Ternary Conservative Phase-field Lattice Boltzmann Method and Its Applications

LBM Working Group Meeting
Institute of Henri Poincare

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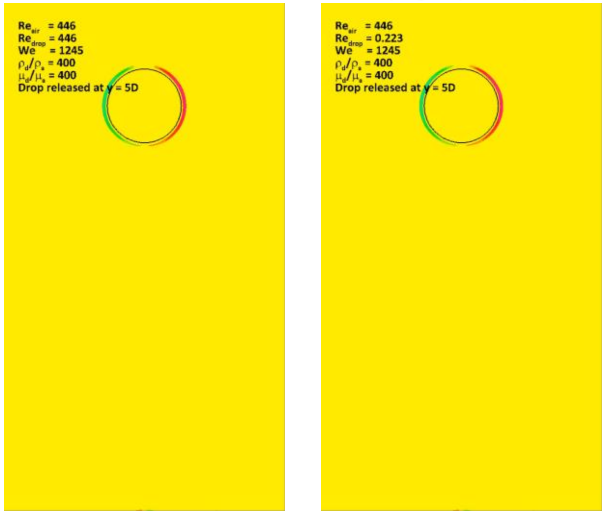
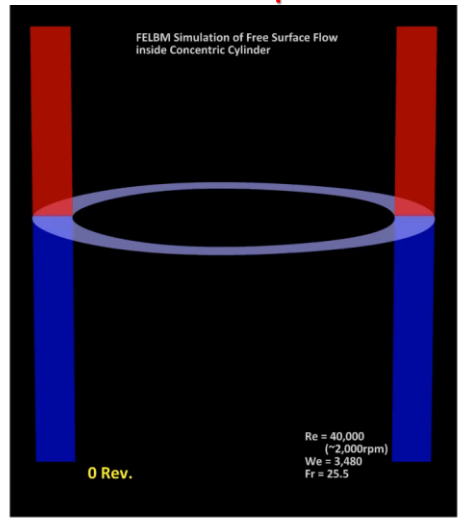
Multi-phase Flow Simulations with LBM

Less viscous (left) and viscous (right) drop impact



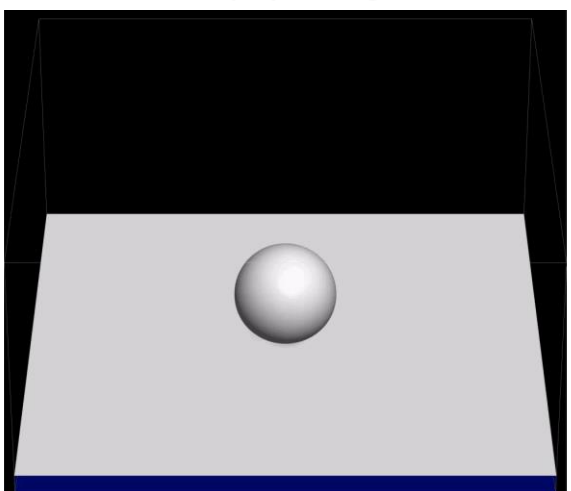
Irmgard, Ray, Morris, Lee, & Nagel, *Soft Matter* 2016

Unstructured two-phase LBM



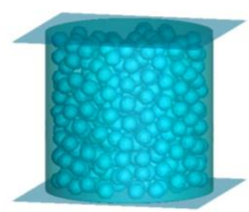
Wardle & Lee, *Comp Math Appl* 2013

Drop Splashing



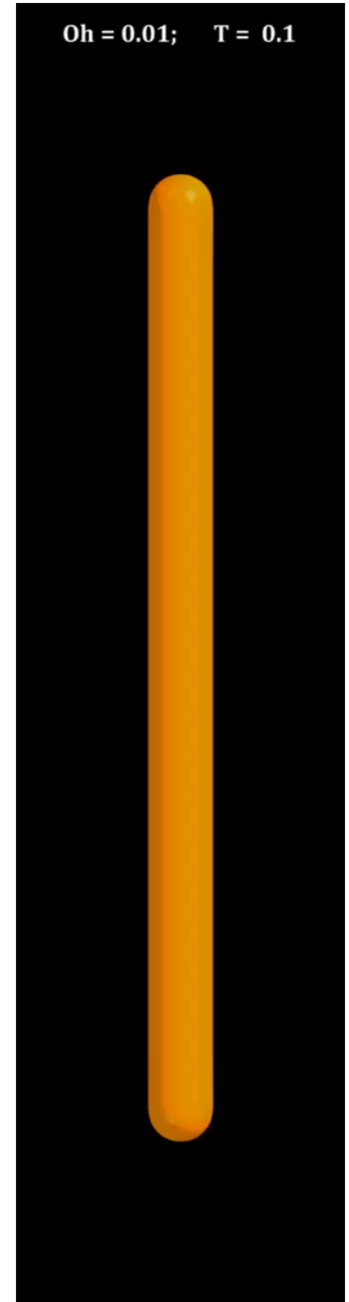
Lee, in preparation

Liquid bridge break-up



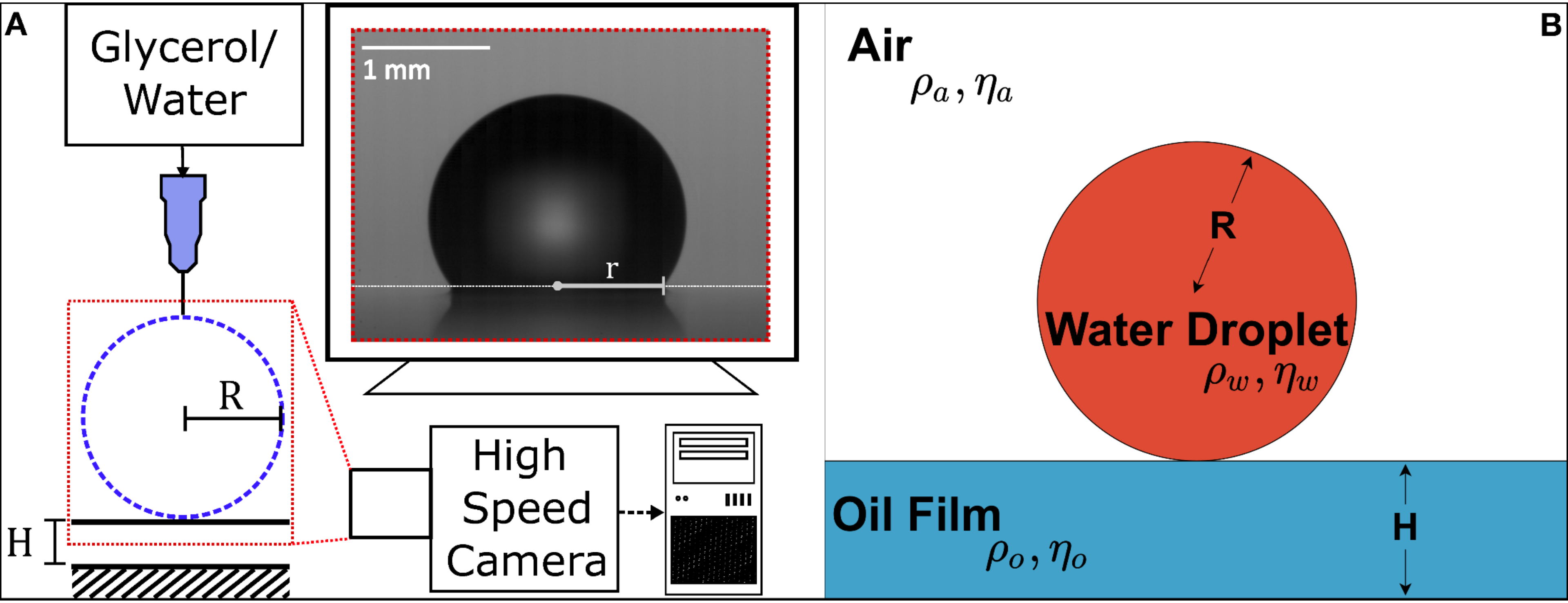
Connington, Miskin, Lee, Morris, Jaeger, IJMF 2015

Breakup of liquid filament



Lee, in preparation

Engulfment of a Drop on Solids Coated by a Film



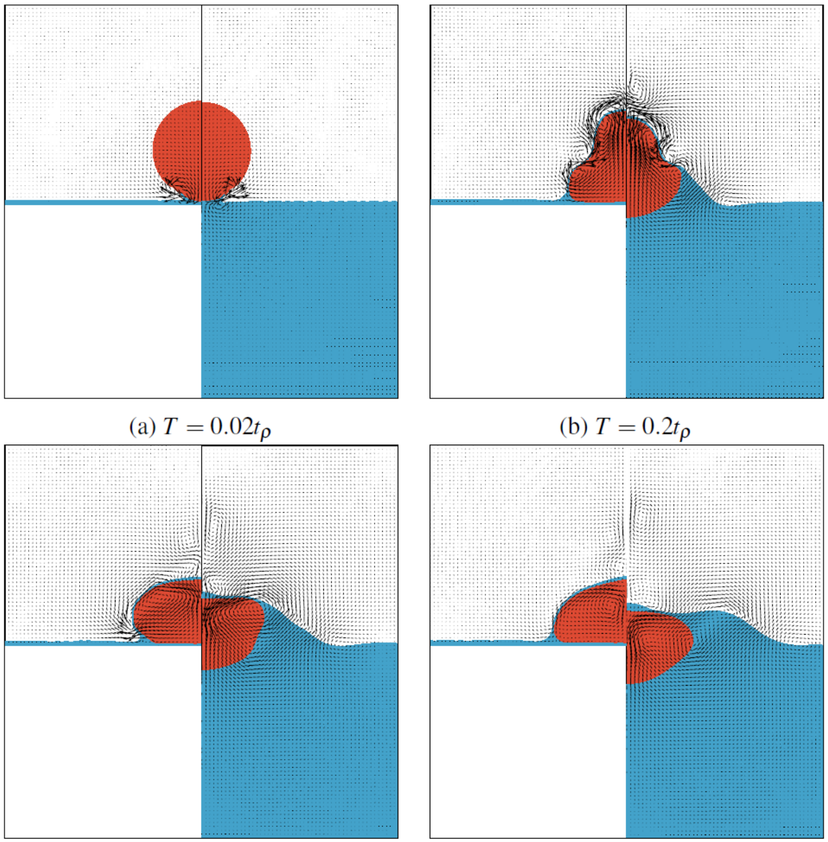
(A) Experimental setup. Water/glycerol pendant drops of radius R~1 mm and viscosity $\eta_w = [0.035 - 0.154] Pa \cdot s$ are brought into contact with a silicone oil film of height H and viscosity $\eta_o = [0.33 - 1.54] Pa \cdot s$. Viscosity ratios are held at 1:10.

(B) Initialization of the droplet spreading simulation.

Note: The dynamics of droplets coalescing with solids coated with a very thin oil film H/R<<1 can be characterized by an inertial time scale $t_\rho = \sqrt{\frac{\rho R^3}{\sigma_{ao}}}$ for Oh<<1 and by a viscous time scale $t_\eta = \frac{\eta_o R}{\sigma_{ao}}$ for Oh>>1 (Carlson 2013), where $Oh = \frac{\eta_o}{\sqrt{\rho_o \sigma_{wo} R}}$.

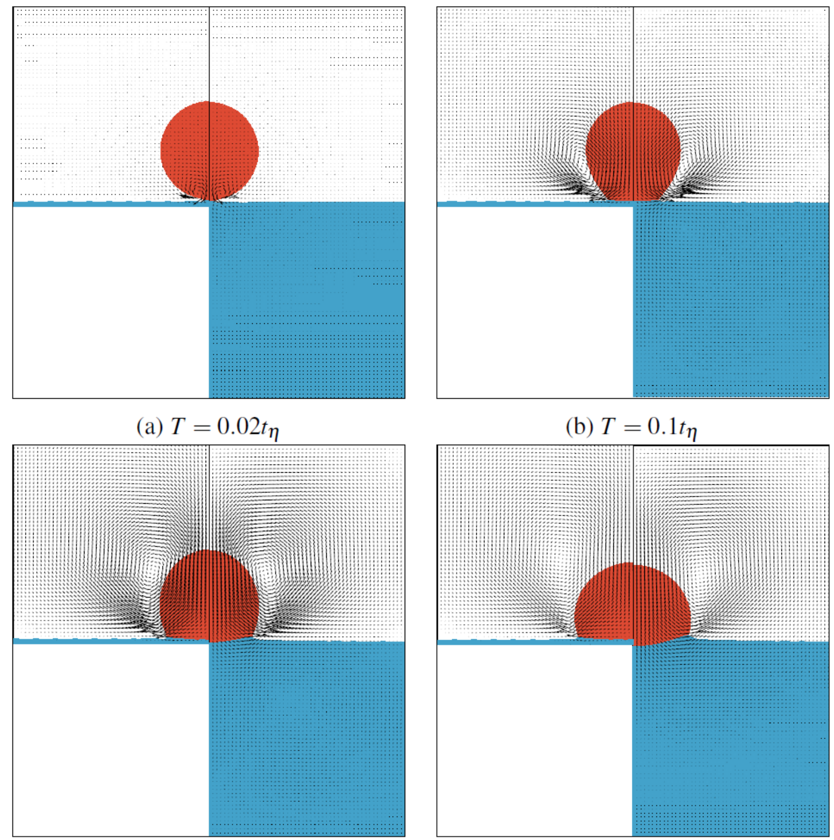
(**Zhao**, Kern, Carlson, and Lee, in preparation)

Engulfment of a Drop on Solids Coated by a Film



(a) $T = 0.02t_\rho$ (b) $T = 0.2t_\rho$ (c) $T = 0.3t_\rho$ (d) $T = 0.4t_\rho$

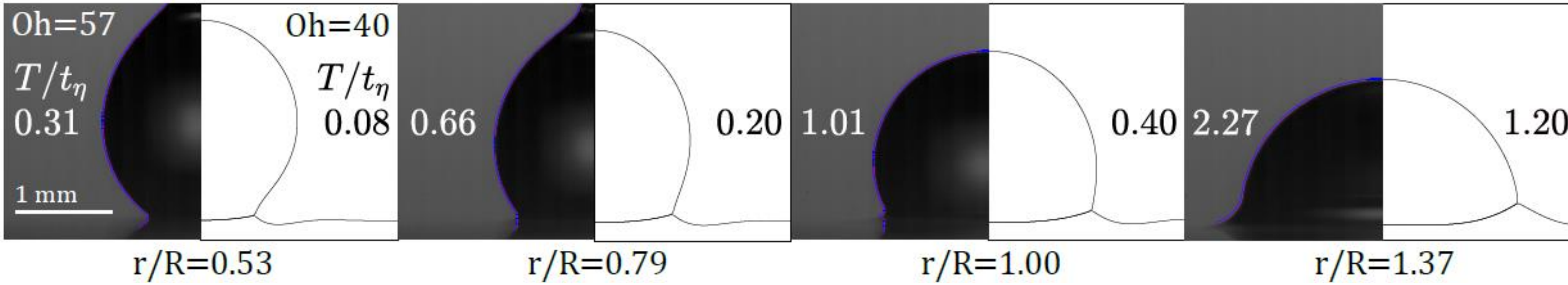
Droplet dynamics on a thin oil film H/R=0.1 and a thick film H/R=4 for Oh=0.07.



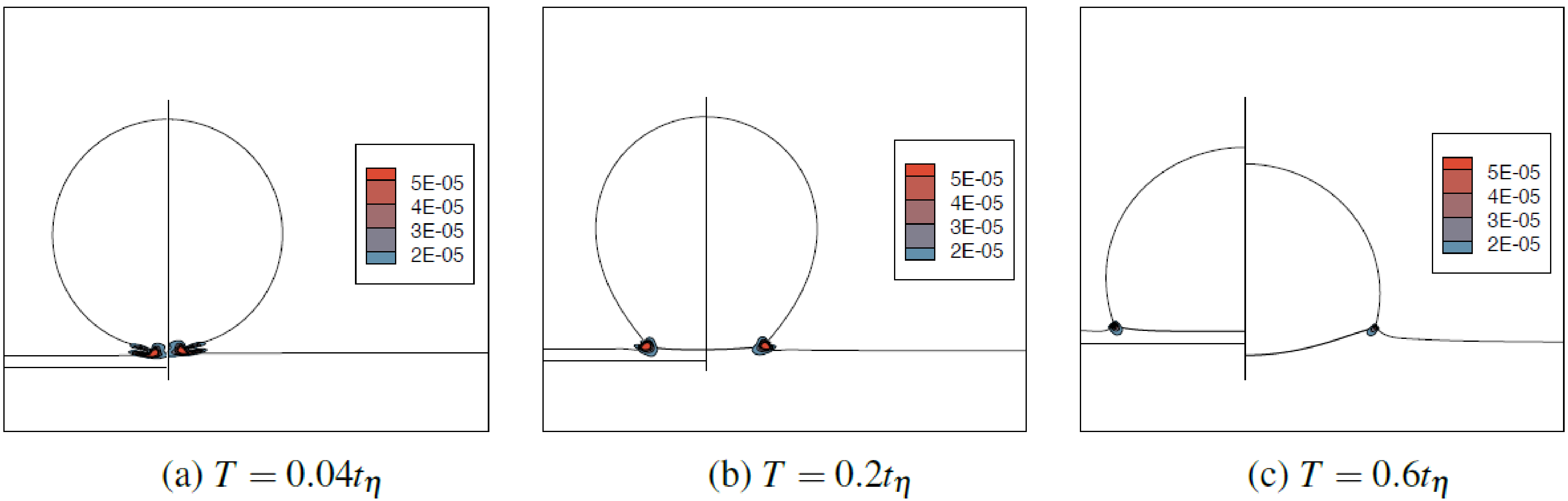
(a) $T = 0.02t_\eta$ (b) $T = 0.1t_\eta$ (c) $T = 0.2t_\eta$ (d) $T = 0.8t_\eta$

Droplet dynamics on a thin oil film H/R=0.1 and a thick film H/R=4 for Oh=5.2.

Engulfment of a Drop on Solids Coated by a Film



Comparison between the simulation and the experiment for H/R=0.2. Simulation: Oh=40. Experiment: Oh=57.



Contour plot of the viscous dissipation of a thin film H/R=0.1 and a thick film H/R=4 for Oh=5.27.

- Model equation: External intermolecular force based single-component two-phase flow model (He et al. 1998 PRE; Lee and Fischer 2006 PRE) and incompressible binary two-phase flow model (He et al. 1999 JCP; Lee and Liu 2010 JCP)

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha = -\frac{1}{\lambda}\left(f_\alpha - f_\alpha^{eq}\right) + \frac{(\boldsymbol{e}_\alpha - \boldsymbol{u}) \cdot \boldsymbol{F}}{\rho c_s^2} f_\alpha^{eq}$$

- External force based model vs. equilibrium free energy model (Wagner & Qi 2006 Physica A) ; External force based model & S-C model (He et al. 1998 PRE): They can be shown equivalent

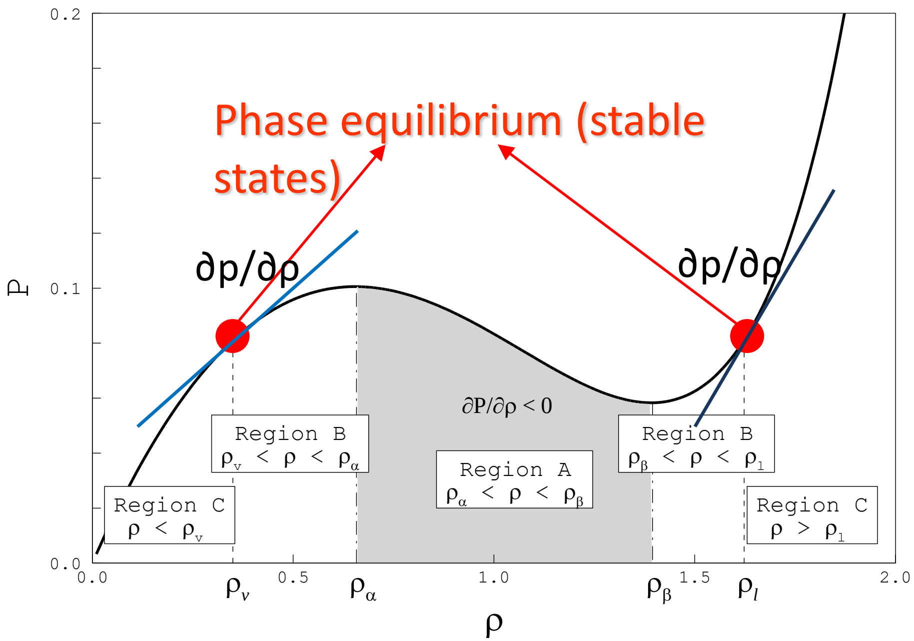
- Other (early) stable models: single-component two-phase flow model (Yuan & Schaefer 2006 PF) and incompressible binary two-phase flow model (Inamuro et al. 2004 JCP; Zheng et al. 2006 JCP)

- Non phase-field model (sharp interface model): Front-tracking LBM (Lallemand 2007 JCP), VOF LBM (Thurey et al. Proc. Vision Mod Visualization 2006) → simpler physics and generally more stable but not necessarily more accurate

Bulk density may fluctuate around equilibrium value

- Momentum equation for non-ideal gas: $\boldsymbol{F} = \nabla \rho c_s^2 - \nabla p_0 + \rho\kappa\nabla\nabla^2\rho$

$$\Rightarrow \rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) = -\underbrace{\nabla p_0}_{crucial\ to\ phase\ separtion} + \underbrace{\rho\kappa\nabla\nabla^2\rho}_{surface\ tension} + \nabla\cdot\Pi$$



P-*ρ* isotherm for van der Waals equation of state

- Region A ($\partial p/\partial \rho<0$) is mechanically unstable

  $\rightarrow$ phase separation

- Speed of sound becomes larger for lower temperature (i.e., larger density ratio)

$$c_s^2 = \frac{\partial p_0}{\partial \rho}$$

Introducing More Terms

- Model equation:

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha = -\frac{1}{\lambda}\left(f_\alpha - f_\alpha^{eq}\right) + \underbrace{\frac{(\boldsymbol{e}_\alpha - \boldsymbol{u}_\alpha)\cdot \boldsymbol{F}}{\rho c_s^2} f_\alpha^{eq}}_{\sim t_\alpha\left(\frac{\boldsymbol{e}_\alpha}{c_s^2} + \frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4}\right)\cdot \boldsymbol{F}}$$

Guo et al. 2002

- Recovered Governing Equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla \rho c_s^2 + \underbrace{\boldsymbol{F}}_{\nabla \rho c_s^2 - \nabla p_0 + \rho\kappa\nabla\nabla^2\rho} + \nabla \cdot \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$$

- Enforcing incompressibility typically requires certain transformation to introduce $-\nabla p^{dynamic}$
- Additional LB equation for passive scalar with the velocity from $\boldsymbol{u} = \frac{1}{\rho}\sum \boldsymbol{e}_\alpha f_\alpha$ and $\rho = \sum h_\alpha$

$$\frac{\partial h_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla h_\alpha = -\frac{1}{\lambda}\left(h_\alpha - h_\alpha^{eq}\right) + \frac{(\boldsymbol{e}_\alpha - \boldsymbol{u}_\alpha)\cdot \boldsymbol{G}}{\rho c_s^2} f_\alpha^{eq}$$

- Recovered scalar transport equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = \nabla \cdot \lambda c_s^2 (\boldsymbol{G} - \boldsymbol{F})$$

- SC force: $\boldsymbol{F} = -g\psi(\boldsymbol{x})\sum_\alpha \psi(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t)\boldsymbol{e}_\alpha = -\nabla\left(\frac{3g c_s^2 \delta_t \psi^2}{2}\right) - \frac{3g c_s^4 \delta_t^3}{8}\psi\nabla\nabla^2\psi$ He et al. PRE 1997

Equilibrium Profile

- Free energy functional: $\Psi = \int \left(E_0 + \frac{\kappa}{2} |\nabla \rho|^2 \right) dV - \int_S \ \rho_s \phi \, dS$

$$E_0 \approx \beta \left(\rho - \rho_{liq}^{sat}\right)^2 \left(\rho - \rho_{vap}^{sat}\right)^2 \qquad \left(\mu_0 = \frac{\partial E_0}{\partial \rho}, p_0 = \rho \frac{\partial E_0}{\partial \rho} - E_0 \right)$$

- In plane interface, density profile (D being interface thickness) is determined such that the energy is minimized ($\mu = \mu_0 - \kappa \nabla^2 \rho$) (Lee and Lin, JCP 2005)

$$\rho(z) = \frac{\rho_{liq}^{sat} + \rho_{vap}^{sat}}{2} + \frac{\rho_{liq}^{sat} - \rho_{vap}^{sat}}{2} \tanh\left(\frac{2z}{D}\right)$$

- Surface tension:

$$\sigma = \frac{\left(\rho_{liq}^{sat} - \rho_{vap}^{sat}\right)^3}{6} \sqrt{2\kappa\beta}, \qquad \kappa = \frac{\beta D^2 \left(\rho_{liq}^{sat} - \rho_{vap}^{sat}\right)^2}{8}$$

- Boundary condition: $\kappa \frac{\partial \rho}{\partial \boldsymbol{n}} = -\phi, \qquad \frac{\partial \mu}{\partial \boldsymbol{n}} = 0$

$$\Omega = \frac{4\phi}{\left(\rho_{liq}^{sat} - \rho_{vap}^{sat}\right)^2 \sqrt{2\kappa\beta}} \text{ (Dimensionless wetting potential)}$$

$$\cos\theta_w = \frac{(1+\Omega)^{3/2} - (1-\Omega)^{3/2}}{2} \text{ (Equilibrium contact angle)}$$

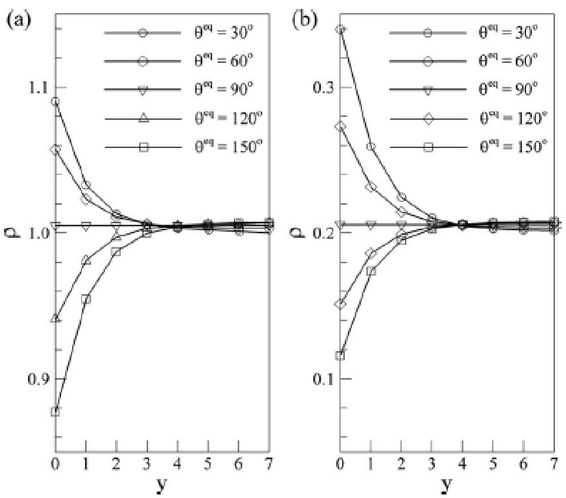


Fig. 1: Density profile in the normal direction to wall (a) liquid (b) vapor

LBM as Phase Field/Diffuse Interface Approach

- Pressure tensor and/or chemical potential are defined such that the system will *phase separate below the critical temperature*
- Interfaces and their associated dynamics will be a natural feature of the simulation
- Ability to handle tortuous interface geometries without having to resort to *interface-tracking schemes* (weakness: necessity for interface to have finite width)
- When exploring systems on a mesoscopic scale it is very reasonable that finite width of a thermodynamic interface is explicitly apparent in the simulation → vital in controlling the dynamics of moving contact line or phase ordering of a fluid
- Stable NS diffuse interface approach is also new (Ding et al. 2007 JCP)

Is LBM Particularly more unstable?

- Phase-field LBM appears to be more stable than NS version of phase-field approach (PF-NS is generally less stable than Level set, FT or VOF-NS)
- Forcing terms are stiff!
  1 – Large density gradient $\boldsymbol{F} = \nabla \rho c_s^2 - \nabla p_0 + \rho\kappa\nabla\nabla^2\rho$
  – Stiff equation of state $\boldsymbol{F} = \nabla \rho c_s^2 - \nabla p_0 + \rho\kappa\nabla\nabla^2\rho$
  – Large surface tension force $\boldsymbol{F} = \nabla \rho c_s^2 - \nabla p_0 + \rho\kappa\nabla\nabla^2\rho$
- Larger speed of sound at large density ratio → sharper interface
- Discretization: Upwind biased vs. Central schemes
- Spurious currents (parasitic currents) → not clear

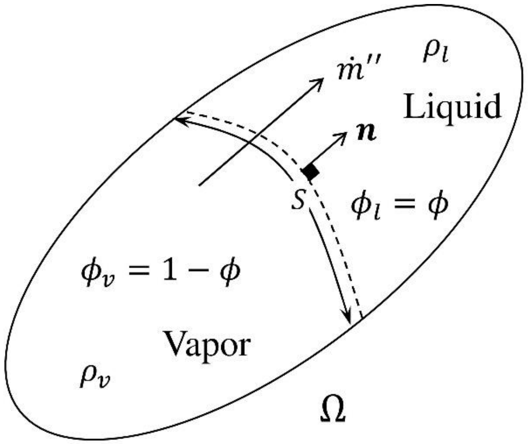
Incompressible Navier-Stokes Equations

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

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

Interface Tracking Equations

$$\frac{\partial\rho}{\partial t} + \boldsymbol{u}\cdot\nabla\rho = \rho\nabla\cdot\boldsymbol{u} \xrightarrow{\nabla\cdot\boldsymbol{u}=0} \frac{\partial\rho}{\partial t} + \boldsymbol{u}\cdot\nabla\rho = 0$$



or define **volume fraction $\boldsymbol{\phi}$** s.t. $\rho = \phi\rho_l + (1-\phi)\,\rho_v$

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

or define **level set function $\boldsymbol{\psi}$** s.t. $|\nabla\psi| = 1$

$$\frac{\partial\psi}{\partial t} + \boldsymbol{u}\cdot\nabla\psi = 0$$

Notes: Local mass conservation and calculation of surface tension

- Due to dispersion and dissipation errors interface tends to oscillate and smear
- VOF: Interface reconstruction is required
- Level set: Reinitialization step is required (Abadie, Aubin, Legendre, *JCP* 2015)

Level-Set Equation

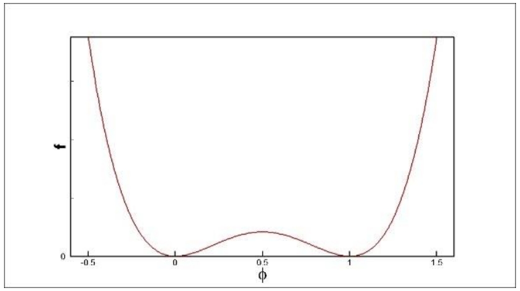
$$\frac{\partial \psi}{\partial t} + \boldsymbol{u} \cdot \nabla \psi = 0 \xrightarrow{Reinitialization} \frac{\partial \psi}{\partial \tau} + s(\psi_0)(|\nabla \psi| - 1) = 0 \overset{S.S.}{\longrightarrow} s(\psi_0)(|\nabla \psi| - 1) = 0$$

at steady state: $|\nabla \psi| = 1$

Note: Interface can shift during reinitialization → Mass conservation problem

Phase Field Equations (Allen-Cahn and Cahn-Hilliard)

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = -M \underbrace{\mu}_{\substack{chemical \\ potential}} = -M \left(\frac{\partial f}{\partial \phi} - \nabla^2 \phi \right)$$

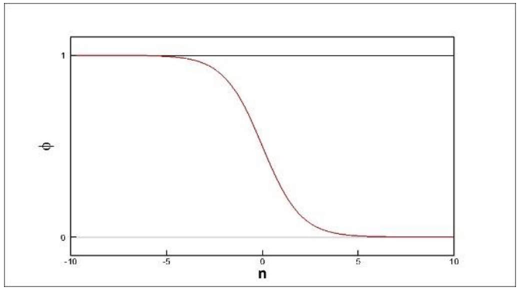


known as **Allen-Cahn** equation.

Notes:

- Pattern formation processes (e.g., solidification)
- Non-conservative due to curvature driven interface

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

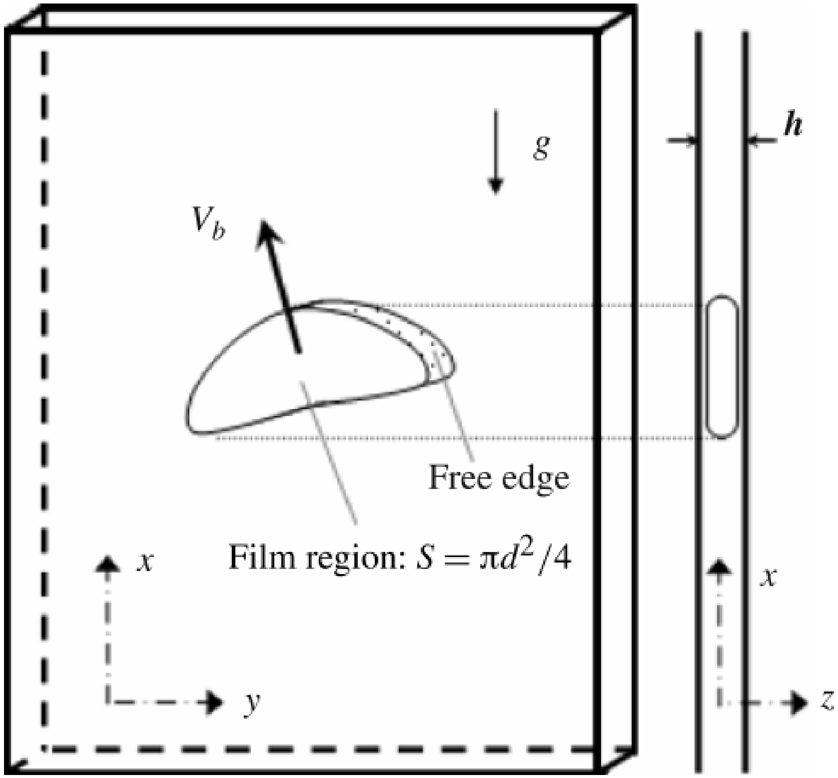


known as **Cahn-Hilliard** equation.

Notes:

- Non-linear high-order spatial derivatives
- Globally conservative but loses mass when curvature is large → $r_c = \left(\frac{\sqrt{3}}{16\pi} DV \right)^{1/3}$

Benchmark I: Bubble Rising within a Thin Gap



- Few numerical simulation of unsteady bubble motion have been performed at high *Reynolds* number
- Detailed study of path oscillations, shape oscillations, and unsteady wake dynamics of high Re bubble flow ($O(10^2) \sim O(10^4)$)
- Dimensionless numbers

$$Bo = \frac{g \Delta\rho d^2}{\sigma}$$

$$Ar = \frac{\sqrt{gd}d}{\nu}$$

$$Re = \frac{\rho_l U_t d}{\eta_l}$$

where g : gravity

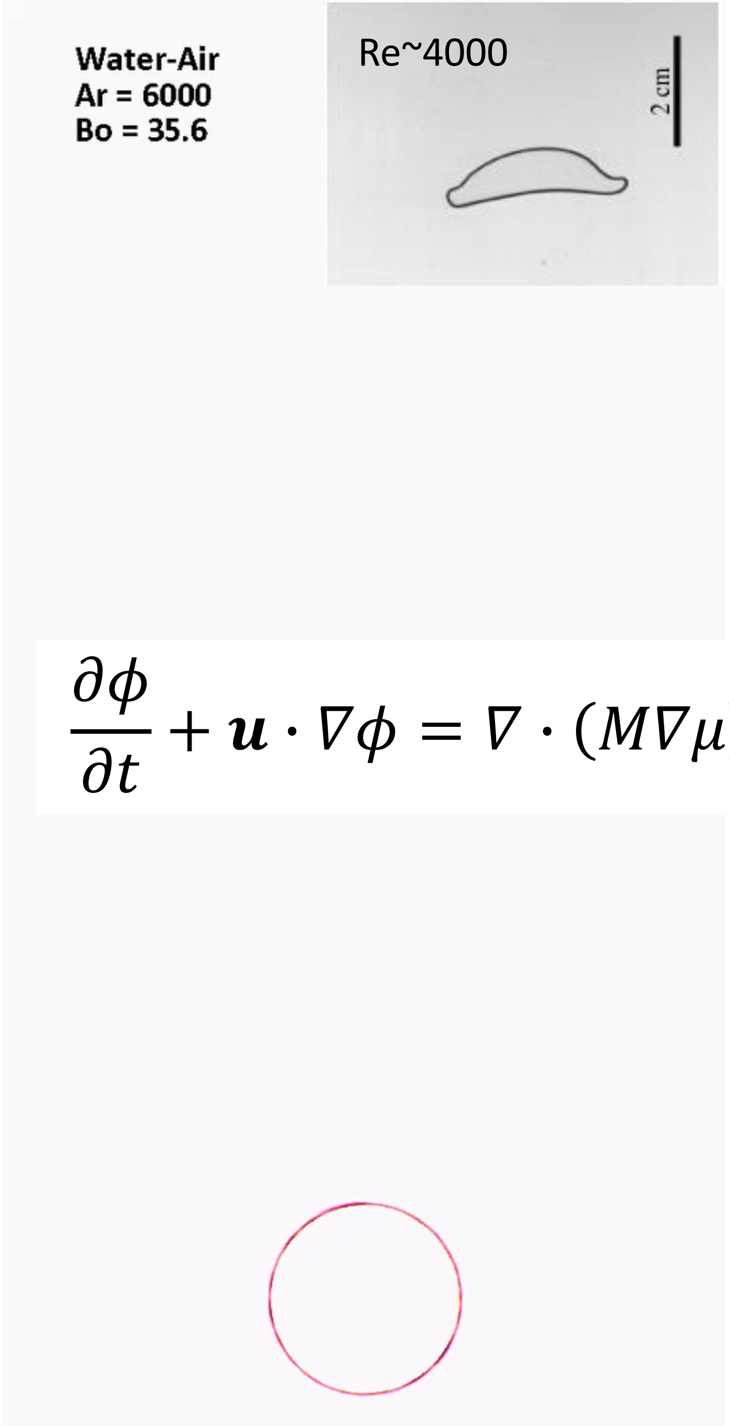
$\Delta\rho$: density difference

σ : surface tension

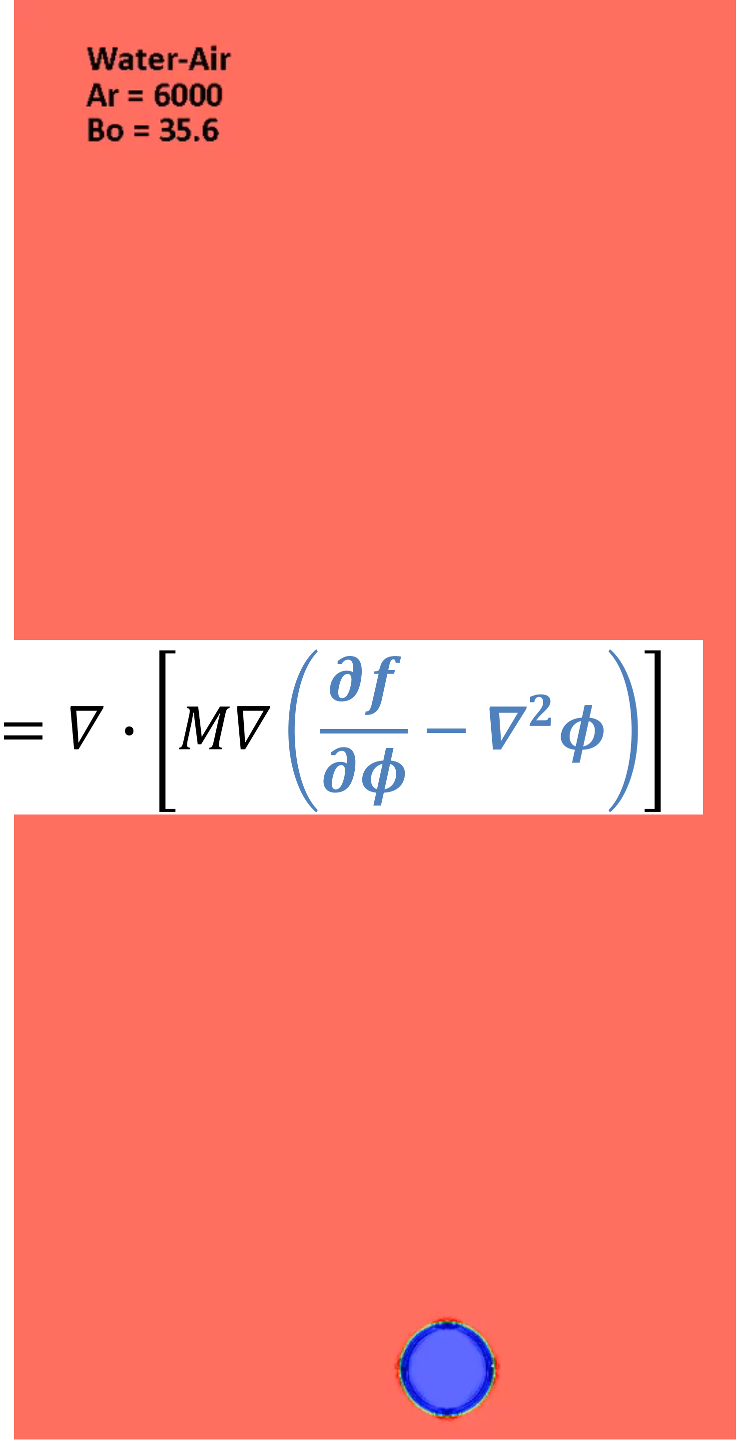
d : bubble diameter

η_l : liquid viscosity

V_t : terminal velocity



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



Hyperbolic Tangent Equilibrium Profile (Chiu & Lin, JCP 2011)

$$\boldsymbol{n} = \frac{\nabla\phi}{|\nabla\phi|}, \qquad \kappa = \nabla\cdot\boldsymbol{n} = \nabla\cdot\frac{\nabla\phi}{|\nabla\phi|}, \qquad \phi = \frac{1}{2}\left[1+\tanh\left(\frac{x}{2\epsilon}\right)\right]$$

$$\frac{\partial\phi}{\partial\boldsymbol{n}} = |\nabla\phi| = \frac{\phi(1-\phi)}{\epsilon}, \qquad \frac{\partial^2\phi}{\partial\boldsymbol{n}^2} = \frac{(\nabla\phi\cdot\nabla)|\nabla\phi|}{|\nabla\phi|} = \frac{\partial f}{\partial\phi} = \frac{\phi(1-\phi)(1-2\phi)}{\epsilon^2}$$

Conservative Phase Field Equation without Curvature Contribution

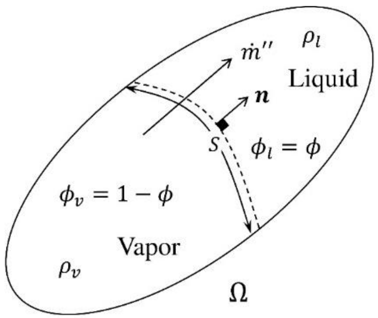
$$\frac{\partial\phi}{\partial t} + \boldsymbol{u}\cdot\nabla\phi = M\left(\nabla^2\phi - \frac{\partial f}{\partial\phi} - |\nabla\phi|\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|}\right) = M\left(\nabla^2\phi - \frac{\partial f}{\partial\phi} - |\nabla\phi|\kappa\right)$$

$$= M\left(\nabla^2\phi - \frac{(\nabla\phi\cdot\nabla)|\nabla\phi|}{|\nabla\phi|} - |\nabla\phi|\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|}\right)$$

$$= M\left(\nabla^2\phi - \frac{\nabla\phi}{|\nabla\phi|}\cdot\nabla\left[\frac{\phi(1-\phi)}{\epsilon}\right] - \frac{\phi(1-\phi)}{\epsilon}\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|}\right)$$

$$= M\nabla\cdot\left(1 - \left[\frac{\phi(1-\phi)}{\epsilon}\right]\frac{1}{|\nabla\phi|}\right)\nabla\phi$$

$$= \frac{4}{\delta}\frac{\nabla\phi_i}{|\nabla\phi_i|}\phi_i(1-\phi_i) - \frac{\phi_i^2}{\sum_{j=1}^{3}\phi_j^2}\sum_{j=1}^{3}\frac{4}{\delta}\frac{\nabla\phi_j}{|\nabla\phi_j|}\phi_j(1-\phi_j)$$



Issues:

- Division by zero ($1/|\nabla\phi|$) possible; could be unstable PDE
- Tend to fragmentize continuous interfaces into droplets and bubbles

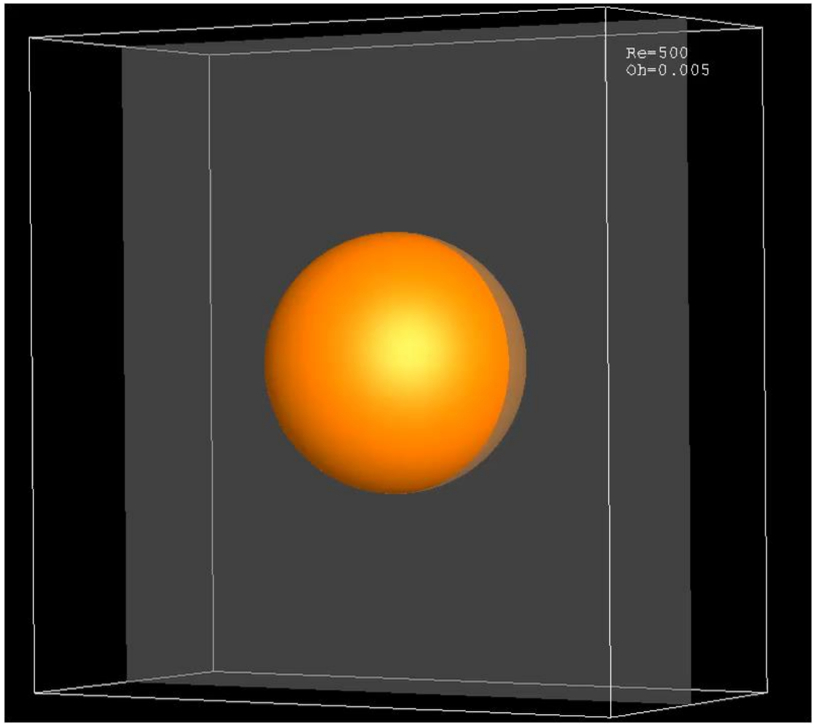
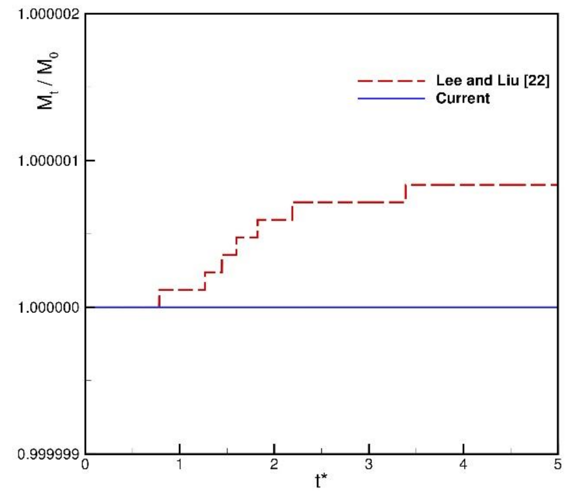


Fig 1: Droplet under Kolmogorov forcing on 128^3 grid



Variation of mass of the system for rising bubble.

Navier-Stokes Equations with Non-ideal Gas EOS

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

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

$$\boldsymbol{F} = \underbrace{\nabla \rho c_s^2}_{\text{Leading order term}} - \rho \nabla (\mu_0 - \kappa \nabla^2 \rho)$$

$$F_\alpha = t_\alpha \left(\frac{\boldsymbol{e}_\alpha}{c_s^2} + \frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u}) \boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4} \right) \cdot \boldsymbol{F}$$

Guo 2002

Lattice Boltzmann (Discrete Boltzmann) Equations

$$\underbrace{\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha}_{Streaming} = \underbrace{-\frac{1}{\lambda} (f_\alpha - f_\alpha^{eq})}_{Collision} + \underbrace{F_\alpha}_{External\ Force}$$

f_α : Particle distribution function ($\sum_\alpha f_\alpha = \rho; \sum_\alpha \boldsymbol{e}_\alpha f_\alpha = \rho \boldsymbol{u}$)

$\boldsymbol{e}_\alpha$: Microscopic particle velocity, e.g. in D2Q9 model

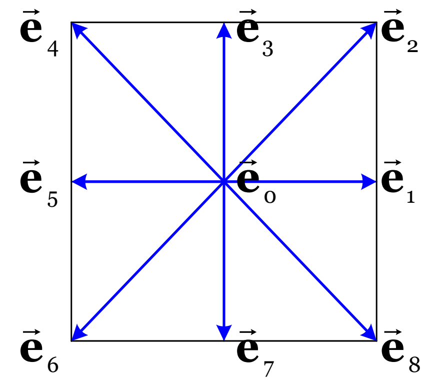
$(e_0 = (0,0);\ e_1 = (1,0); e_2 = (1,1); \ldots; e_8 = (1,-1))$

f_α^{eq}: Equilibrium distribution function

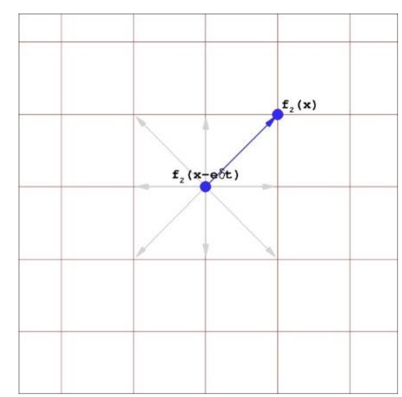
$$f_\alpha^{eq} = t_\alpha \rho \left(1 + \frac{\boldsymbol{e}_\alpha \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{e}_\alpha \boldsymbol{e}_\alpha - c_s^2 \boldsymbol{I}) : \boldsymbol{u}\boldsymbol{u}}{2 c_s^4} \right)$$

λ : Relaxation time ($\eta = \rho \lambda c_s^2$, c_s: speed of sound)

Set of 1st order hyperbolic PDEs with constant advection velocities
(Nonlinearity is considered in f_α^{eq})



9 velocity model (2D)



From DBE to Lattice Boltzmann Equation (LBE): Standard Approach

- Discretize DBE along characteristics over time δt

$$\int_t^{t+\delta t} \left(\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha\right) dt' = -\int_t^{t+\delta t} \frac{1}{\lambda}\left(f_\alpha - f_\alpha^{eq}\right) dt' + \int_t^{t+\delta t} F_\alpha dt'$$

- Applying Crank-Nicolson scheme to integrate RHS

$$f_\alpha(\boldsymbol{x}, t+\delta t) - f_\alpha(\boldsymbol{x} - \boldsymbol{e}_\alpha \delta t, t) = -\left.\frac{f_\alpha - f_\alpha^{eq}}{2\tau}\right|_{(\boldsymbol{x}-\boldsymbol{e}_\alpha\delta t, t)} + \left.\frac{\delta t}{2} F_\alpha\right|_{(\boldsymbol{x}-\boldsymbol{e}_\alpha\delta t, t)} - \left.\frac{f_\alpha - f_\alpha^{eq}}{2\tau}\right|_{(\boldsymbol{x}, t+\delta t)} + \left.\frac{\delta t}{2} F_\alpha\right|_{(\boldsymbol{x}, t+\delta t)}$$

- Introduction of modified particle distribution functions (He et al. 1998)

$$\bar{f}_\alpha = f_\alpha + \frac{f_\alpha - f_\alpha^{eq}}{2\tau} - \frac{\delta t}{2} F_\alpha \qquad \& \qquad \bar{f}_\alpha^{eq} = f_\alpha^{eq} - \frac{\delta t}{2} F_\alpha$$

- LBE

$$\bar{f}_\alpha(\boldsymbol{x}, t+\delta t) - \bar{f}_\alpha(\boldsymbol{x} - \boldsymbol{e}_\alpha \delta t, t) = -\left.\frac{\bar{f}_\alpha - \bar{f}_\alpha^{eq}}{\tau + 1/2}\right|_{(\boldsymbol{x}-\boldsymbol{e}_\alpha\delta t, t)} + \left.\delta t\, F_\alpha\right|_{(\boldsymbol{x}-\boldsymbol{e}_\alpha\delta t, t)}$$

- This equation can be solved in two steps: Collision & Streaming
- Non-local forcing requires particular attention: truncation errors due to time and space discretizations may not be balanced

Strang & Force Splitting

- Strang Splitting: A method to compute f_α^{n+1} from f_α^{n} (Dellar 2013)

$$f_\alpha^{n+1} = C_\lambda^I\left(\frac{\delta t}{2}\right) \circ S_{\boldsymbol{e}_\alpha}(\delta t) \circ C_\lambda^E\left(\frac{\delta t}{2}\right) f_\alpha^n$$

- Here, $C_\lambda^I\left(\frac{\delta t}{2}\right)$ and $C_\lambda^E\left(\frac{\delta t}{2}\right)$ represent numerical operator for following ODE

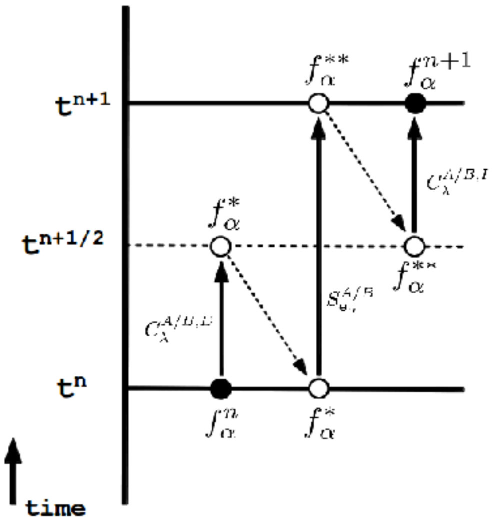
$$\frac{df_\alpha}{dt} = -\frac{f_\alpha - f_\alpha^{eq}}{\lambda} + F_\alpha^{**}$$

  over a half time-step. Superscripts *E* and *I* indicate explicit and implicit Euler time-stepping schemes

- $S_{\boldsymbol{e}_\alpha}(\delta t)$ is numerical operator for

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha = F_\alpha^{*}$$

  over full time-step



- Strang splitting: $F_\alpha = F_\alpha^{*} + F_\alpha^{**}$

Proposed Force Splitting

- $S_{\boldsymbol{e}_\alpha}(\delta t)$: Hyperbolic equation with a source term, which can be fairly stiff

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha = F_\alpha^*$$

- It is desired that F_α^* is close to $\boldsymbol{e}_\alpha \cdot \nabla f_\alpha$ to the leading order, for instance $F_\alpha^* \sim t_\alpha \boldsymbol{e}_\alpha \cdot \nabla \rho c_s^2$, so that their difference is small

- Here we choose the following force splitting (Patel & Lee 2016)

$$F_\alpha^* = t_\alpha \left(\frac{\boldsymbol{e}_\alpha}{c_s^2} \right) \cdot \boldsymbol{F} \quad \text{and} \quad F_\alpha^{**} = t_\alpha \left(\frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4} \right) \cdot \boldsymbol{F}$$

such that

$$\sum\nolimits_\alpha F_\alpha^{**} = 0 \quad \text{and} \quad \sum\nolimits_\alpha \boldsymbol{e}_\alpha F_\alpha^{**} = 0$$

and thus collisions do not change conservative moments

Navier-Stokes Equations with Non-ideal Gas EOS

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

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

$$\boldsymbol{F} = \underbrace{\nabla \rho c_s^2}_{\text{Leading order term}} - \rho \nabla(\mu_0 - \kappa \nabla^2 \rho)$$

$$F_\alpha = t_\alpha \left(\frac{\boldsymbol{e}_\alpha}{c_s^2} + \frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4}\right) \cdot \boldsymbol{F}$$

Guo 2002

Lattice Boltzmann (Discrete Boltzmann) Equations

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha = -\frac{1}{\lambda}(f_\alpha - f_\alpha^{eq}) + \underbrace{t_\alpha \left(\frac{\boldsymbol{e}_\alpha}{c_s^2}\right) \cdot \nabla \rho c_s^2}_{F_\alpha^*} + \underbrace{t_\alpha \left(\frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4}\right) \cdot \nabla \rho c_s^2}_{F_\alpha^{**}}$$

Introduction of modified particle distribution functions

$$\bar{f}_\alpha = f_\alpha + \frac{f_\alpha - f_\alpha^{eq}}{2\tau} - \frac{\delta t}{2} t_\alpha \left(\frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4}\right) \cdot \nabla \rho c_s^2$$

$$\bar{f}_\alpha^{eq} = f_\alpha^{eq} - \frac{\delta t}{2} t_\alpha \left(\frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4}\right) \cdot \nabla \rho c_s^2$$

Collision step after combining $C_\lambda^I\left(\frac{\delta t}{2}\right)$ and $C_\lambda^E\left(\frac{\delta t}{2}\right)$:

$$\bar{f}_\alpha(\boldsymbol{x}, t + \delta t) - \bar{f}_\alpha(\boldsymbol{x}, t) = -\left.\frac{\bar{f}_\alpha - \bar{f}_\alpha^{eq}}{\tau + 1/2}\right|_{(\boldsymbol{x},t)} + \delta t\, t_\alpha \left.\left(\frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})\boldsymbol{e}_\alpha - \boldsymbol{u} c_s^2}{c_s^4}\right) \cdot \nabla \rho c_s^2\right|_{(\boldsymbol{x},t)}$$

From DBE to Lattice Boltzmann Equation (LBE)

- Discretize $S^A_{\boldsymbol{e}_\alpha}(\delta t)$ along characteristics over time δt

$$\int_t^{t+\delta t} \left(\frac{\partial \bar{f}_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla \bar{f}_\alpha \right) dt' = \int_t^{t+\delta t} F^*_\alpha \, dt'$$

- Applying Crank-Nicolson scheme to integrate RHS

$$\bar{f}_\alpha(\boldsymbol{x}, t+\delta t) - \bar{f}_\alpha(\boldsymbol{x} - \boldsymbol{e}_\alpha \delta t, t) = \frac{\delta t}{2} \left(\frac{t_\alpha}{c_s^2} \right) \boldsymbol{e}_\alpha \cdot \nabla \rho c_s^2 \Big|_{(\boldsymbol{x} - \boldsymbol{e}_\alpha \delta t, t)} + \frac{\delta t}{2} \left(\frac{t_\alpha}{c_s^2} \right) \boldsymbol{e}_\alpha \cdot \nabla \rho c_s^2 \Big|_{(\boldsymbol{x}, t+\delta t)}$$

- How to discretize *directional derivative* $\delta t \boldsymbol{e}_\alpha \cdot \nabla \rho$?

  - Discretization along characteristics:

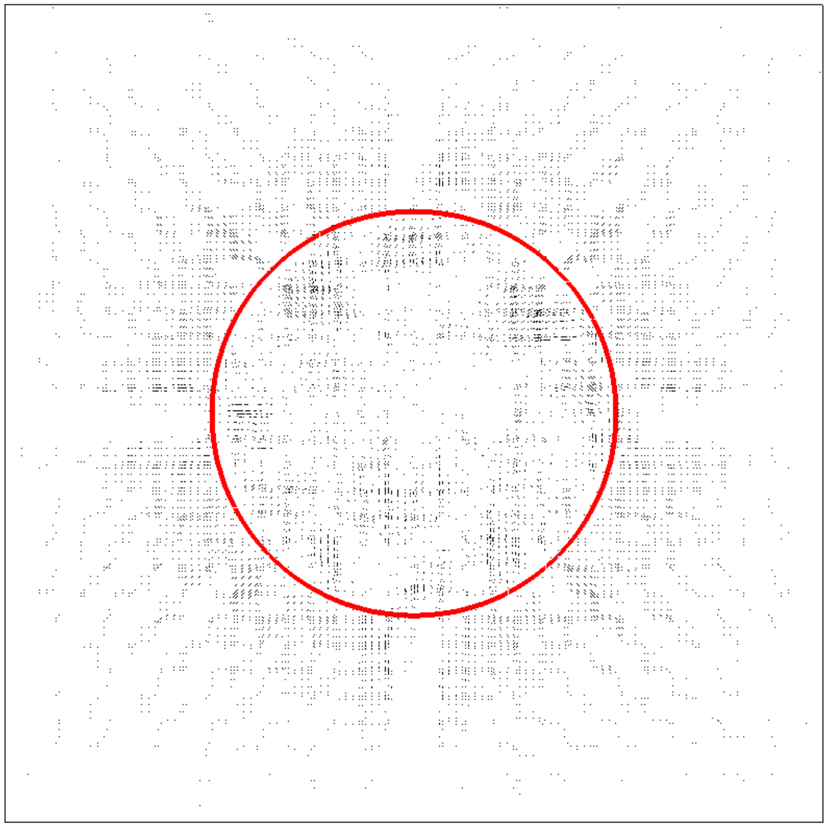
$$\delta t \boldsymbol{e}_\alpha \cdot \nabla \rho = \frac{1}{2} [\rho(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta t) - \rho(\boldsymbol{x} - \boldsymbol{e}_\alpha \delta t)]$$

  - Isotropic finite difference (Lee & Lin 2005; Kumar 2004)

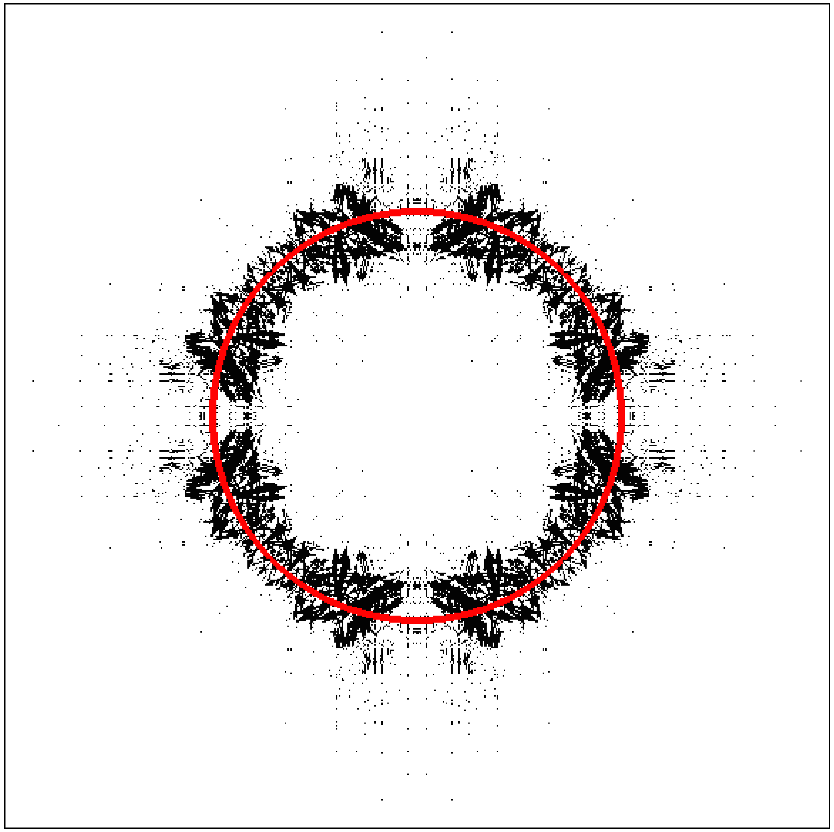
$$\delta t \boldsymbol{e}_\alpha \cdot \nabla \rho = \boldsymbol{e}_\alpha \cdot \sum_{\alpha \neq 0} \frac{t_\alpha \boldsymbol{e}_\alpha [\rho(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta t) - \rho(\boldsymbol{x} - \boldsymbol{e}_\alpha \delta t)]}{2 c_s^2}$$

Numerical Test: ρu field of a 2D Stationary Drop

- $\Omega := [-1,1]^2$ filled with quadrilateral spectral elements, $\frac{\rho_l}{\rho_v} = 10$
- Uniform mesh of size $E = 32 \times 32$ and $N = 5$, after 10^6 time steps



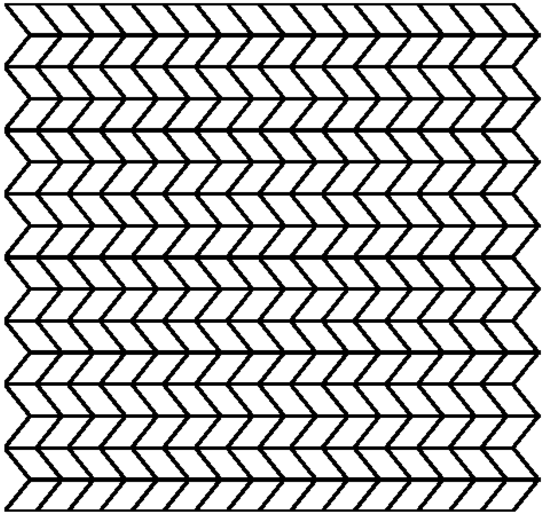
SAS-DBM, vectors magnified by 10^{15}

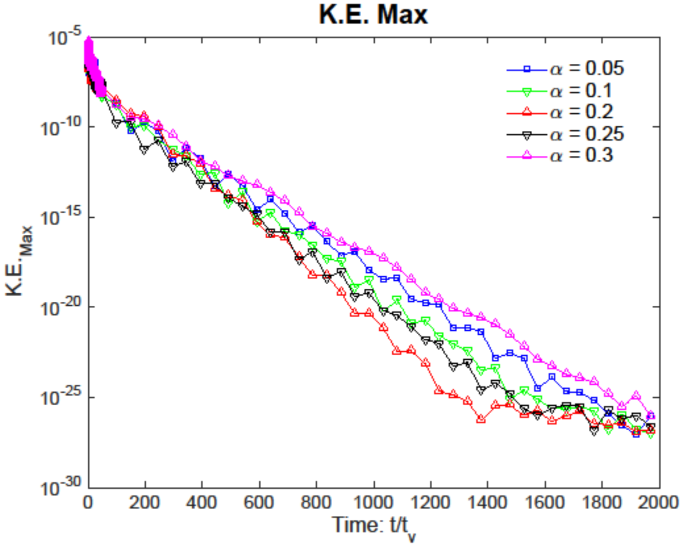


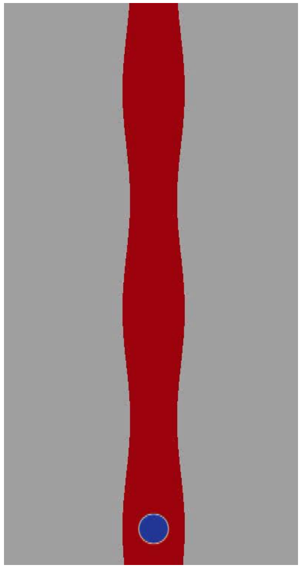
SANS-DBM, vectors magnified by 10^2

Numerical Test: 2D Stationary Drop on Perturbed Mesh

- $\Omega := [-1,1]^2$ filled with quadrilateral spectral elements, $\frac{\rho_l}{\rho_v} = 10$
- Non-uniform mesh of size $E = 16 \times 16$ and variable $La = \frac{\sigma 2 R_0}{\rho \nu^2} = 10^3$







Perturbed mesh with zig-zagged distribution. The degree of perturbation is based on the skewness coefficient $\alpha = \tan\theta$

Summary

- Cahn-Hilliard LBM performs well but suffers local mass conservation when local curvature effect is large
- To correct mass conservation error for low resolution simulation, derivative-free conservative phase-field LBM has been proposed, which possesses excellent Galilean invariant property, numerical efficiency, and accuracy.
- Moment-based fully derivative-free model lacks robustness of finite difference version, which needs to be improved.
- A force splitting scheme based on the Strang splitting is proposed and tested for two-phase lattice Boltzmann equation
- Discretization along characteristics is consistent with LB framework, more stable, and delivers better quality solutions.

$$\boldsymbol{F} = \underbrace{\nabla \rho c_s^2}_{\text{Leading order term}} - \rho \nabla (\mu_0 - \kappa \nabla^2 \rho)$$

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