubble shape

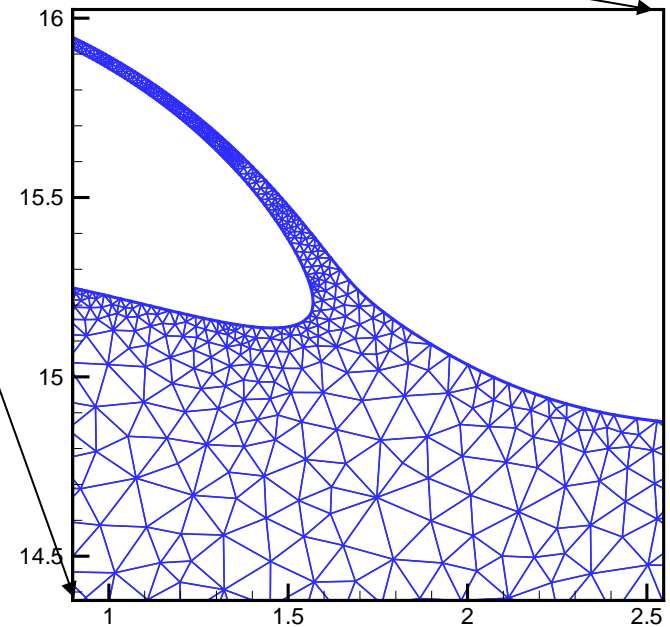
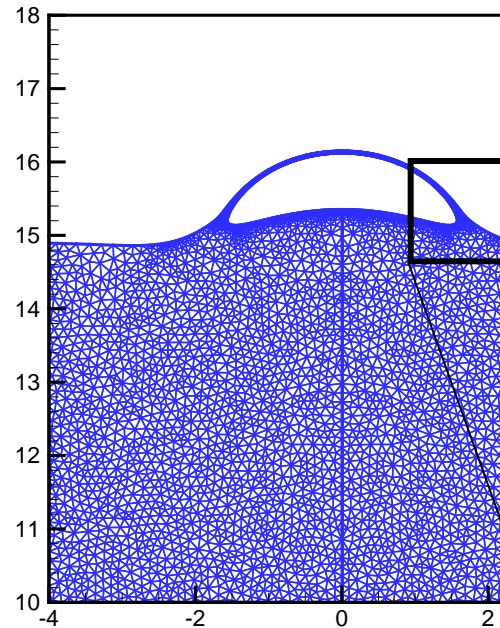
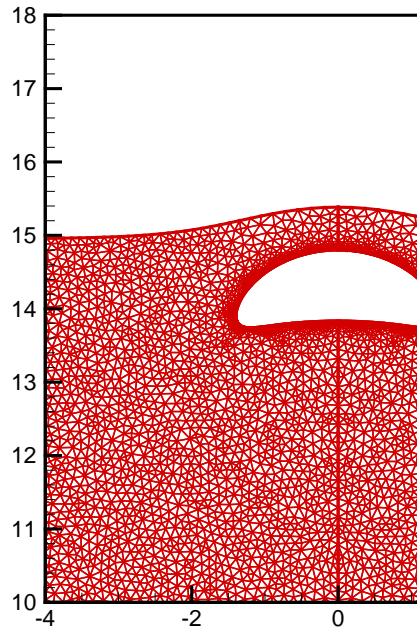
$Re=9.69$, $We=7.64$



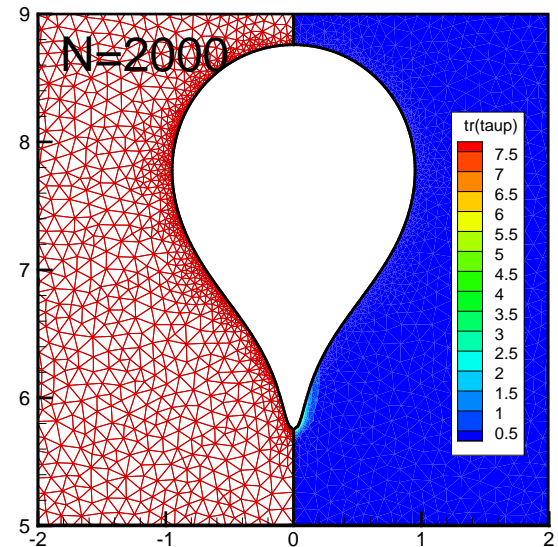
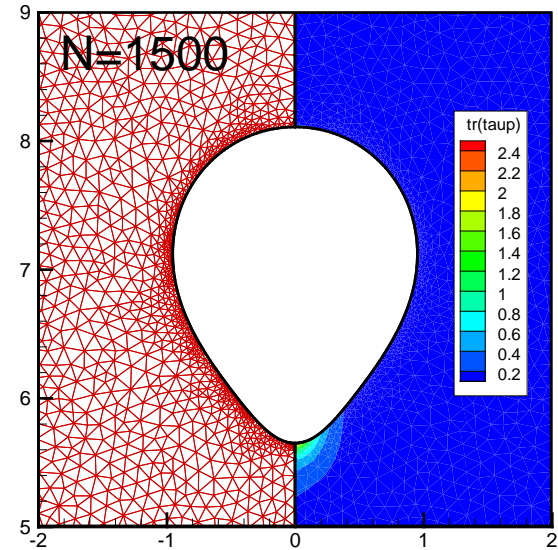
Rising velocity

$$U_\infty(\text{numer.}) = 0.995U_\infty(\text{exp.})$$

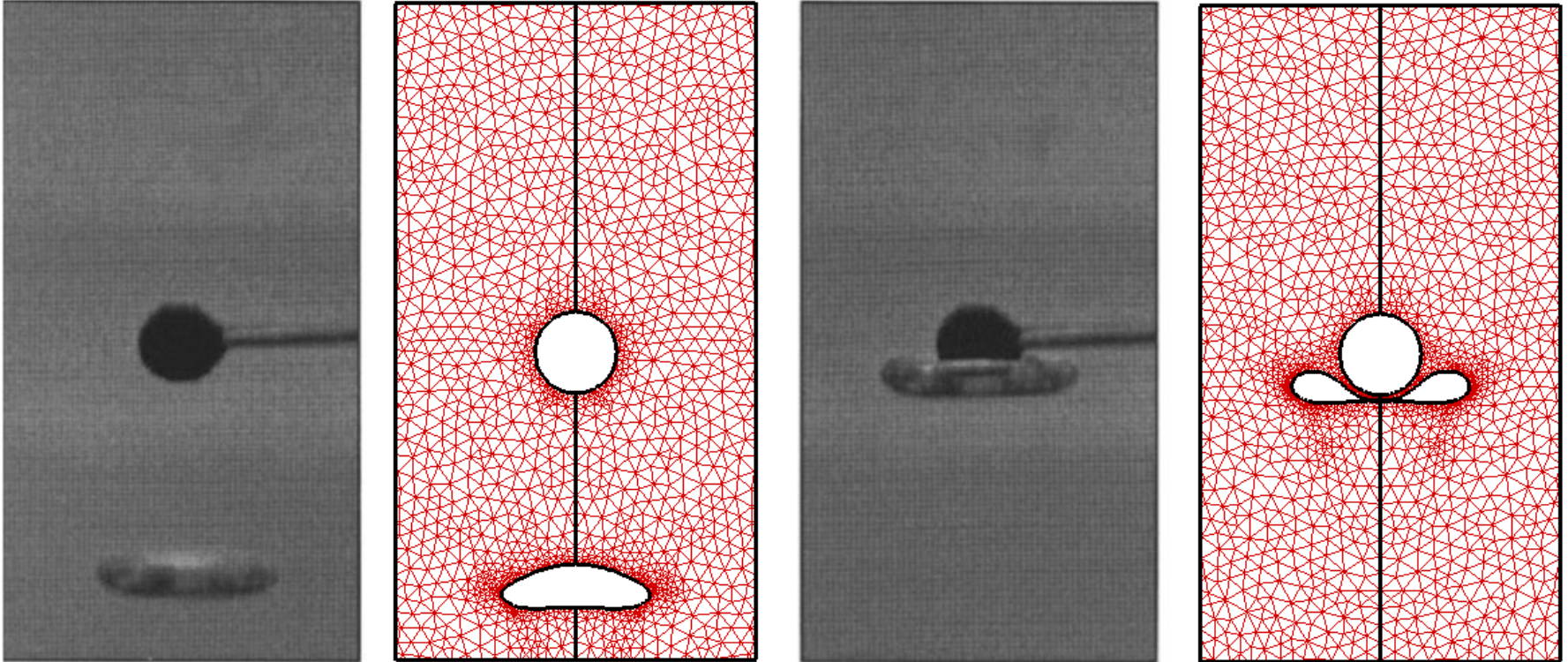
When bubble approaches surface



Rising bubble in a viscoelastic liquid



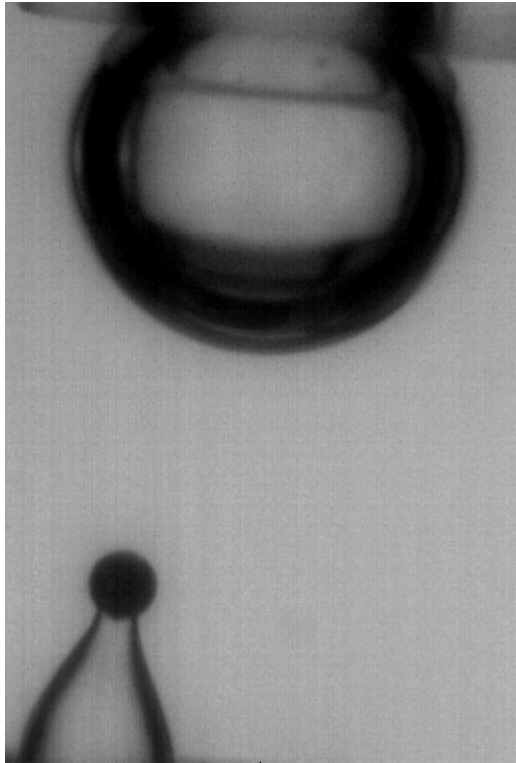
Particle-bubble collision



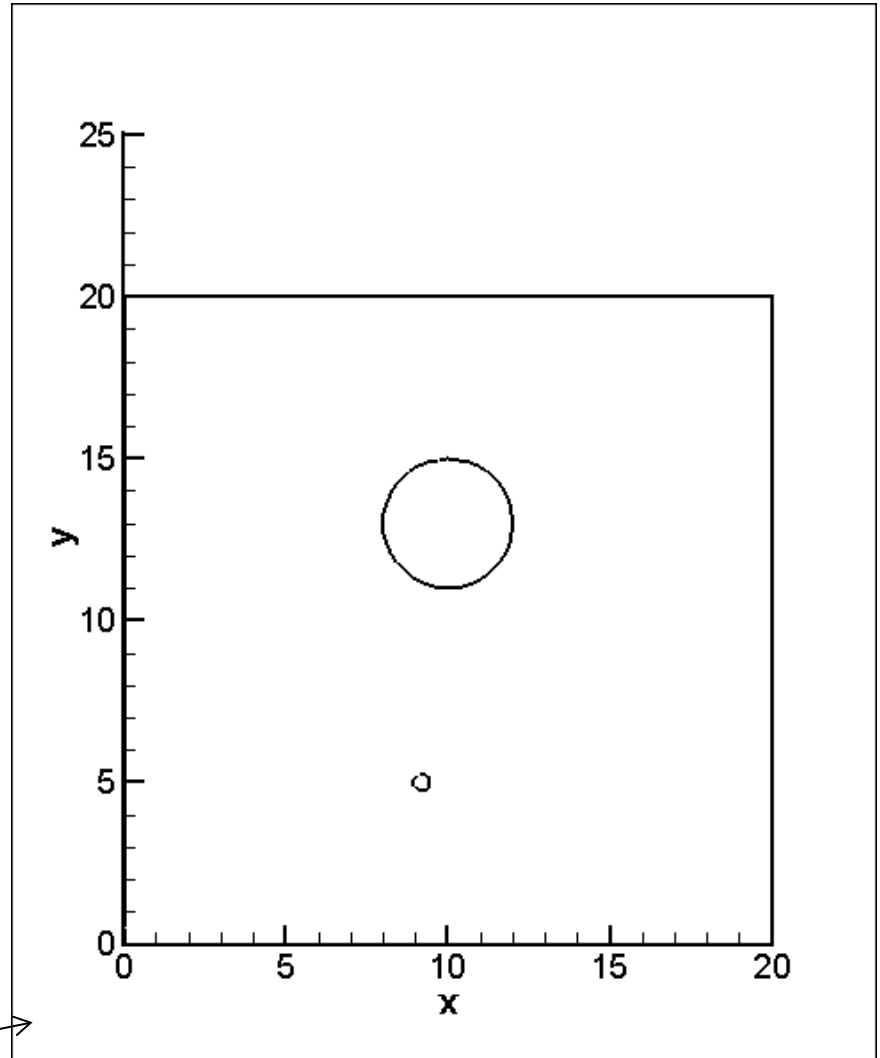
Collision between a rising bubble and a stationary particle
 $d_p=0.5\text{cm}$, $d_b=1.2\text{cm}$, 80 wt% glycerin solution

(Experimental by Hong, Fan & Lee, *Int J. Multiphase Flow*, 1999)

Oblique collision (qualitative comparison)

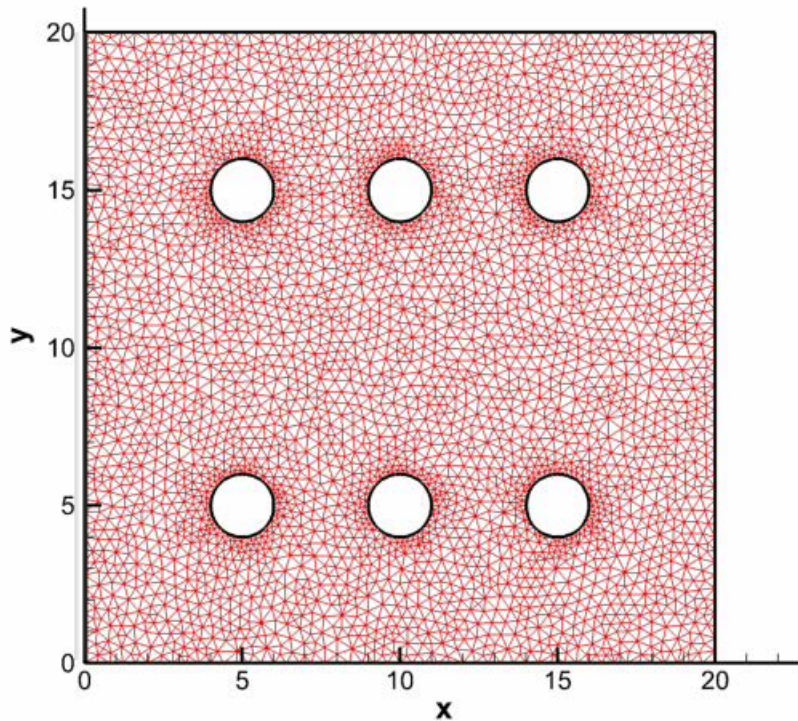


Experiment by Y. Yang ($Re = 80$)

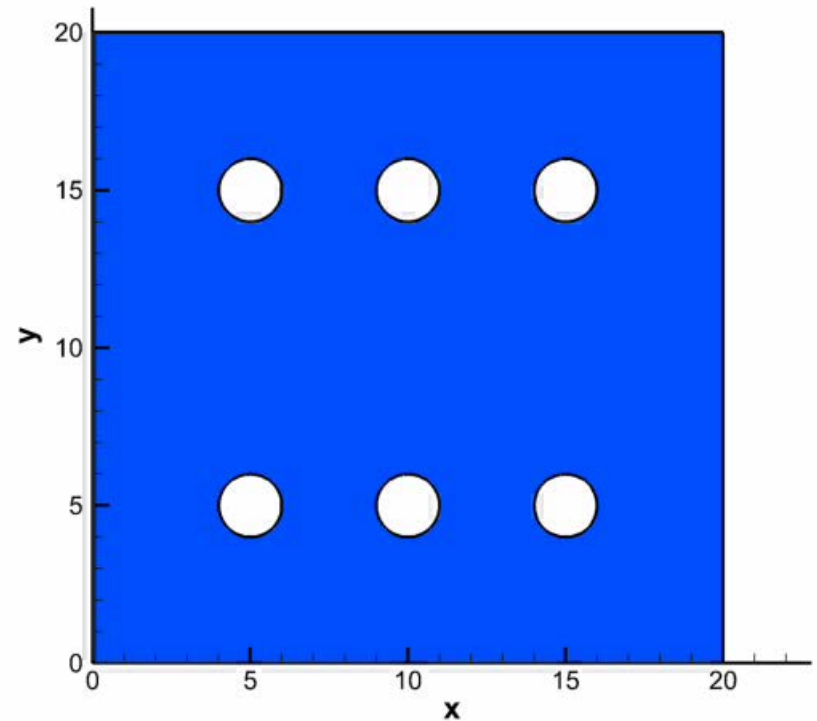


ALE, 2D planar, ($Re = 20$)

Multiple particle-bubble interaction (2D planar)

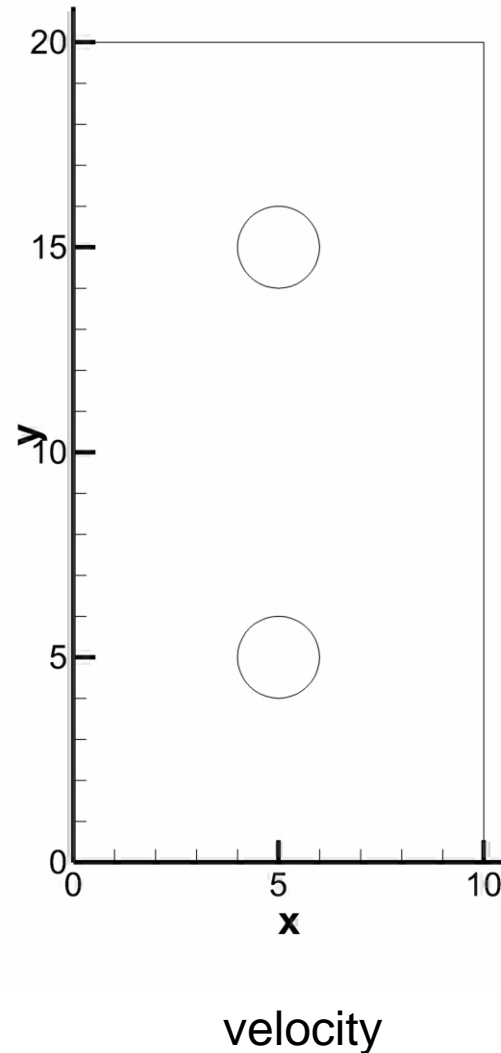
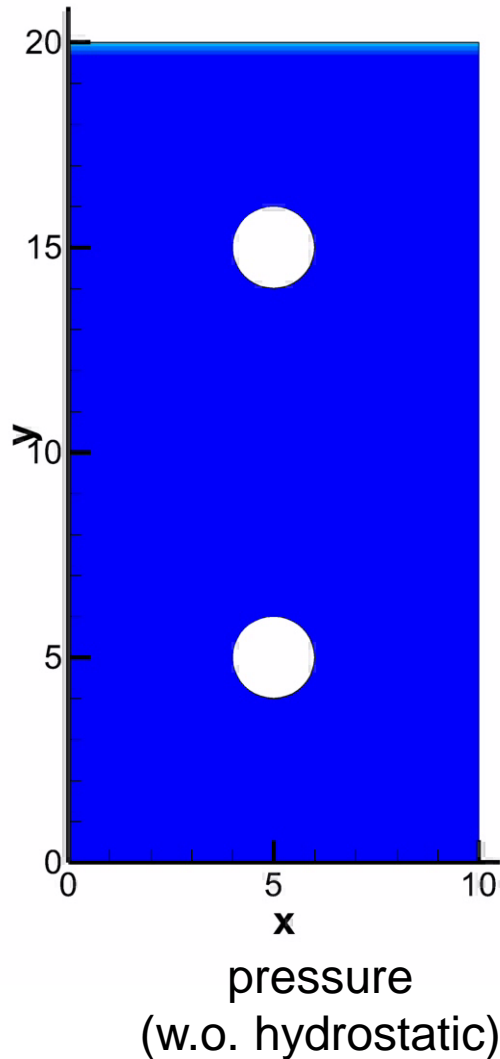


Mesh



pressure

Head-on collision



Input:

$$\rho_p = 2, \rho = 1$$

$$g_y = -1, \mu = 1$$

$$r_p = r_b = 1$$

$$\sigma = 1$$

Output:

$$V \approx 0.25$$

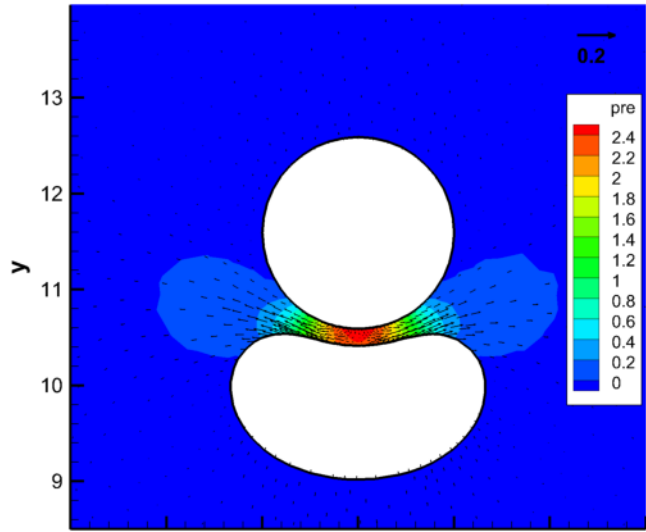
$$\text{Re} = \frac{\rho V r}{\mu} \approx 0.25$$

$$\text{Ca} = \frac{\mu V}{\gamma} \approx 0.25$$

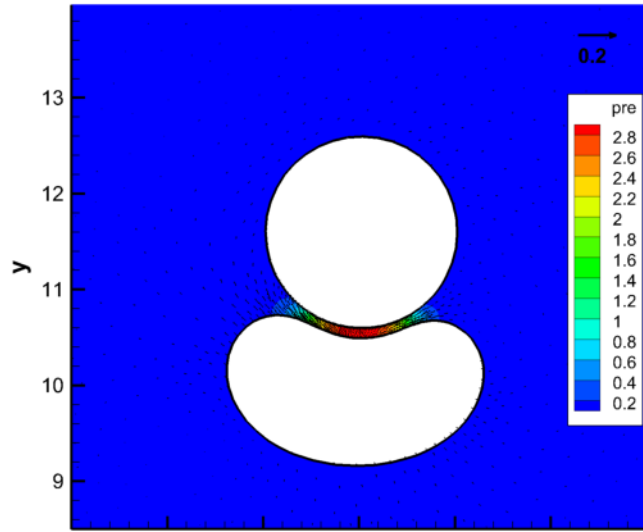
$$\text{Bo} = \frac{\rho g r^2}{\gamma} = 1$$

Pressure & velocity

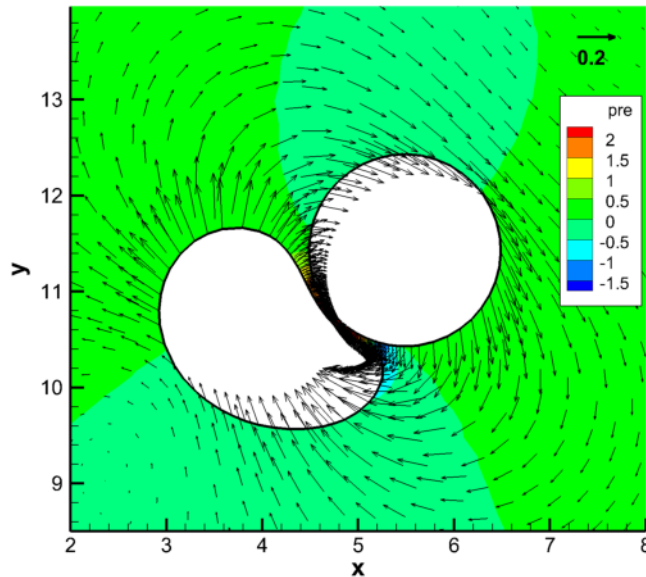
t=23.48



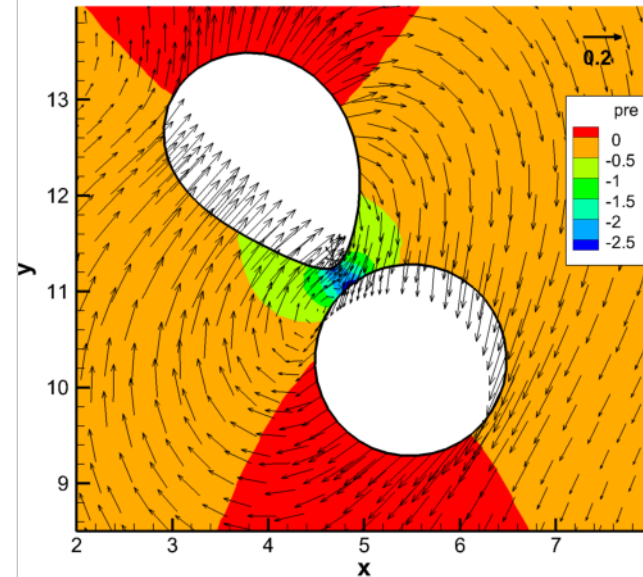
t=33.48



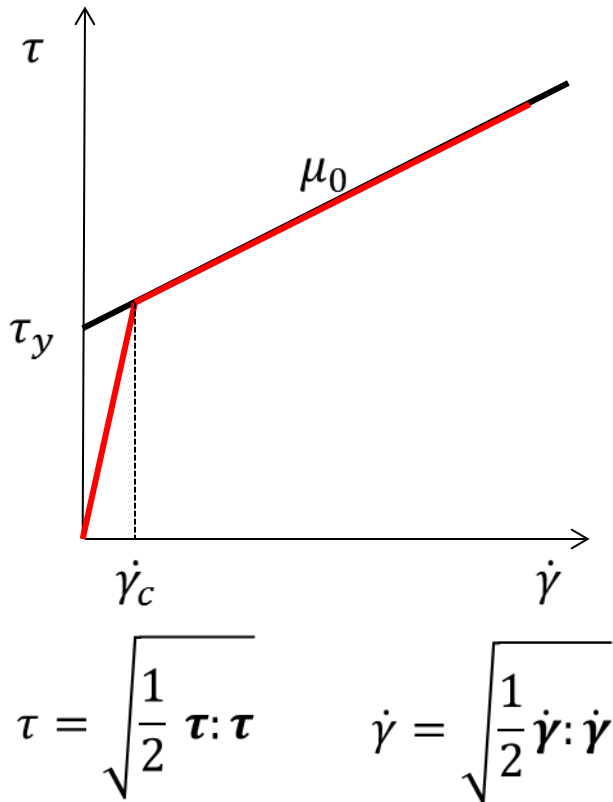
t=43.46



t=49.72



Bingham fluid



$$\dot{\boldsymbol{\gamma}} = \nabla \mathbf{u} + \nabla \mathbf{u}^T$$

Bingham model

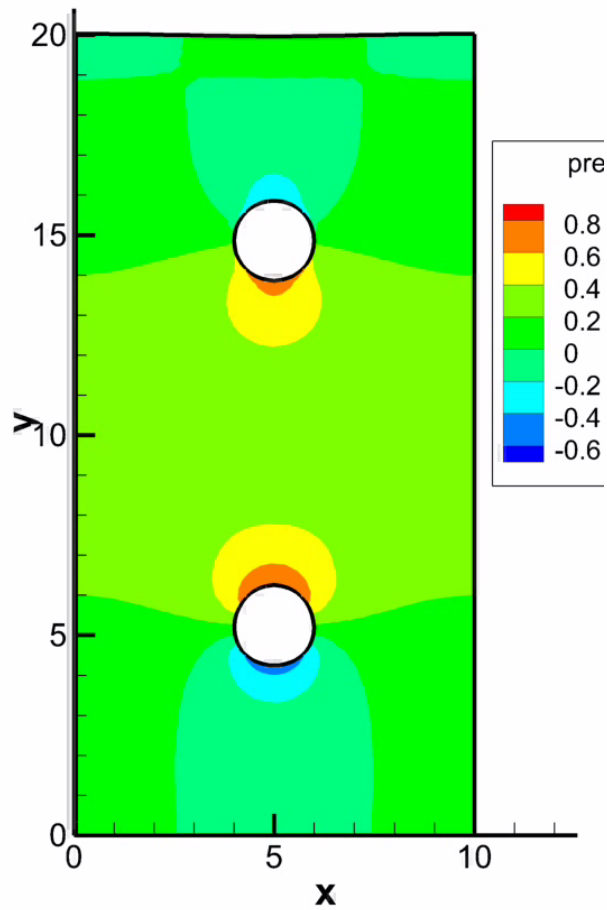
$$\begin{cases} \dot{\boldsymbol{\gamma}} = 0, & \tau \leq \tau_y \\ \tau = \tau_y + \mu_0 \dot{\boldsymbol{\gamma}}, & \tau > \tau_y \end{cases}$$

A simple regularization

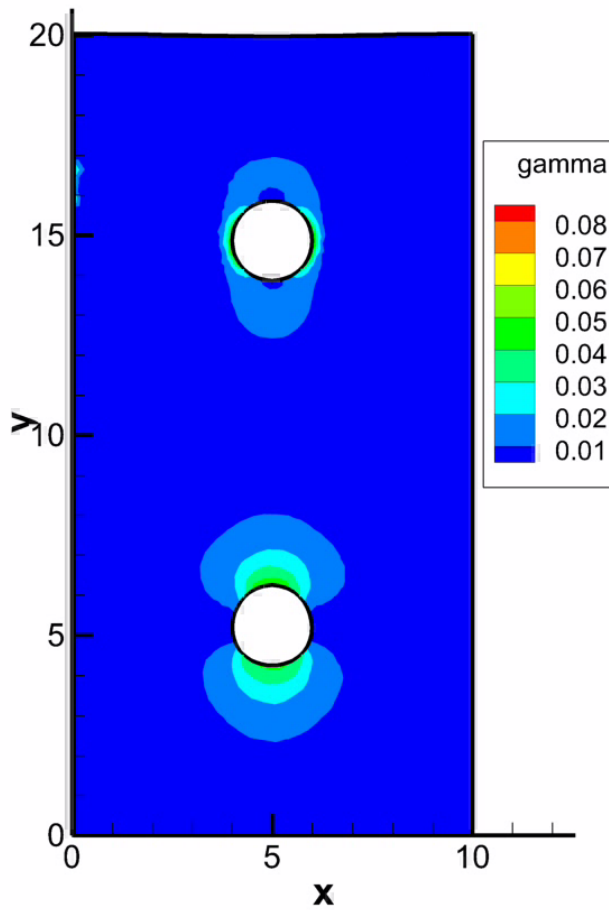


$$\mu(\dot{\boldsymbol{\gamma}}) = \begin{cases} \mu_0 + \frac{\tau_y}{\dot{\gamma}_c \left(2 - \frac{\dot{\boldsymbol{\gamma}}}{\dot{\gamma}_c}\right)}, & \dot{\boldsymbol{\gamma}} \leq \dot{\gamma}_c \\ \mu_0 + \frac{\tau_y}{\dot{\boldsymbol{\gamma}}}, & \dot{\boldsymbol{\gamma}} > \dot{\gamma}_c \end{cases}$$

$$\boldsymbol{\tau} = \mu \dot{\boldsymbol{\gamma}}$$



pressure



Rate-of-strain

$$\tau_y = 0.1$$

$$\dot{\gamma}_c = 0.01$$

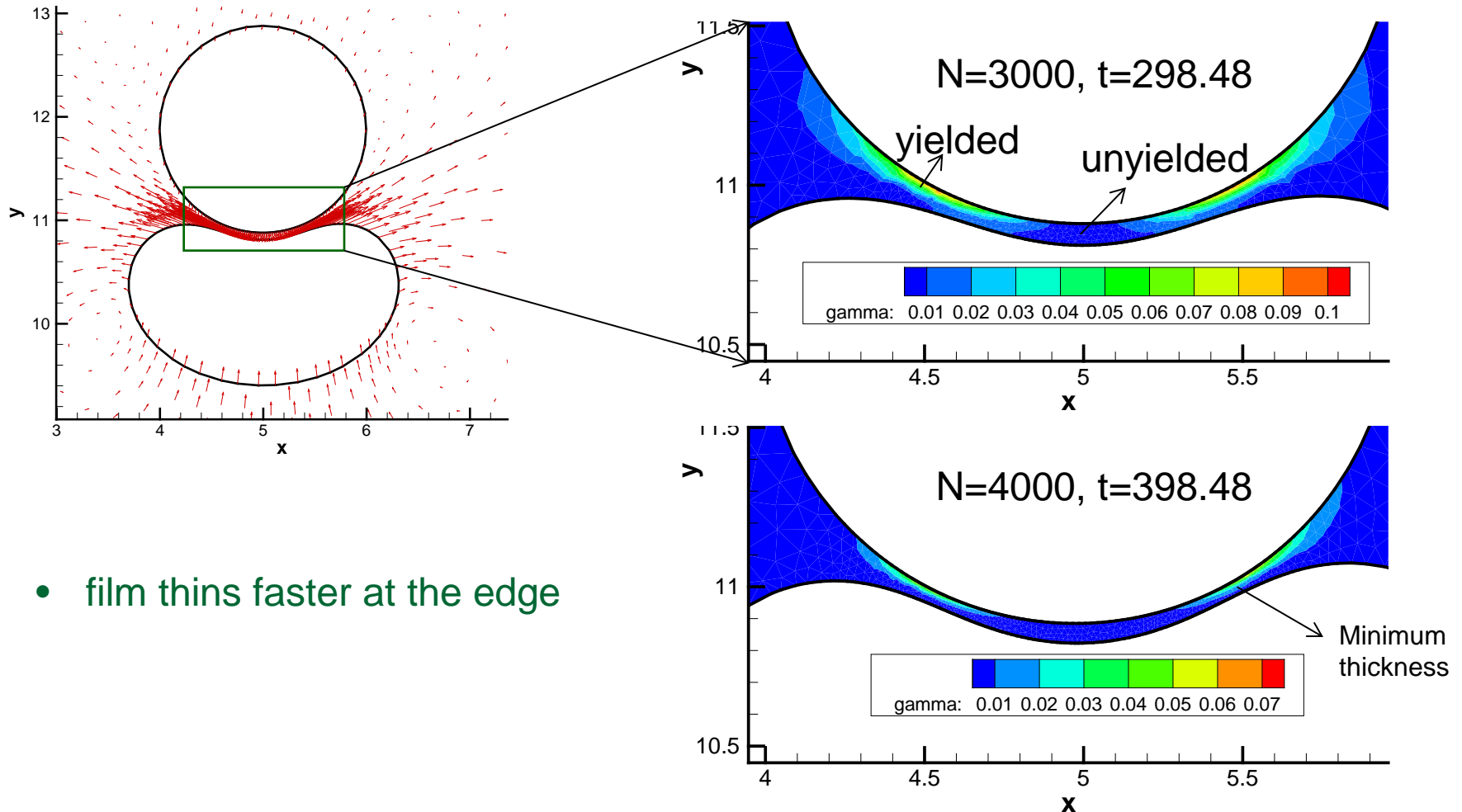
Yielded region:
 $\dot{\gamma} \geq 0.01$

Bingham number:

$$Bn = \frac{\tau_y R}{\mu_0 V} \sim O(1)$$

- Longer contact time due to unyielded region

Film drainage in Bingham fluid



- film thins faster at the edge

Summary

■ Advantages of ALE

- Accurate tracking of moving boundaries
- Easy incorporation of matching conditions on moving boundaries

■ Disadvantages

- Topological transition of moving boundaries
- 3D bubble surface mesh generation and adaptation

■ An optimal direction

- Hybrid ALE-interface capturing method

Thank you!