Lattice Boltzmann Method

I. Fluid Model

- Mesoscopic particle description of a fluid, where particle distribution functions evolve and flow across the domain

$f(\bar{r},\bar{e},t)\,d\bar{r}\,d\bar{e} = dN(\bar{r},\bar{e},t)$

$\bar{r}$: spatial degrees of freedom
$\bar{e}$: particle velocity degrees of freedom
f : particle distribution function
dN : number of particles occupying phase space volume $d\bar{r}\,d\bar{e}$.

- Macroscopic fluid quantities : velocity moments of f

$\rho(\bar{r},t) = \int f(\bar{r},\bar{e},t)\,d\bar{e}$ number density

$\bar{u}(\bar{r},t) = \frac{1}{\rho(\bar{r},t)} \int \bar{e} f(\bar{r},\bar{e},t)\,d\bar{e}$ fluid velocity

$E(\bar{r},t) = \frac{1}{2} m \frac{1}{\rho(\bar{r},t)} \int (\bar{e}-\bar{u})^2 f(\bar{r},\bar{e},t)\,d\bar{e}$ kinetic energy

II. Equilibrium Distribution

- borrow from kinetic theory of gases: Spread of velocities of a gas in thermal equilibrium given by the Maxwell-Boltzmann distribution

$$f^{eq}(\bar{r},\bar{e},t) = \rho(\bar{r},t)\left(\frac{m}{2\pi k_B T}\right)^{D/2} \exp\left\{-\frac{m(\bar{e}-\bar{u})^2}{2k_B T}\right\}$$

D: spatial dimension (D=2 for us)

- How is Maxwell-Boltzmann distribution adapted for Lattice Boltzmann?

1. Low Mach Expansion : $|\bar{u}| \ll \sqrt{\frac{k_B T}{m}} \equiv C_s$: effective speed of sound

2. Phase Space Discretization $f^{eq}(\bar{r},\bar{e},t) \to f^{eq}(\bar{r}_{ij},\bar{e}_{kl},t_n)$ where

$$\bar{r}_{ij} = \delta_x (i\hat{x} + j\hat{y})$$
$$\bar{e}_{kl} = \frac{\delta_x}{\delta_t}(k\hat{x} + l\hat{y})$$
$$t_n = n\delta_t$$

Start with Low Mach Expansion, retaining terms up to 2nd order in $\bar{u}$

$$f^{eq}(\bar{r},\bar{e},t) = \rho(\bar{r},t)\frac{m}{2\pi k_B T} \exp\left\{-\frac{m\bar{e}^2}{2k_B T}\right\} \exp\left\{\frac{m\bar{e}\cdot\bar{u}}{k_B T}\right\} \exp\left\{-\frac{m\bar{u}^2}{2k_B T}\right\}$$

$$\approx \rho(\bar{r},t)\frac{m}{2\pi k_B T}\exp\left\{\frac{-m\bar{e}^2}{2k_BT}\right\}\left[1+\frac{m\bar{e}\cdot\bar{u}}{k_BT}+\frac{1}{2}\left(\frac{m\bar{e}\cdot\bar{u}}{k_BT}\right)^2\right]\left[1-\frac{m\bar{u}^2}{2k_BT}\right]$$

$$\approx \rho(\bar{r},t)\frac{m}{2\pi k_B T}\exp\left\{\frac{-m\bar{e}^2}{2k_BT}\right\}\left[1+\frac{m\bar{e}\cdot\bar{u}}{k_BT}+\frac{1}{2}\left(\frac{m\bar{e}\cdot\bar{u}}{k_BT}\right)^2-\frac{m\bar{u}^2}{2k_BT}\right]$$

∴ with Low Mach Expansion, in 2D

$$f^{eq}(\bar{r},\bar{e},t) = \rho(\bar{r},t)\frac{m}{2\pi k_B T}\exp\left\{-\frac{m\bar{e}^2}{2k_BT}\right\}\Big[\underbrace{1+\frac{m\bar{e}\cdot\bar{u}}{k_BT}+\frac{1}{2}\left(\frac{m\bar{e}\cdot\bar{u}}{k_BT}\right)^2-\frac{m\bar{u}^2}{2k_BT}}_{\substack{\text{polynomial } \psi(e_x,e_y) \\ \text{degree 2 in } e_x \text{ and } e_y}}\Big]$$

Next is phase space discretization

Goal: Discretization must <u>exactly</u> preserve local velocity moments of f

$$\int f(\bar{r},\bar{e},t)\,d\bar{e} = \sum_{\bar{e}_{kl}} f(\bar{r}_{ij},\bar{e}_{kl},t_n) = \rho(\bar{r}_{ij},t_n)$$

$$\frac{1}{\rho(\bar{r},t)}\int \bar{e} f(\bar{r},\bar{e},t)\,d\bar{e} = \frac{1}{\rho(\bar{r}_{ij},t_n)}\sum_{\bar{e}_{kl}} \bar{e}_{kl} f(\bar{r}_{ij},\bar{e}_{kl},t_n) = \bar{u}(\bar{r}_{ij},t_n)$$

Look at conserving number density as our example case. Plugging in f^{eq} into the integral gives us

$$\rho\frac{m}{2\pi k_BT}\int \exp\left\{-\frac{m(e_x^2+e_y^2)}{2k_BT}\right\}\psi(e_x,e_y)\,de_x\,de_y \quad \text{with polynomial } \psi$$

Define $\varepsilon_x = \dfrac{e_x}{\sqrt{2k_BT/m}}$ $\qquad \varepsilon_y = \dfrac{e_y}{\sqrt{2k_BT/m}}$

$$\rightarrow \frac{\rho}{\pi}\int \exp\left\{-(\varepsilon_x^2+\varepsilon_y^2)\right\}\psi\,d\varepsilon_x\,d\varepsilon_y$$

Exact Gaussian-type quadrature exists such that

$$\frac{\rho}{\pi}\int \exp\left\{-(\varepsilon_x^2+\varepsilon_y^2)\right\}\psi\,d\varepsilon_x\,d\varepsilon_y = \frac{\rho}{\pi}\sum_{k,l}\omega_k\omega_l\,\psi(\varepsilon_{x_k},\varepsilon_{y_l})$$

The exponential weighting function in integrand means this is a case of Gauss-Hermite quadrature.

What order quadrature rule to choose? In general,

$n+1$-point quadrature rule → recover integral exactly if ψ is a polynomial of degree $2n+1$ or less. Right now, ψ is a polynomial of degree 2 in e_x, e_y. But we also want our quadrature rule to match higher order velocity moments like fluid velocity and kinetic energy, which would go up to degree 4. So we choose a <u>3</u>-point quadrature rule.

3-Point Gauss-Hermite Quadrature, in 2D

$$\varepsilon_{x_k} = \left\{ -\sqrt{\frac{3}{2}},\ 0\ \sqrt{\frac{3}{2}} \right\} = \varepsilon_{y_l}$$

Define $c \equiv \sqrt{\frac{3k_BT}{m}} \equiv \frac{\delta_x}{\delta_t}$ "lattice speed" - how fast the particles move.

$$e_{x_k} = \left\{ -\sqrt{\frac{3k_BT}{m}},\ 0,\ \sqrt{\frac{3k_BT}{m}} \right\} = e_{y_l}$$

$$= \{-c, 0, c\}$$

Notice that $c_s = \sqrt{\frac{k_BT}{m}}$ so $c_s^2 = \frac{c^2}{3}$

Pressure $p = \rho c_s^2$

$$\omega_k = \left\{ \frac{\sqrt{\pi}}{6},\ \frac{2\sqrt{\pi}}{3},\ \frac{\sqrt{\pi}}{6} \right\} = \omega_l$$

* Turn to slides for tabulated $\bar{e}_\alpha, \omega_\alpha$, now using a single linear index for 2D.

$$\therefore\ \frac{\rho}{\pi}\int \exp\left\{-(\varepsilon_x^2+\varepsilon_y^2)\right\}\psi\, d\varepsilon_x d\varepsilon_y = \frac{\rho}{\pi}\sum_{\alpha=0}^{8}\omega_\alpha \psi(\bar{e}_\alpha)$$

$$= \frac{\rho}{\pi}\sum_{\alpha=0}^{8}\omega_\alpha\left[1 + \frac{m\bar{e}_\alpha\cdot\bar{u}}{k_BT} + \frac{1}{2}\left(\frac{m\bar{e}_\alpha\cdot\bar{u}}{k_BT}\right)^2 - \frac{m\bar{u}^2}{2k_BT}\right]$$

$$= \frac{\rho}{\pi}\sum_{\alpha=0}^{8}\omega_\alpha\left[1 + 3\frac{\bar{e}_\alpha\cdot\bar{u}}{c^2} + \frac{9}{2}\left(\frac{\bar{e}_\alpha\cdot\bar{u}}{c^2}\right)^2 - \frac{3}{2}\frac{\bar{u}^2}{c^2}\right] = \rho$$

Same correspondence should happen for higher moments.

$$\rho(\bar{r}_{ij}, t_n) = \sum_{\alpha=0}^{8} f_\alpha(\bar{r}_{ij}, t_n)$$

$$\bar{u}(\bar{r}_{ij}, t_n) = \frac{1}{\rho(\bar{r}_{ij}, t_n)}\sum_{\alpha=0}^{8}\bar{e}_\alpha f_\alpha(\bar{r}_{ij}, t_n)$$

$$f_\alpha^{eq}(\bar{r}_{ij}, t_n) = \rho(\bar{r}_{ij}, t_n)\frac{\omega_\alpha}{\pi}\left[1 + 3\frac{\bar{e}_\alpha\cdot\bar{u}}{c^2} + \frac{9}{2}\left(\frac{\bar{e}_\alpha\cdot\bar{u}}{c^2}\right)^2 - \frac{3}{2}\frac{\bar{u}^2}{c^2}\right]$$

III. Transport Equation

Flow of particle distribution functions in space and time is governed by Boltzmann transport equation.

$$\frac{\partial f_\alpha}{\partial t} + \bar{e}_\alpha\cdot\bar{\nabla} f_\alpha = \Omega(f_\alpha)$$ Ω is a collision operator

First order explicit Euler step in time, and first order forward finite difference in space discretize the transport equation:

$$\frac{f_\alpha(\bar{r}_{ij}, t_n+\delta_t) - f_\alpha(\bar{r}_{ij}, t_n)}{\delta_t} + c\,\frac{f_\alpha(\bar{r}_{ij}+\bar{e}_\alpha\delta_t, t_n+\delta_t) - f_\alpha(\bar{r}_{ij}, t_n+\delta_t)}{\delta_x} = \Omega(f_\alpha(\bar{r}_{ij}, t_n))$$

recall $c = \frac{\delta_x}{\delta_t}$

$$\rightarrow\ f_\alpha(\bar{r}_{ij}+\bar{e}_\alpha\delta_t, t_n+\delta_t) = f_\alpha(\bar{r}_{ij}, t_n) + \delta_t\,\Omega(f_\alpha(\bar{r}_{ij}, t_n))$$

Common choice for collision operator is Bhatnagar-Gross-Krook (BGK) operator

$\rightarrow f_\alpha(\bar{r}_{ij} + \bar{e}_\alpha \delta_t, t_n + \delta_t) = f_\alpha(\bar{r}_{ij}, t_n) - \frac{1}{\tau}\left(f_\alpha(\bar{r}_{ij}, t_n) - f_\alpha^{eq}(\bar{r}_{ij}, t_n)\right)$ (δ_t absorbed into relaxation constant)

τ is related to kinematic viscosity: $\nu = \frac{2\tau - 1}{6} c^2 \delta_t$

Simulation Steps: see slides

Boundary conditions: see slides