Lattice Boltzmann Method in Multiphase Transport Phenomena

Research Overview

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Motivation

Applications:

- CO_2 mineralization, gas densification, and gas diffusion
- Solute transport and phase distribution
- Relative permeabilities - wettability

Why a new code?:

- 3D version for arbitrary domains, forces, and boundary conditions
- Future parallelization
- Coupling with other transport equations

Fortran 90, Object Oriented, LBM code for multi-component (N_c) mixtures. Output in VTK format.

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The Lattice Boltzmann Method - Formulation

The Lattice Boltzmann Method is based on kinetic theory, that states:

$$\underbrace{\frac{\partial f_i(x,t)}{\partial t} + \mathbf{c}_i \frac{\partial f_i(x,t)}{\partial x}}_{\text{Streaming - DF Advection}} = \underbrace{\mathbf{\Omega}}_{\text{Collision}} \tag{1}$$

What in its discretized form[1] becomes:

$$f_i(x + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(x,t) = -\mathbf{M}^{-1}\mathbf{S}[\mathbf{m}(x,t) - \mathbf{m}^{\mathrm{eq}}] + \hat{F}_i \tag{2}$$

where $\mathbf{m}$ are vectors of moments, $\mathbf{S}$ is a relaxation diagonal matrix, and $\mathbf{M}$ is a fixed matrix depending on DnQm. $\mathbf{m}^{\mathrm{eq}} = f(f_i^{\mathrm{eq}}, \mathbf{F})$.

[1] Going from 1 to 2, what about spatial derivative?

Macroscopic variables

Density and velocity are computed as follows:

$$\rho = \sum_i f_i \qquad \mathbf{u} = \sum_i \mathbf{c}_i f_i \tag{3}$$

Two important constitutive equations:

$$f_i^{\text{eq}} = \rho\omega_i \left[1 + \frac{\vec{u}\cdot\vec{\mathbf{c}_i}}{c_s^2} + \frac{(\vec{u}\cdot\vec{\mathbf{c}_i})^2}{2c_s^4} - \frac{\vec{u}\cdot\vec{u}}{2c_s^2}\right]$$

$$\hat{F}_i = \frac{\mathbf{F}}{\rho}\frac{\vec{u}-\vec{\mathbf{c}_i}}{c_s^2} f_i^{\text{eq}}$$

where **F** is defined in the multiphase problem, as the Shan Cheng force:

$$\mathbf{F} = -G\psi(x)\sum_i \omega_i \psi(x + \mathbf{c}_i\delta t)\mathbf{c}_i \quad \psi := \sqrt{\frac{2(P^{\text{EoS}} - c_s^2\rho)}{G\delta t c_s^2}} \tag{4}$$

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Dynamic Validations

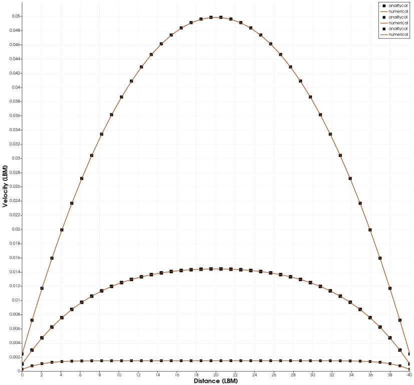
The main validation sources are: analytical solutions, Cheng's codes, qualitative physics understanding.

Single phase:

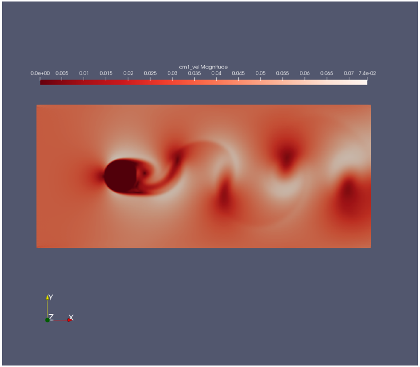
- Channel flow ($\mathbf{F}$ & ∇p-driven)
- Couette flow (plates)
- Cylinder (turbulent)
- Cavity flow
- Porous medium

Multiphase:

- Static droplet
- Oscillation droplet
- Falling droplet



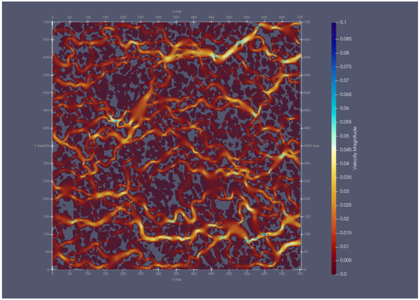
(a) **F**-driven channel flow



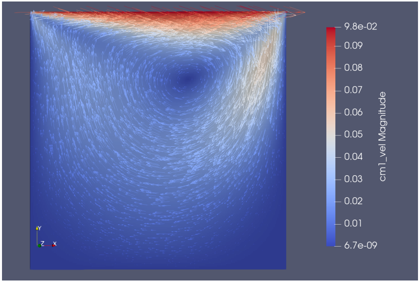
(b) Turbulent flow around cylinder

Figure: Results with direct source for quantitative comparisons.

Single phase validations (qualitative)



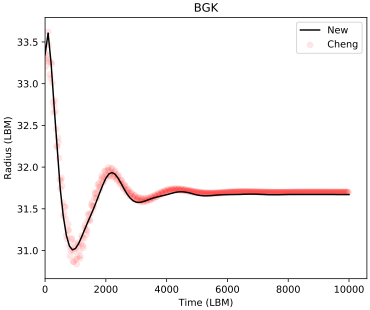
(a) Arbitrary porous medium (real image).



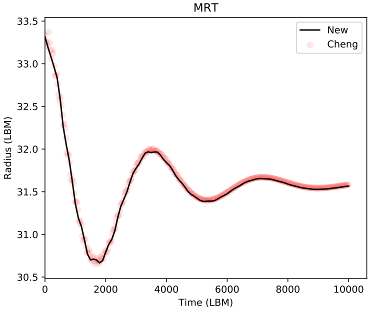
(b) Cavity flow, imposing a velocity on the upper wall.

Figure: Single phase cases qualitatively demonstrating the ability of modeling arbitrary porous media and arbitrary boundary conditions.

Multiphase single component - Oscillating droplet



(a) BGK

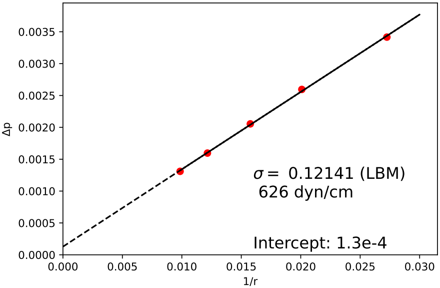


(b) MRT

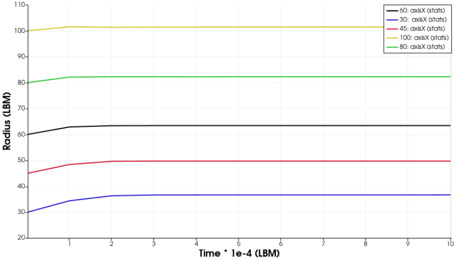
Figure: Oscillation droplet case. Viscosities are different in each case.

Static results - Young Laplace

$P_c = \frac{\sigma}{r}$, for a 2D geometry. $\sigma = 0.12141$. Here, $r = R_e$, the equilibrium radius.



(a) Young-Laplace validation



(b) Evolution of R_e for the static cases.

Figure: Young Laplace and R_e change due to thermodynamic inconsistency.

Oscillating droplet

$R_{x,0} = 60, R_{y,0} = 0.9R_{x,0}$, in a grid of 400x400. $\tau_l = \tau_v = 0.56$, to reduce the viscous dissipation.

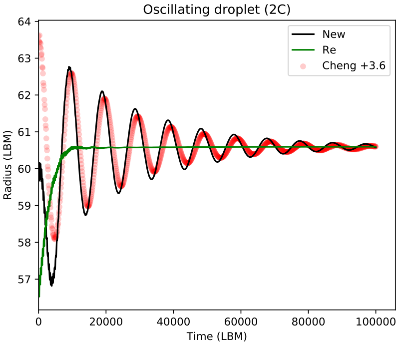


Figure: Oscillation of the X axis compared with Cheng's solution.

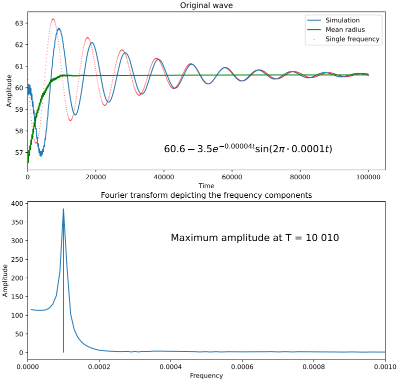


Figure: Maximum amplitude at $T_n = 10010$.

Analytical solution:

$$T_a = 2\pi \left[\frac{n(n^2 - 1)\sigma}{\rho_l R_e^3} \right]^{-0.5} \tag{5}$$

Giving a period $T_a = 9989$. This gives a relative error of 2%.

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- Main properties
  - Surface tension
  - Body forces
  - Viscosity and density ratio
  - Boundary conditions
- Bond and Morton numbers fix $R_e = \frac{u_t d_b}{\nu_l}$

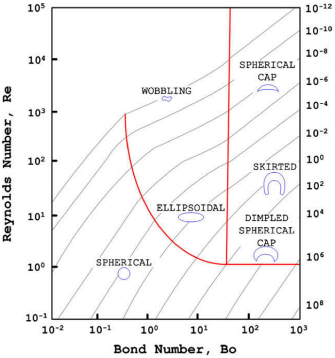
$$B_o = \frac{g \Delta \rho d_b^2}{\sigma}$$

$$M_o = \frac{g \Delta \rho \mu_l^4}{\sigma^3 \rho_l^2}$$

- The drag coefficient, C_D, function of R_e, and defined as:

$$C_D = \frac{4 \Delta \rho g d_b}{3 u_t^2 \rho_l}$$

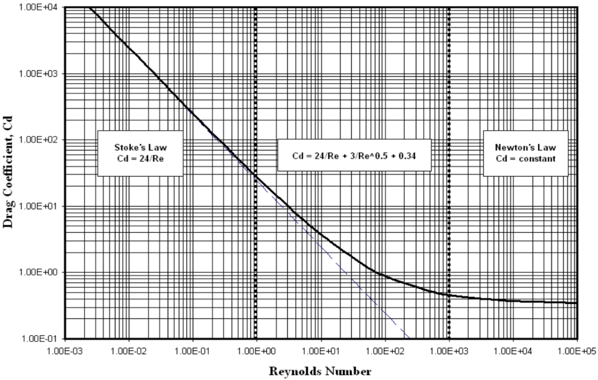
  resulting from a drag and gravity force balance.



Taken from Amaya-Bower L., Lee T. Single bubble rising dynamics for moderate Reynolds number using Lattice Boltzmann Method. Computer and Fluids. 2010.

Experimental relationship of C_D with R_e

The constants may change due to the 2D approximation.



Taken from API Specifications for Oil and Gas Separators and PNG 480 Handout. L. Ayala, H. Emami-M.

Considerations

Goal
Test the pseudopotential approach for partially misc. mixtures, under the action of gravity.

Methodology
Test different flow regimes based on Bond (Eotvos) and Morton numbers. Validate against **terminal velocities and bubble shapes.**

$$R_e = \frac{\rho_l u_b d_b}{\mu_l}$$

$$B_o = \frac{g \Delta \rho d_b^2}{\sigma} \quad M_o = \frac{g \Delta \rho \mu_l^4}{\sigma^3 \rho_l^2}$$

A thermodynamic state fixes $\rho, \Delta\rho, \sigma$. At a given temperature, in a single component case, some values are provided $(\rho, \Delta\rho)$ and others can be obtained by simulating the static droplet (σ).

Procedure

- Select B_o
- Calculate the gravity $g = \frac{B_o \sigma}{\Delta \rho d_b^2}$
- Select M_o
- Calculate $\mu_l^4 = \frac{M_o \sigma^3 \rho_l^2}{g \Delta \rho}$
- Select the viscosity ratio
- Calculate $\mu_g = \mu_l * \frac{\mu_g}{\mu_l}$

The LBM parameters are thus fixed:

$$\tau = \frac{\nu}{c_s^2} + \frac{\Delta t}{2}$$

Try single component and then the multicomponent case.

Simulation setup (Amaya)

Domain: (!) 200x360 mesh (2D)
Fluid: Water at 485.33 K ($T_r = 0.75$), and $P_r = 0.092$.
$\rho_l^0 = 7.679$ (), $\rho_v^0 = 0.109$. $\rho_L/\rho_g = 70$.
$\tau_l = 210.5$. $\tau_g = 0.8$. μ_l/μ_g =10.

Initial condition: Spherical droplet with $d_o = 40$, and $w_o = 8$.

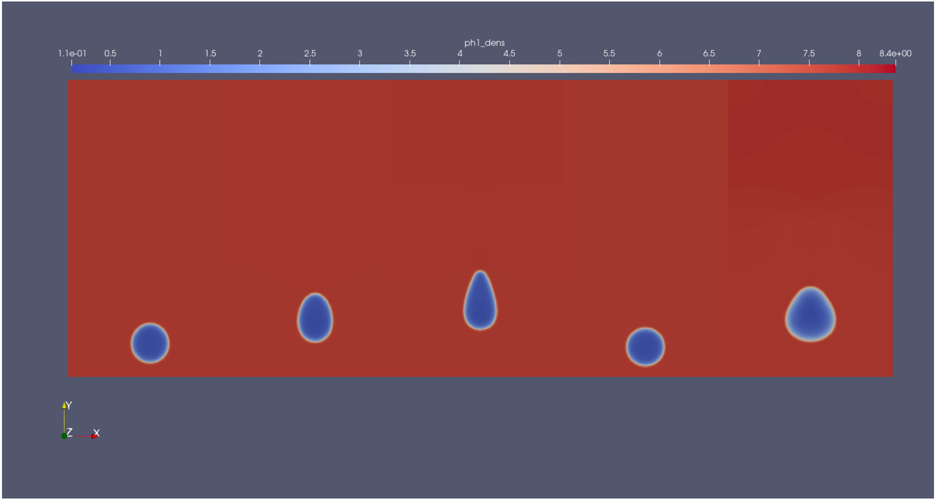
Boundary conditions: No-slip condition on all boundaries.

Parameters: Shan-Chen G=-1.0.
Beta = 0.9
Time = 10000 ($\approx 10\sqrt{\frac{d_b}{g}}$)

Single static simulation:
$\Delta\rho = 7.2$ (7.7-0.5), $d_s = 40.0$,
$\Delta P =$ 8.5e-3 - 5.87e-3 = 2.623e-3
$\sigma = \Delta P \cdot r = 0.05254$.
First, the single component case was tested as follows:

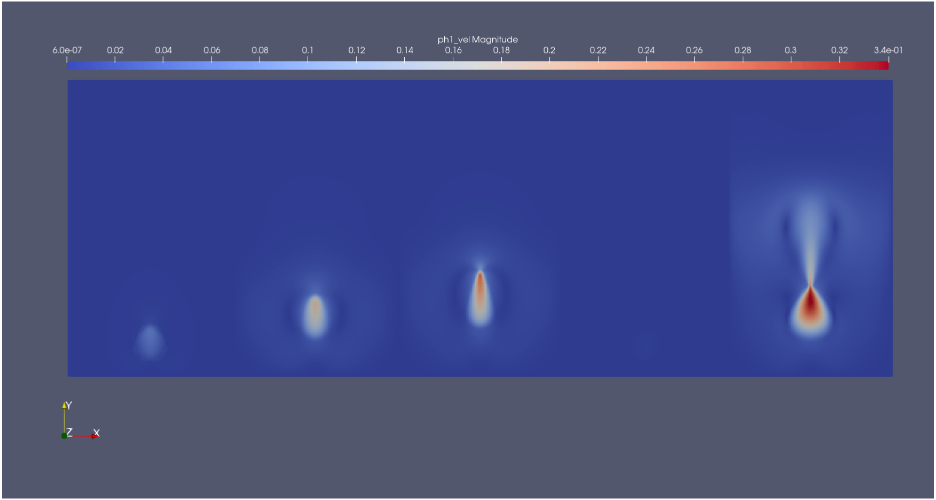
1. $B_o = 1$. $M_o =$ 3e-5. $\mu_R = 100$.
2. $B_o = 10$. $M_o =$ 2e-2. $\mu_R = 10$.
3. $B_o = 10$. $M_o =$ 2e-2. $\mu_R = 100$.
4. $B_o = 0.1$. $M_o =$ 1e-2. $\mu_R = 100$.
5. $B_o = 22$. $M_o =$ 8.4e-4. $\mu_R = 100$.

Preliminary Results



Bubble shapes

Preliminary Results



Velocity field

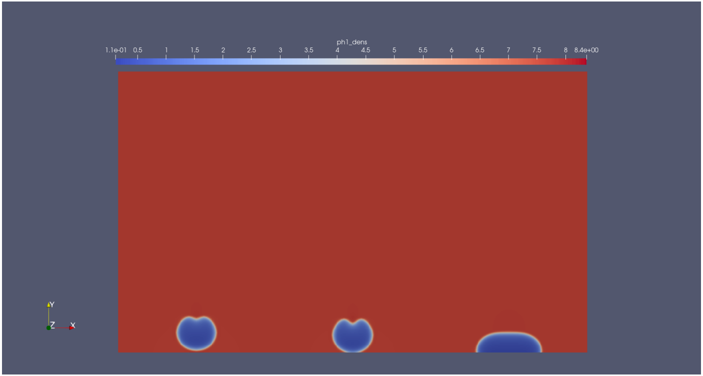
Difficulties in single phase

- Reach low Morton values (due to restrictions in kinematic viscosity).
- Reach high Bond numbers (high gravity)
- The cap shapes are not being observed, and the ellipsoidal tends to be more triangular.
- Hard to change Bond with fixed σ. System becomes unstable with other values of G.

Increasing the Morton number

Trying to make the liquid more viscous (at $B_o = 10$), seems to not allow the bubble to rise ($M_o = 8e6$), which later collapses.

- $\tau_g = 0.52$. $\tau_l = 47$
- $\tau_g = 2.0$. $\tau_l = 47$
- $\tau_g = 0.92$. $\tau_l = 4.7$



Velocity field

Potential solutions

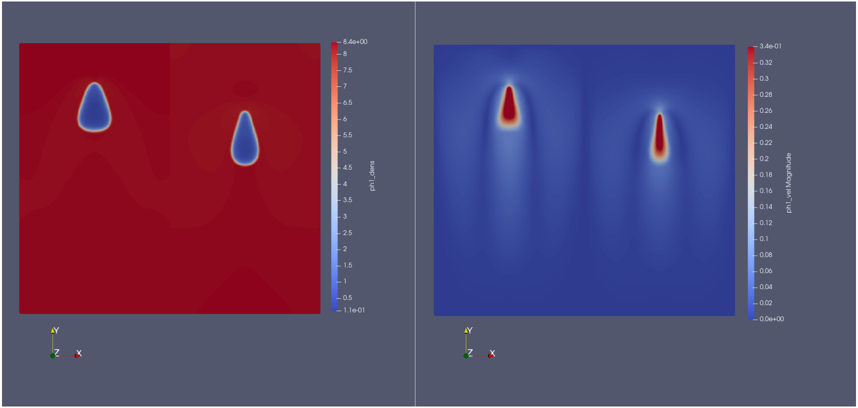
- Fix MRT parameters
- Consider an implicit scheme
- Compare against the usual Shan-Chen force which may provide better stability

MC case with the beta model

Using the same mixture that was used for the oscillating droplet, with a viscosity ratio of 10, two cases were run:

- $B_o = 10$, $M_o =$ 5e-3.
- $B_o = 10$, $M_o =$ 5e-4.

Multicomponent case - First approach



Density and Velocity field

Difficulties in single phase

- Same as in single component
- Reach stable simulations
- Seems that walls are affecting more the shape than in the single component

Thank you!