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Simulation of rising bubbles using a new multiple relaxation time lattice Boltzmann method coupled with level set interface capturing

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- General LBE with single relaxation collision based on Maxwell equilibrium

$$\frac{\partial f_k}{\partial t} + e_k.\nabla f_k = \frac{1}{\tau}(f_k - f_k^{eq}) + \frac{(e_k - u_i)\cdot F_i}{\rho c_s^2} f_k^{eq}$$

- Recovers the nearly incompressible N.E. equations through the Chapman-Enskog expansion

$$\partial_t(\rho u_j) + \partial_i(\underbrace{\frac{1}{3}\rho\delta_{ij}}_{P} + \rho u_i u_j) - \underbrace{\frac{1}{3}\left(\tau - \frac{1}{2}\right)}_{\nu}\partial_i\left[\partial_j(\rho u_i) + \partial_i(\rho u_j)\right] = F_j$$

- Pressure is simply recovered by an equation of state (EOS)

ideal gas EOS $\quad P = \frac{1}{3}\rho$

Continuum Surface Force (CSF) form of LBM

- Turn the N.E. into a desired form for LBM (Mehravaran, 2011)

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla P}{\rho(\phi)} - \frac{\nabla \cdot \left(\mu(\phi)(\nabla \mathbf{u} + \nabla \mathbf{u}^T)\right)}{\rho(\phi)} = -\frac{\sigma \kappa(\phi) \mathbf{n}(\phi) \delta_\varepsilon(\phi)}{\rho(\phi)}$$

- Assume virtual variables $\bar{\rho} = 1$ and $\bar{\mu} = \mu/\rho$ and move the $\frac{\nabla P}{\rho(\phi)}$ to the rhs

$$\bar{\rho}(\phi)\partial_t u + \bar{\rho}(\phi)\mathbf{u} \cdot \nabla \mathbf{u} + \nabla P - \bar{\mu}(\phi)\nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) = \bar{F}$$

- The new rhs force takes the form

$$\bar{F} = -\frac{\sigma \kappa(\phi) \mathbf{n}(\phi) \delta_\varepsilon(\phi)}{\rho(\phi)} + \frac{\nabla \mu(\phi) \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T)}{\rho(\phi)} + \nabla P \left(1 - \frac{1}{\rho(\phi)}\right)$$

▶ Time Integration

- Forward Euler for the collision term, Crank-Nicolson for the forces

$$f_k(x+e_k\Delta t, t+\Delta t) = f_k(x,t) - \sum_j \Lambda_{k,j}(f_j(x,t) - f_j^{eq}(x,t)) + \frac{\Delta t}{2} S_k\Big|_{(x,t)} + \frac{\Delta t}{2} S_k\Big|_{(x+e_k\Delta t, t+\Delta t)}$$

$$\text{where} \qquad S_k = \frac{(e_{k,i} - u_i)\cdot \bar{F}_i}{\rho c_s^2} f_k^{eq}$$

- Recast into an explicit form for $g_k = f_k - \frac{\Delta t}{2} S_k$

$$g_k(x+e_k\Delta t, t+\Delta t) = g_k(x,t) - \sum_j \Lambda_{k,j}(g_j(x,t) - g_j^{eq}(x,t)) + (I - \frac{1}{2}\Lambda_{k,j}) S_j(x,t)$$

Velocity $\bar{\rho} u_i = \sum_k e_{k,i} g_k + 0.5 \bar{F}_i$, Pressure $P = \frac{\bar{\rho}}{3} = \frac{1}{3}\sum_k g_k$

Force Discretization; Central differencing approach

- discretization along major directions; (X, Y)
- central differences for $\nabla \mathbf{u}, \nabla \phi, \nabla P$ (∇a in general)

$$\frac{\partial a(x,y)}{\partial x} = \frac{a(x+h,y) - a(x-h,y)}{2h}$$

$$\frac{\partial a(x,y)}{\partial y} = \frac{a(x,y+h) - a(x,y-h)}{2h}$$

- perform the dot product of the force terms as in

$$S_k = \frac{(e_{k,i} - u_i) \cdot \bar{F}_i}{\rho c_s^2} f_k^{eq}$$

Force Discretization; Directional approach

- discretizing the $(e_k \cdot \nabla)$ terms along the lattice directions, e_k
- central differences for $(e_k \cdot \nabla \mathbf{u})$ and $(e_k \cdot \nabla \phi)$
- $P \approx O(f_k)$, so we perform an averaged differencing for $(e_k \cdot \nabla P)$ (Lee, Lin, 2005)

$$(e_k \cdot \nabla P)^C = \frac{P(x+e_k\Delta t) - P(x-e_k\Delta t)}{2}$$

$$(e_k \cdot \nabla P)^B = \frac{-P(x+2e_k\Delta t) + 4P(x+e_k\Delta t) - 3P(x)}{2}$$

Averaged difference $$(e_k \cdot \nabla P)^{Avg} = \frac{(e_{k,i} \cdot \partial_i P)^C + (e_{k,i} \cdot \partial_i P)^B}{2}$$

▸ Solving the Level Set equation

$$\partial_t \phi + \mathbf{u} \cdot \nabla \phi = 0 \qquad \text{where} \qquad \phi(\mathbf{x}) = 0 \quad at \quad X = \Gamma$$

- 2nd order Runge-Kutta time integration
- 5th order WENO finite difference for the convective term
- weighted reinitialization to the approximated signed distance function every $\triangle T$

$$\phi_{new} = \alpha \phi_{dist} + (1 - \alpha) \phi_{old}$$

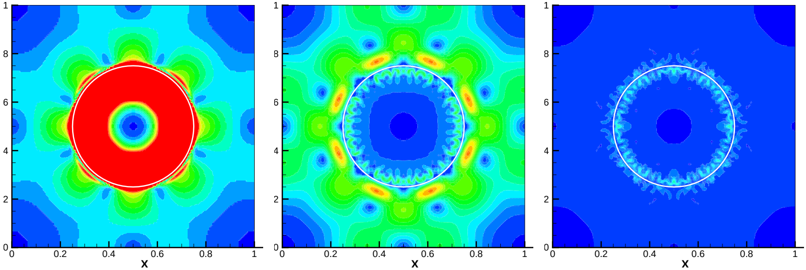
- regularized *Heaviside* function $H(\phi)$, for density and viscosity profiles

$$\begin{cases} \rho(\phi) = \rho_l H(\phi) + \rho_g (1 - H(\phi)) \\ \mu(\phi) = \mu_l H(\phi) + \mu_g (1 - H(\phi)) \end{cases}$$

▶ Static bubble; Case 1

Density ratio : $\rho_l/\rho_g = 10$ Viscosity ratio: $\mu_l/\mu_g = 10$

Spurious velocity level



Shan-Chen	LBM-LevelSet app. 1	LBM-LevelSet app. 2
$U_{max} = 3 \times 10^{-4}$	$U_{max} = 9.8 \times 10^{-6}$	$U_{max} = 4.8 \times 10^{-6}$

▶ Static bubble; Case 1

Pressure and velocity errors

Shan-Chen LB Model

$1/h$	40	80	160	320
U_{max}	6.5e-5	1.4e-4	3.00e-4	6.24e-4
$\lvert\triangle P - \sigma/r_0\rvert/(\sigma/r_0)$	0.0453	0.0172	0.0017	0.0023

LBM-Level Set, Approach 1

$1/h$	40	80	160	320
U_{max}	5.8e-5	3.00e-5	9.8e-6	7.4e-6
$\lvert\triangle P - \sigma/r_0\rvert/(\sigma/r_0)$	0.0108	0.0126	0.0087	0.0058

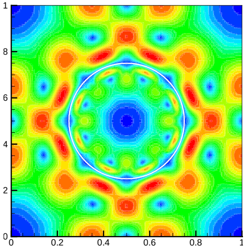
LBM-Level Set, Approach 2

$1/h$	40	80	160	320
U_{max}	1.93e-5	8.2e-6	4.6e-6	2.6e-6
$\lvert\triangle P - \sigma/r_0\rvert/(\sigma/r_0)$	0.0277	0.0147	0.0086	0.0060

Numerical Results

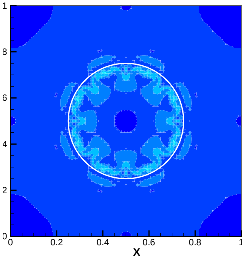
▶ Static bubble; Case 2

Density ratio : $\frac{\rho_l}{\rho_g} = 1000$ Viscosity ratio : $\frac{\mu_l}{\mu_g} = 100$



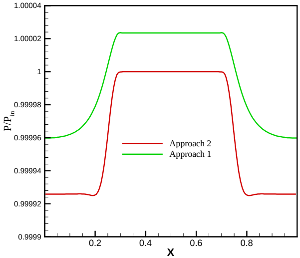
Spurious vel., App. 1

$U_{max} = 3.0 \times 10^{-6}$



Spurious vel., App. 2

$U_{max} = 8.4 \times 10^{-7}$



Pressure profile

- **Static bubble; Test Case 2**

Pressure and velocity errors

LBM-Level Set, Approach 1

$1/h$	40	80	160	320
U_{max}	4.7e-6	5.0e-6	3.0e-6	2.1e-6
$\lvert \triangle P - \sigma/r_0 \rvert / (\sigma/r_0)$	0.7520	0.4250	0.1331	0.0249

LBM-Level Set, Approach 2

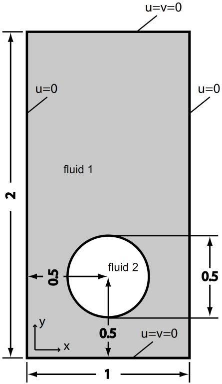
$1/h$	40	80	160	320
U_{max}	5.7e-6	4.1e-6	8.4e-7	3.6e-7
$\lvert \triangle P - \sigma/r_0 \rvert / (\sigma/r_0)$	0.1611	0.0211	0.0080	0.0060

▶ Rising bubble; Test Case 1

"Proposal for quantitative benchmark computations of bubble dynamics" (2007)

Hysing, S.; Turek, S.; Kuzmin, D.; Parolini, N.; Burman, E.; Ganesan, S.; Tobiska, L.

see www.featflow.de/benchmarks/

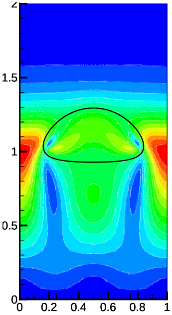


ρ_l/ρ_g	μ_l/μ_g	Eo	Re
10	10	10	35

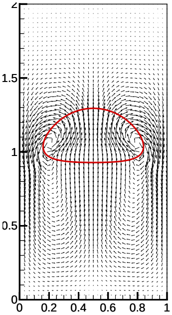
$$Eo = \frac{4\rho_l g r_0^2}{\sigma} \quad , \quad Re = \frac{\rho_l \sqrt{g}(2r_0)^{3/2}}{\mu_l}$$

▶ Rising bubble; Test Case 1

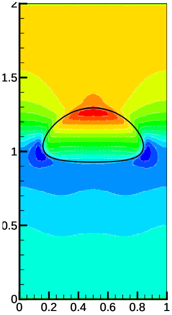
Bubble at $T = 3$, Grid: 160×320



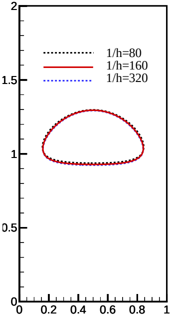
Velocity contour



Velocity vectors



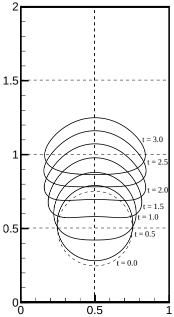
Pressure contour



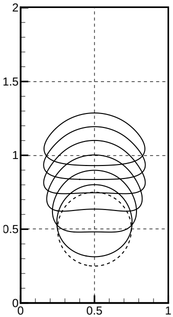
Interface

▶ Rising bubble; Test Case 1

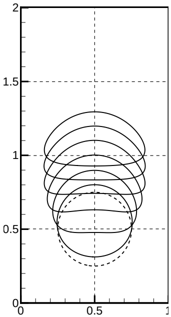
Benchmarking time evolution, $0 < T < 3$



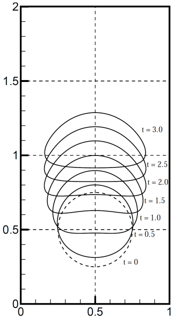
Shan-Chen



LBM-LS App. 1

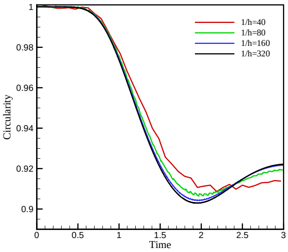


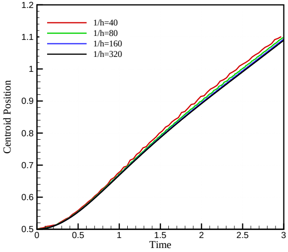
LBM-LS App. 2

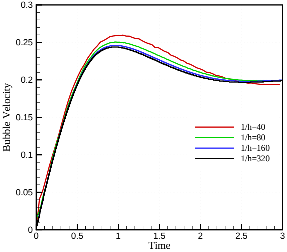


FeatFLOW

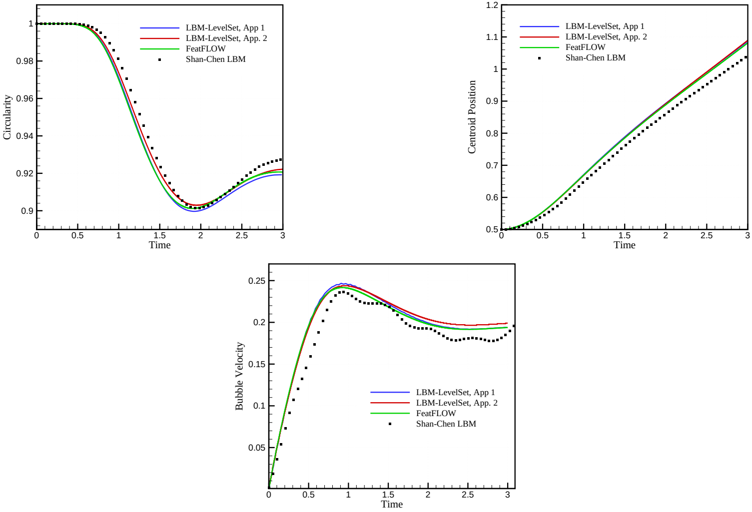
▶ **Rising bubble; Test Case 1** ⇒ LBM-LS Approach 2, grid effect, $0 < T < 3$







- **Rising bubble; Test Case 1** $\Rightarrow$ Benchmark comparison, 320×640, $0 < T < 3$



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- **Rising bubble; Test Case 1**

Error Reduction Rate

LBM-Level Set, Approach 1

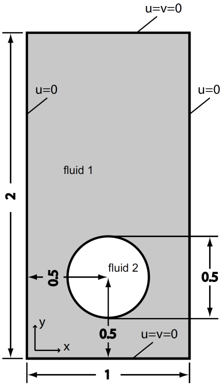
$1/h$	$\| e_1 \|$	ROC_1	$\| e_2 \|$	ROC_2	$\| e_\infty \|$	ROC_∞
Rise Velocity						
40	0.076750		0.149206		0.177204	
80	0.028549	1.426712	0.053590	1.477261	0.055123	1.684686
160	0.007367	1.954169	0.013609	1.977321	0.024643	1.161464

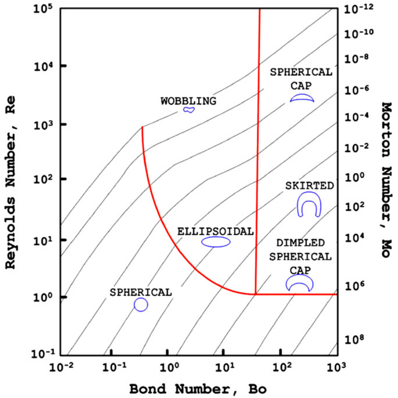
LBM-Level Set, Approach 2

$1/h$	$\| e_1 \|$	ROC_1	$\| e_2 \|$	ROC_2	$\| e_\infty \|$	ROC_∞
Rise Velocity						
40	0.096958		0.051369		0.046389	
80	0.042549	1.188226	0.021663	1.245647	0.020337	1.189679
160	0.013890	1.615036	0.000692	1.644344	0.000757	1.424072

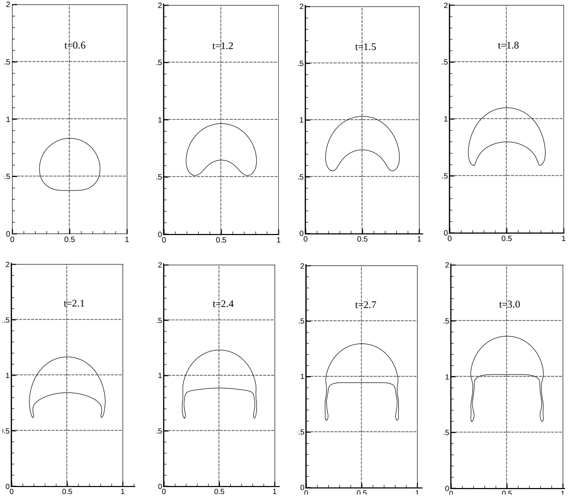
▶ Rising bubble; Test Case 2

ρ_l/ρ_g	μ_l/μ_g	Eo	Re
1000	100	125	35



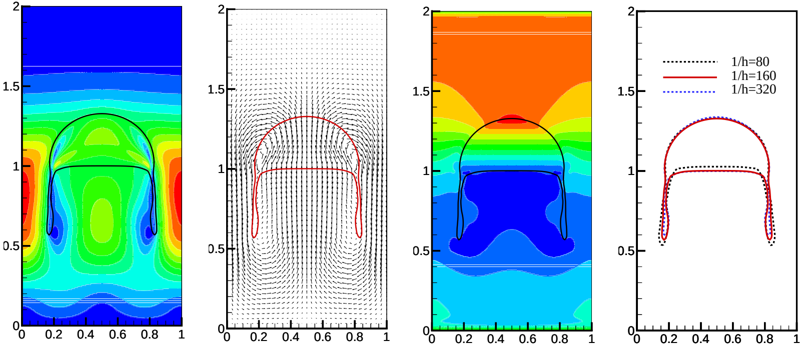


▶ **Rising bubble; Test Case 2** LBM-LS Approach 2, 160×160, $0 < T < 3$



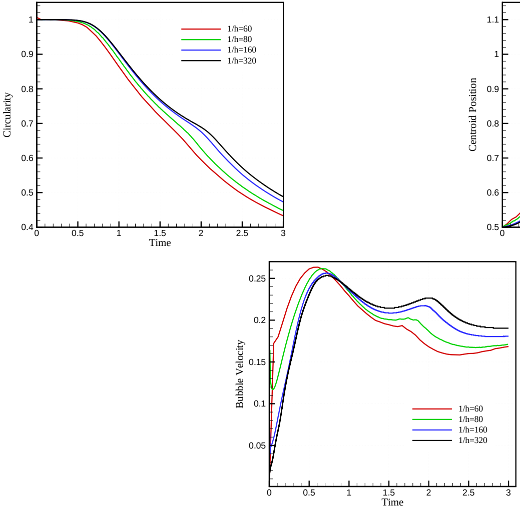
▶ Rising bubble; Test Case 2

Bubble at $T = 3$, Grid: 160×320



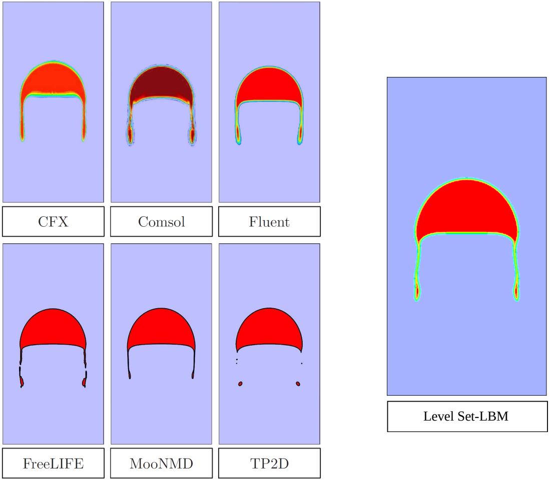
Velocity contour | Velocity vectors | Pressure contour | Interface

▶ **Rising bubble; Test Case 2** ⇒ LBM-LS Approach 2, grid effect, $0 < T < 3$

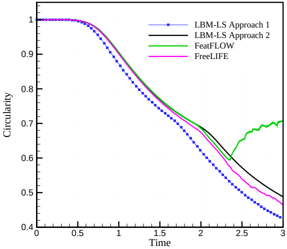


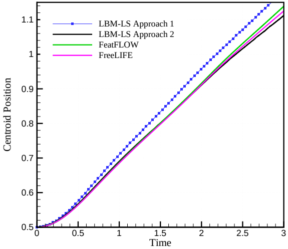
Numerical Results

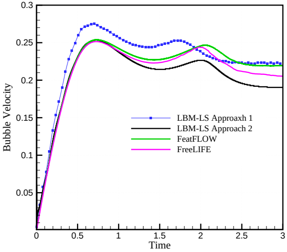
- **Rising bubble; Test Case 2** $\Rightarrow$ Benchmarking the picture norm!



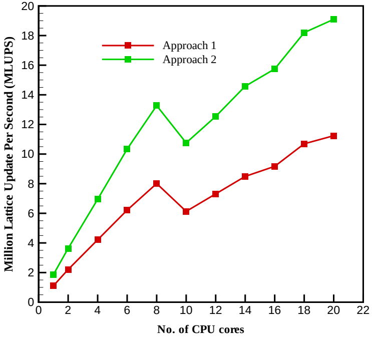
▶ **Rising bubble; Test Case 2** ⇒ Benchmark comparison, 320×640, $0 < T < 3$







▶ **Computational Performance**



- OpenMP implementation on Intel Xeon 1.65 MHz (up to 20 cores)
- Scaling for moderate Nr. of cores keeps a linear trend
- The modified discretization asks for $\approx$ 40% more computational time
- The level set module only adds $\approx$ 18% of extra computational cost

Summary and Conclusions

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- A 2nd order multiphase flow solver is designed by means of coupling LBM and Level set
- Sharp interfaces, low spurious velocities and accurate pressure recovery as compared to monolithic Shan-Chen model
- Large density and viscosity ratios attained using the Averaged-Directional force discretization and MRT collision
- High degree of stability and isotropy via the Averaged-Directional approach
- Maintains the nice properties of LBM; highly scalable for HPC purposes
- Extensive benchmarking; accuracy comparable to that from FEM-based FeatFLOW solutions (www.featflow.de/benchmarks)

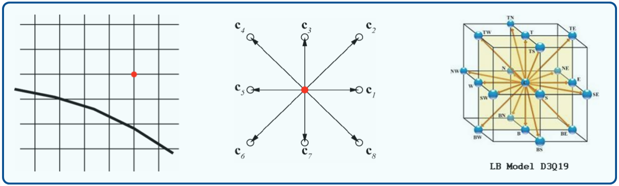
Thanks for your attention!

Outlook

- Use more robust reinitialization tools for updating the level set
- Use higher order approximations for normals and curvature
- Add local multi-block mesh refinements around the interface
- Implementation on graphics processing units (GPU)
- Extend the model towards complex and computationally demanding problems e. g. visco-elastic fluids

The continuous Boltzmann equation discretized in phase space

$$\frac{\partial f_k}{\partial t} + e_k.\nabla f_k = \Omega_c - \frac{F}{\rho} \cdot \nabla_e f$$



Hydrodynamic moments

$$\rho = \sum_k f_k \qquad , \qquad \rho u_i = \sum_k e_{i,k} f_k$$

- Surface tension boundary condition adds to the N.E. equation via a smeared out delta funcion across the interface Γ

$$\rho(\phi)\partial_t \mathbf{u} + \rho(\phi)\mathbf{u}\cdot\nabla\mathbf{u} + \nabla P - \nabla\cdot\left(\mu(\phi)(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right) = -\sigma\kappa(\phi)\delta_\varepsilon(\phi)\mathbf{n}(\phi)$$

- Interface is captured by solving for the implicit level set function

$$\partial_t\phi + \mathbf{u}\cdot\nabla\phi = 0 \quad , \quad \phi(\mathbf{x}) = 0 \quad at \quad X = \Gamma$$

ϕ is initialized to and maintained as a "signed distance function"

- Normal $\mathbf{n}(\phi)$ and curvature $\kappa(\phi)$ obtained via direct differentiation of ϕ

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \quad , \quad \kappa = \nabla\cdot\mathbf{n}$$

$$\bar{F} = \underbrace{\frac{\nabla\mu(\phi)\cdot(\nabla\mathbf{u}+\nabla\mathbf{u}^T)}{\rho(\phi)}}_{F_\mu:\ \text{viscosity jump}} \quad - \quad \underbrace{\frac{\sigma\kappa(\phi)\delta_\varepsilon(\phi)\nabla\phi}{\rho(\phi)}}_{F_\sigma:\ \text{surface tension}} \quad + \quad \underbrace{\nabla P\left(1-\frac{1}{\rho(\phi)}\right)}_{F_p:\ \text{pressure jump}}$$

▶ Multiple Relaxation Time LBM

- transform the distribution functions into the moment space

$$\hat{f} = \mathbb{T} f = (\rho, e, e^2, \rho u_x, q_x, \rho u_y, q_y, \sigma_{xx}, \sigma_{yy})^T$$

- modify the collision operator for the moment space

$$\Omega = \Lambda(f - f^{eq}) \quad \Rightarrow \quad \Omega = \mathbb{T}^{-1}\hat{\Lambda}(\hat{f} - \hat{f}^{eq})$$

- moments relax through their individual relaxation times

$$\hat{\Lambda} = \mathrm{diag}\{s_0, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8\}$$

- proper choice of relaxation times is crucial

$$\hat{\Lambda} = \mathrm{diag}\{1, s_1, s_2, 1, s_4, 1, s_4, s_7, s_7\}$$

$$s_1 = 0.3 \quad , \quad s_2 = 1 \quad , \quad s_4 = 0.7 \quad , \quad s_7 = 1/\tau$$

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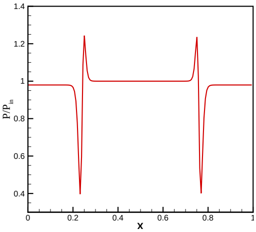
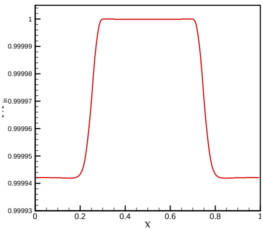
- **Static bubble; Case 1**

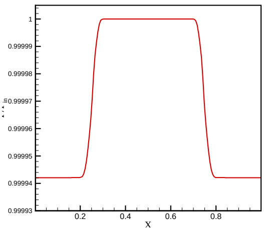
Pressure profile across the interface



Shan-Chen

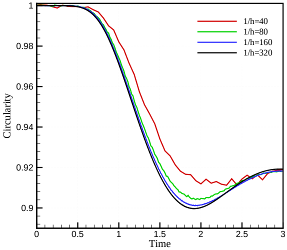


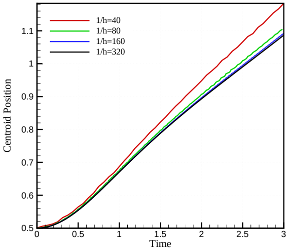
LBM-LevelSet app. 1

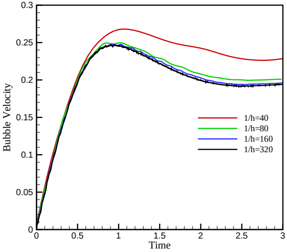


LBM-LevelSet app. 2

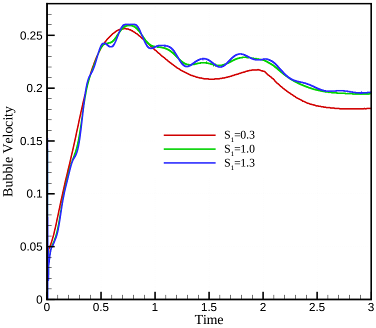
▶ **Rising bubble; Test Case 1** $\Rightarrow$ LBM-LS Approach 1, grid effect, $0 < T < 3$



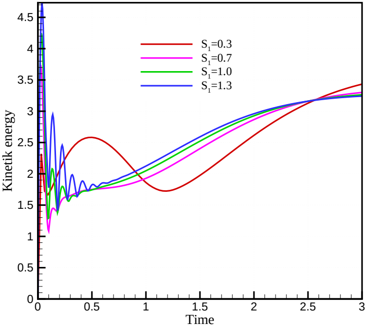




▶ **Relaxation time study**



Rising Bubble



Static Bubble

S_1 corresponds to the energy mode of the flow. A good choice is to under-relax for faster relaxation towards equilibrium!