Modeling and simulation of capsules using lattice Boltzmann method

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Outline

Background

Numerical Methods

- Lattice Boltzmann method for fluid
- Immersed boundary method for capsules;

Numerical Results

Future Work

Background

- Natural, artificial and biological capsules and cells abound in nature, biology and technology.
- Desirable properties:
  - Ability to deform and accommodate the shapes of capillaries and microchannels
  - Ability to withstand the shearing action of an imposed flow
  - Capacity to transport materials in a protect way and release it in a timely fashion
- Fundamental research is necessary: The flow-induced deformation of liquid capsules in simple shear flow.
- Difficulties:
  - Deformable
  - Strong fluid-structure interaction

A Priori Derivation of Lattice Boltzmann Equation

The Boltzmann Equation with BGK approximation:

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = \int [f_1' f_2' - f_1 f_2] d\mu \approx -\frac{1}{\lambda}[f - f^{(0)}] , \quad f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t) . \quad (1)$$

The Boltzmann-Maxwellian equilibrium distribution function:

$$f^{(0)} = \rho \, (2\pi\theta)^{-D/2} \, \exp\left[-\frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2\theta} \right], \quad (2)$$

The macroscopic quantities are the hydrodynamic moments of f or $f^{(0)}$:

$$\rho = \int f d\boldsymbol{\xi} = \int f^{(0)} d\boldsymbol{\xi} , \quad (3a)$$

$$\rho \boldsymbol{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi} = \int \boldsymbol{\xi} f^{(0)} d\boldsymbol{\xi} , \quad (3b)$$

$$\rho \varepsilon = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f d\boldsymbol{\xi} = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f^{(0)} d\boldsymbol{\xi} . \quad (3c)$$

Integral Solution of Continuous Boltzmann Equation

Rewrite the Boltzmann BGK Equation in the form of ODE:

$$D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)} , \qquad D_t \equiv \partial_t + \boldsymbol{\xi} \cdot \nabla . \tag{4}$$

Integrate Eq. (4) over a time step δ_t along characteristics:

$$\begin{aligned} f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) &= e^{-\delta_t/\lambda} f(\boldsymbol{x}, \boldsymbol{\xi}, t) \\ &+ \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^{t'/\lambda} f^{(0)}(\boldsymbol{x} + \boldsymbol{\xi} t', \boldsymbol{\xi}, t + t') \, dt' . \end{aligned} \tag{5}$$

By Taylor expansion, and with $\tau \equiv \lambda/\delta_t$, we obtain:

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) - f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau}[f(\boldsymbol{x}, \boldsymbol{\xi}, t) - f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi}, t)] + \mathcal{O}(\delta_t^2) . \tag{6}$$

Note that a *finite-volume* scheme or higher-order schemes can also be formulated based upon the integral solution.

Three necessary steps to derive LBE:[1,2]

1. Low Mach number expansion of the distribution functions;
2. Discretize $\boldsymbol{\xi}$-space with necessary and min. number of $\boldsymbol{\xi}_\alpha$;
3. Discretization of $\boldsymbol{x}$ space according to $\{\boldsymbol{\xi}_\alpha\}$.

Low Mach Number ($\boldsymbol{u} \approx 0$) Expansion of the distribution functions $f^{(0)}$ and f up to $\mathcal{O}(\boldsymbol{u}^2)$ is sufficient to derive the Navier-Stokes equations:

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \left\{1 + \frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{\theta} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2\theta^2} - \frac{\boldsymbol{u}^2}{2\theta}\right\} + \mathcal{O}(\boldsymbol{u}^3)\,. \tag{7a}$$

$$f = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \sum_{n=0}^{2} \frac{1}{n!} \mathsf{a}^{(n)}(\boldsymbol{x},\, t) : \mathsf{H}^{(n)}(\boldsymbol{\xi})\,, \tag{7b}$$

where $\mathsf{a}^{(0)} = 1$, $\mathsf{a}^{(1)} = \boldsymbol{u}$, $\mathsf{a}^{(2)} = \boldsymbol{u}\boldsymbol{u} - (\theta - 1)\mathsf{I}$, and $\{\mathsf{H}^{(n)}(\boldsymbol{\xi})\}$ are generalized Hermite polynomials.

[1] X. He and L.-S. Luo, *Phys. Rev. E* **55**:R6333 (1997).

[2] X. Shan and X. He, *Phys. Rev. Lett.* **80**:65 (1998).

Discretization and Conservation Laws

The conservation laws are preserved exactly, if the hydrodynamic moments (ρ, $\rho\boldsymbol{u}$, and $\rho\epsilon$) are evaluated exactly:

$$I = \int \boldsymbol{\xi}^m f^{(\mathrm{eq})} d\boldsymbol{\xi} = \int \exp(-\boldsymbol{\xi}^2/2\theta)\psi(\boldsymbol{\xi}) d\boldsymbol{\xi}, \tag{8}$$

where $0 \le m \le 3$, and $\psi(\boldsymbol{\xi})$ is a polynomial in $\boldsymbol{\xi}$. The above integral can be evaluated by quadrature:

$$I = \int \exp(-\boldsymbol{\xi}^2/2\theta)\psi(\boldsymbol{\xi}) d\boldsymbol{\xi} = \sum_j W_j \exp(-\boldsymbol{\xi}_j^2/2\theta)\psi(\boldsymbol{\xi}_j) \tag{9}$$

where $\boldsymbol{\xi}_j$ and W_j are the abscissas and the weights. Then

$$\rho = \sum_\alpha f_\alpha^{(\mathrm{eq})} = \sum_\alpha f_\alpha, \qquad \rho\boldsymbol{u} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha^{(\mathrm{eq})} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha, \tag{10}$$

where $f_\alpha \equiv f_\alpha(\boldsymbol{x}, t) \equiv W_\alpha f(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t)$, and $f_\alpha^{(\mathrm{eq})} \equiv W_\alpha f^{(\mathrm{eq})}(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t)$.

The quadrature must preserve the conservation laws *exactly*!

Example: 9-bit LBE Model with Square Lattice

In two-dimensional Cartesian (momentum) space, set

$$\psi(\boldsymbol{\xi}) = \xi_x^m \xi_y^n,$$

the integral of the moments can be given by

$$I = (\sqrt{2\theta})^{(m+n+2)} I_m I_n, \qquad I_m = \int_{-\infty}^{+\infty} e^{-\zeta^2} \zeta^m d\zeta, \tag{11}$$

where $\zeta = \xi_x / \sqrt{2\theta}$ or $\xi_y / \sqrt{2\theta}$.
The second-order Hermite formula ($k = 2$) is the *optimal* choice to evaluate I_m for the purpose of deriving the 9-bit model, *i.e.*,

$$I_m = \sum_{j=1}^{3} \omega_j \zeta_j^m.$$

Note that the above quadrature is *exact* up to $m = 5 = (2k+1)$.

Discretization of Velocity $\boldsymbol{\xi}$-Space (9-bit Model)

The three abscissas in momentum space (ζ_j) and the corresponding weights (ω_j) are:

$$\begin{array}{lll} \zeta_1 = -\sqrt{3/2}\,, & \zeta_2 = 0\,, & \zeta_3 = \sqrt{3/2}\,, \\ \omega_1 = \sqrt{\pi}/6\,, & \omega_2 = 2\sqrt{\pi}/3\,, & \omega_3 = \sqrt{\pi}/6\,. \end{array} \tag{12}$$

Then, the integral of moments becomes:

$$I = 2\theta \left[\omega_2^2 \psi(\mathbf{0}) + \sum_{\alpha=1}^{4} \omega_1 \omega_2 \psi(\boldsymbol{\xi}_\alpha) + \sum_{\alpha=5}^{8} \omega_1^2 \psi(\boldsymbol{\xi}_\alpha) \right] , \tag{13}$$

where

$$\boldsymbol{\xi}_\alpha = \begin{cases} (0,\, 0) & \alpha = 0, \\ (\pm 1,\, 0)\sqrt{3\theta},\ (0,\, \pm 1)\sqrt{3\theta}, & \alpha = 1-4, \\ (\pm 1,\, \pm 1)\sqrt{3\theta}, & \alpha = 5-8. \end{cases} \tag{14}$$

Identifying

$$W_\alpha = (2\pi\,\theta)\,\exp(\boldsymbol{\xi}_\alpha^2/2\theta)\,w_\alpha\,, \tag{15}$$

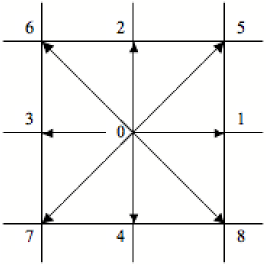
with $c \equiv \delta_x/\delta_t = \sqrt{3\theta}$, or $c_s^2 = \theta = c^2/3$, δ_x is the lattice constant, then:

$$\begin{aligned} f_\alpha^{(\mathrm{eq})}(\boldsymbol{x},\,t) &= W_\alpha\,f^{(\mathrm{eq})}(\boldsymbol{x},\,\boldsymbol{\xi}_\alpha,\,t) \\ &= w_\alpha\,\rho\left\{1 + \frac{3(\boldsymbol{c}_\alpha\cdot\boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{c}_\alpha\cdot\boldsymbol{u})^2}{2c^4} - \frac{3\boldsymbol{u}^2}{2c^2}\right\}, \end{aligned} \tag{16}$$

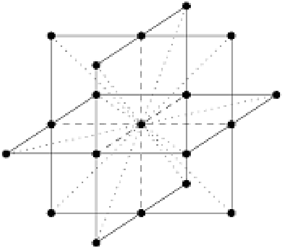
where weight coefficient w_α and discrete velocity $\boldsymbol{c}_\alpha$ are:

$$w_\alpha = \begin{cases} 4/9, \\ 1/9, \\ 1/36, \end{cases} \quad \boldsymbol{c}_\alpha = \boldsymbol{\xi}_\alpha = \begin{cases} (0,\,0), & \alpha = 0\,, \\ (\pm 1,\,0)\,c,\ (0,\,\pm 1)\,c, & \alpha = 1 - 4, \\ (\pm 1,\,\pm 1)\,c, & \alpha = 5 - 8. \end{cases} \tag{17}$$

With $\{\boldsymbol{c}_\alpha | \alpha = 0,\,1,\,\ldots,\,8\}$, a square lattice structure is constructed in the physical space.



D2Q9



D3Q19

D3Q19 cubic lattice:

$$w_\alpha = \begin{cases} 1/3, \\ 1/18, \\ 1/36, \end{cases} \quad \boldsymbol{c}_\alpha = \begin{cases} (0,\,0,\,0), & \alpha = 0\,, \\ (\pm 1,\,0,\,0)\,c,\ (0,\,\pm 1,\,0)\,c,\ (0,\,0,\,\pm 1)\,c, & \alpha = 1-6, \\ (\pm 1,\,\pm 1,\,\pm 1)\,c, & \alpha = 7-18. \end{cases}$$

LBE: Numerical Procedure

1. Choose particle velocity model
2. Given initial ρ_0, $\boldsymbol{u}_0$
3. Calculate equilibrium distribution function

$$f_\alpha^{(\mathrm{eq})}(\boldsymbol{x},\, t) = w_\alpha\, \rho \left\{ 1 + \frac{3(\boldsymbol{c}_\alpha \cdot \boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{c}_\alpha \cdot \boldsymbol{u})^2}{2c^4} - \frac{3\boldsymbol{u}^2}{2c^2} \right\}$$

4. Collision + Streaming

$$f_\alpha(\boldsymbol{x} + \boldsymbol{c}_\alpha \delta_t,\, \boldsymbol{c}_\alpha,\, t + \delta_t) - f_\alpha(\boldsymbol{x},\, \boldsymbol{c}_\alpha,\, t) = -\frac{1}{\tau}[f(\boldsymbol{x},\, \boldsymbol{c}_\alpha,\, t) - f^{(\mathrm{eq})}(\boldsymbol{x},\, \boldsymbol{c}_\alpha,\, t)]$$

5. Calculate ρ, $\boldsymbol{u}$

$$\rho = \sum_\alpha f_\alpha, \qquad \rho \boldsymbol{u} = \sum_\alpha \boldsymbol{c}_\alpha f_\alpha$$

Performing Taylor expansion in time and space:

$$(\partial_t + \boldsymbol{c}_\alpha \cdot \nabla) f_\alpha + \varepsilon \frac{1}{2} (\partial_t + \boldsymbol{c}_\alpha \cdot \nabla)^2 f_\alpha = \frac{1}{\varepsilon} \Omega_\alpha \tag{18}$$

Chapman-Enskog expansion:

$$\frac{\partial}{\partial t} = \varepsilon \frac{\partial}{\partial t_1} + \varepsilon^2 \frac{\partial}{\partial t_2} + \ldots, \qquad \frac{\partial}{\partial x} = \varepsilon \frac{\partial}{\partial x_1}, \tag{19}$$

For distribution function:

$$f_\alpha = f_\alpha^{(\mathrm{eq})} + \varepsilon f_\alpha^{(\mathrm{neq})}, \qquad f_\alpha^{(\mathrm{neq})} = f_\alpha^{(1)} + \varepsilon f_\alpha^{(2)} + \mathcal{O}(\varepsilon^2) \tag{20}$$

For collision operator,

$$\Omega_\alpha(f) = \Omega_\alpha(f^{(\mathrm{eq})}) + \varepsilon \frac{\partial \Omega_\alpha(f^{(\mathrm{eq})})}{\partial f_\beta} f_\beta^{(1)} + \varepsilon^2 \tag{21}$$

$$\left(\frac{\partial \Omega_\alpha(f^{(\mathrm{eq})})}{\partial f_\beta} f_\beta^{(2)} + \frac{\partial^2 \Omega_\alpha(f^{(\mathrm{eq})})}{\partial f_\beta \partial f_\gamma} f_\beta^{(1)} f_\gamma^{(1)} \right) + \mathcal{O}(\varepsilon^3) .$$

LBE Hydrodynamics: Chapman-Enskog Procedure

Order ε^0

$$(\partial_{t_1} + \boldsymbol{c}_\alpha \cdot \nabla_1) f_\alpha^{(\mathrm{eq})} = -\frac{1}{\tau} f_\alpha^{(1)} \tag{22}$$

Order ε^1

$$\left[\partial_{t_2} + (1 - \frac{2}{\tau})\partial_{t_1} + \boldsymbol{c}_\alpha \cdot \nabla_1\right] f_\alpha^{(1)} = -\frac{f_\alpha^{(2)}}{\tau} \tag{23}$$

Constraints:

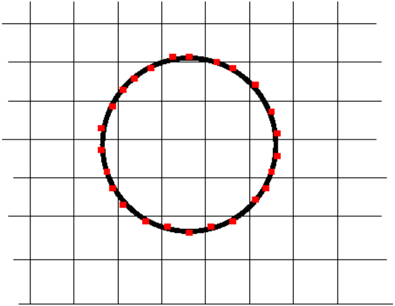
$$\sum_\alpha f_\alpha^{(\mathrm{eq})} = \rho \quad \sum_\alpha f_\alpha^{(k)} = 0, \quad \sum_\alpha \boldsymbol{c}_\alpha f_\alpha^{(\mathrm{eq})} = \rho \boldsymbol{u} \quad \sum_\alpha \boldsymbol{c}_\alpha f_\alpha^{(k)} = 0 \tag{24}$$

Hydrodynamical Equations:

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0\,. \tag{25a}$$

$$\partial_t (\rho \boldsymbol{u}) + \boldsymbol{\nabla} \cdot \Pi = 0\,. \tag{25b}$$

LBE Boundary Condition: Immersed Boundary Method



- It uses the Cartesian mesh for the fluid.
- Assuming the boundaries are immersed in the fluid.
- Boundaries are represented by a set of boundary points. (independent of grid points)

Immersed Boundary Method

- The immersed boundary moves at the local fluid velocity
- Boundary deformation generates force based on constitutive law
- This force is distributed into the flow field.
- The interaction between the fluid and immersed boundary is modeled by Dirac delta function.

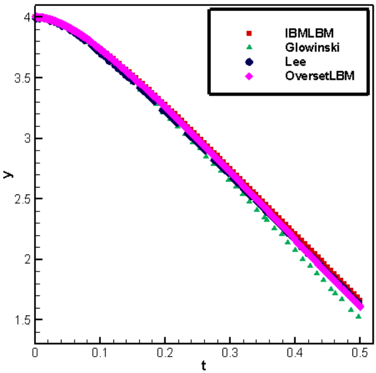
Immersed Boundary Method

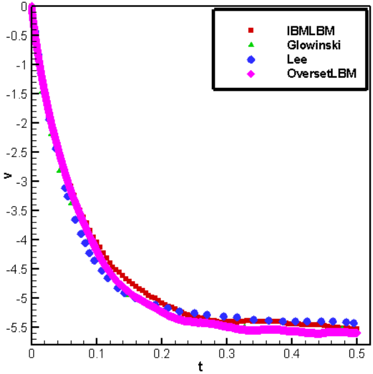
Immersed boundary is not the computational boundary in the flow solver. A singular force field is added in the governing equations.

Advantages:

- Discrete equations of motion are identical at all mesh points. (inside, outside or near the edge of boundary)
- Boundary can have undergoing time-dependent motions
- No need to generate grids each time

Sedimentation of one particle (movie)



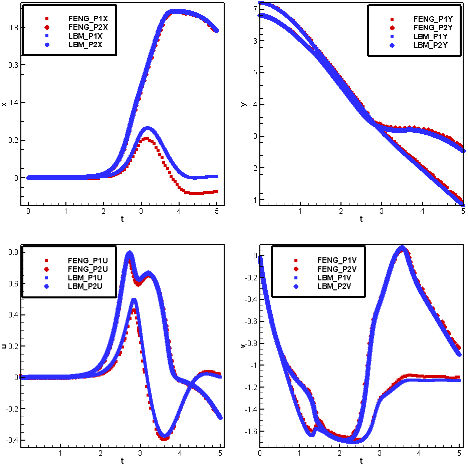


History of particle y position

History of translation velocity

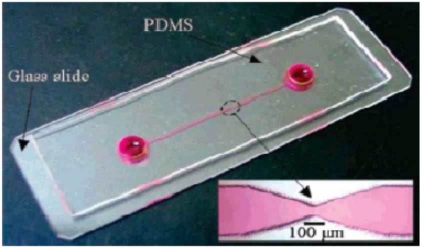
Results

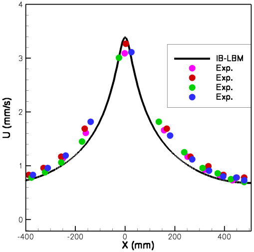
Sedimentation of two particles (movie)



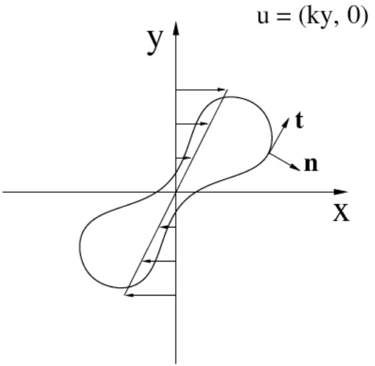
Results

Particle transport in a converge-diverge channel (movie)





Deformation of biconcave capsule in shear flow (movie)



Future work

- Effect of membrane constitutive law and analyze the force on capsule deformation.
- Multiple capsules motion in microvessels.