Introduction to the lattice Boltzmann method

Burkhard Dünweg

Max Planck Institute for Polymer Research
Ackermannweg 10, D-55128 Mainz, Germany

duenweg@mpip-mainz.mpg.de

B. D. & A. J. C. Ladd, arXiv:0803.2826v2,
Advances in Polymer Science 221, 89 (2009)

Introduction

Low Mach numbers, Navier-Stokes

Chapman–Enskog

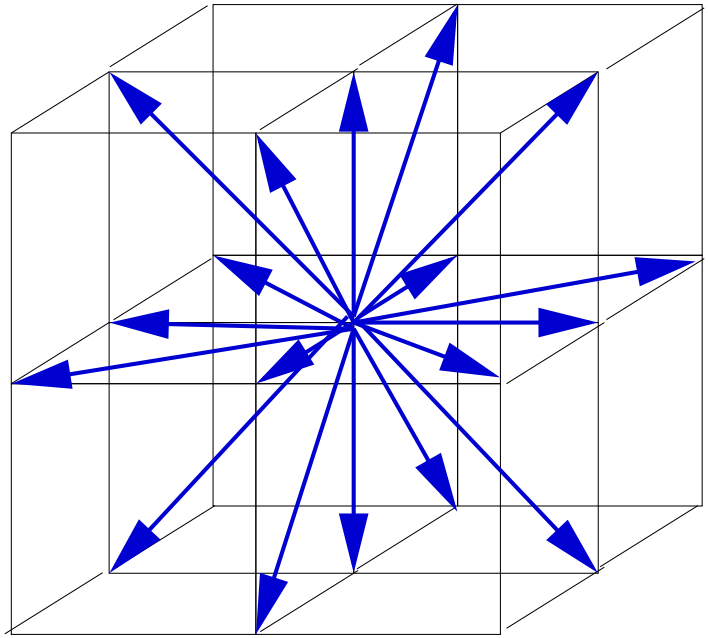
Building an LB model

Equilibrium populations

Linear collision operator

Statistical mechanics

Lattice Boltzmann



- linearized Boltzmann equation (kinetic theory of gases)
- fully discretized
- sites $\vec{r}$, lattice spacing a
- time t, time step h

- $\vec{c}_i$ small set of velocities
- $\vec{c}_i h$ connects two sites
- $n_i(\vec{r}, t)$: real number, mass density on site $\vec{r}$ corresponding to velocity $\vec{c}_i$

$$n_i(\vec{r} + \vec{c}_i h, t + h) = n_i^\star(\vec{r}, t) = n_i(\vec{r}, t) + \Delta_i \left\{ n_i(\vec{r}, t) \right\}$$

Lattice Boltzmann algorithm

- $\rho = \sum_i n_i$
- $\vec{j} = \sum_i n_i \vec{c}_i$, $\vec{u} = \vec{j}/\rho$
- $\overleftrightarrow{\Pi} = \sum_i n_i \vec{c}_i \otimes \vec{c}_i$
- $n_i^{eq}(\rho, \vec{u}) = w_i \rho \left(1 + \frac{\vec{u}\cdot\vec{c}_i}{c_s^2} + \frac{(\vec{u}\cdot\vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2}\right)$, such that
- $\sum_i n_i^{eq} = \rho$
- $\sum_i n_i^{eq} \vec{c}_i = \vec{j}$
- $\sum_i n_i^{eq} \vec{c}_i \otimes \vec{c}_i = \rho c_s^2 + \rho \vec{u} \otimes \vec{u}$
- linear relaxation: $\Delta_i = \sum_j L_{ij}(n_j - n_j^{eq})$
- streaming

remarks:

- $\overleftrightarrow{\Pi}$ relaxation rates determine viscosities
- thermal noise: Langevin stress term in $\overleftrightarrow{\Pi}$

Goal of this lecture

- What is the connection between lattice Boltzmann and Navier–Stokes?
- Why 19 velocities?
- Where does the equilibrium distribution come from?
- What are the "magic numbers" w_i?
- Relaxation rates $\leftrightarrow$ viscosities?
- How to put in noise?

Some philosophical remarks

$$n_i(\vec{r} + \vec{c}_i h, t + h) = n_i^\star(\vec{r}, t) = n_i(\vec{r}, t) + \Delta_i \left\{ n_i(\vec{r}, t) \right\}$$

$$\rho = \sum_i n_i$$

$$\vec{j} = \rho \vec{u} = \sum_i n_i \vec{c}_i$$

$$\sum_i \Delta_i = \sum_i \Delta_i \vec{c}_i = 0$$

- mass conservation
- momentum conservation
- locality
- rotational symmetry (lattice!)
- Galilei invariance (finite number of velocities)

- only $u \ll c_i$
- only $u \ll c_s$
- $Ma = u/c_s \ll 1$
- low Mach number $\Rightarrow$ compressibility does not matter $\Rightarrow$ equation of state does not matter $\Rightarrow$ choose ideal gas!

m_p particle mass:

$$p = \frac{\rho}{m_p} k_B T$$

$$c_s^2 = \frac{\partial p}{\partial \rho} = \frac{1}{m_p} k_B T$$

$$p = \rho c_s^2$$

$$k_B T = m_p c_s^2$$

Necessity of thermal fluctuations

- Ideal gas, temp. T, particle mass m_p, sound speed c_s:

$$k_B T = m_p c_s^2$$

- $c_s \sim a/h$ (a lattice spacing, h time step)
- c_s as small as possible

Example (water):
mass density $\rho = 10^3 kg/m^3$
sound speed realistic: $1.5 \times 10^3 m/s$
sound speed artificial: $c_s = 10^2 m/s$
temperature $T \approx 300K$, $k_B T = 4 \times 10^{-21} J$
particle mass: $m_p = 4 \times 10^{-25} kg$

	macroscopic scale	molecular scale
lattice spacing	$a = 1mm$	$a = 1nm$
time step	$h = 10^{-5} s$	$h = 10^{-11} s$
mass of a site	$m_a = 10^{-6} kg$	$m_a = 10^{-24} kg$
"Boltzmann number"	$Bo = (m_p/m_a)^{1/2} = 6 \times 10^{-10}$	$Bo = (m_p/m_a)^{1/2} = 0.6$

Where we want to get

$$\partial_t \rho + \partial_\alpha j_\alpha = 0$$

$$\partial_t j_\alpha + \partial_\beta \left(\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta \right) = \partial_\beta \sigma_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \eta_{\alpha\beta\gamma\delta} \partial_\gamma u_\delta$$

$$\eta_{\alpha\beta\gamma\delta} = \left(\zeta - \frac{2}{3}\eta \right) \delta_{\alpha\beta}\delta_{\gamma\delta} + \eta \left(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma} \right)$$

- η shear viscosity
- ζ bulk viscosity

Chapman–Enskog expansion

Multi–time scale analysis: $\varepsilon \ll 1$ (e. g. $\varepsilon = 10^{-3}$):

$$\vec{r}_1 = \varepsilon \vec{r}$$

interpretation: "coarse–grained ruler":
$1\mu m$ instead of $978nm$

$$t_1 = \varepsilon t$$

interpretation: "coarse–grained clock":
$1ns$ instead of $837ps$

$$t_2 = \varepsilon^2 t$$

interpretation: "yet more coarse–grained clock":
$1\mu s$ instead of $976ns572ps$

- t_1 to capture wave–like phenomena
- t_2 to capture diffusive phenomena
- location in space and time: read off $\vec{r}_1$, t_1, t_2

$$\vec{r} = \varepsilon^{-1}\vec{r}_1$$

$\vec{r}_1$ fixed $\Rightarrow$ $\vec{r}$ varies with ε $\Rightarrow$

$$\begin{aligned} n_i &= n_i^{(0)} + \varepsilon n_i^{(1)} + O(\varepsilon^2) \\ \Delta_i &= \Delta_i^{(0)} + \varepsilon \Delta_i^{(1)} + \varepsilon^2 \Delta_i^{(2)} + O(\varepsilon^3) \end{aligned}$$

$$\sum_i \Delta_i^{(k)} = \sum_i \Delta_i^{(k)} \vec{c}_i = 0$$

LBE:

$$n_i(\vec{r}_1 + \varepsilon \vec{c}_i h, t_1 + \varepsilon h, t_2 + \varepsilon^2 h) - n_i(\vec{r}_1, t_1, t_2) = \Delta_i(\vec{r}_1, t_1, t_2)$$

- Taylor expansion wrt ε
- $\varepsilon \longrightarrow 0$ corresponds to macroscopic limit

ε orders

- ε^0:

$$\Delta_i^{(0)} = 0$$

- ε^1:

$$\left(\partial_{t_1} + \vec{c}_i \cdot \partial_{\vec{r}_1}\right) n_i^{(0)} = h^{-1} \Delta_i^{(1)}$$

- ε^2:

$$\begin{aligned} & \partial_{t_2} n_i^{(0)} + \frac{h}{2} \left(\partial_{t_1} + \vec{c}_i \cdot \partial_{\vec{r}_1}\right)^2 n_i^{(0)} \\ + \quad & \left(\partial_{t_1} + \vec{c}_i \cdot \partial_{\vec{r}_1}\right) n_i^{(1)} = h^{-1} \Delta_i^{(2)} \end{aligned}$$

or

$$\partial_{t_2} n_i^{(0)} + \frac{1}{2} \left(\partial_{t_1} + \vec{c}_i \cdot \partial_{\vec{r}_1}\right) \left(n_i^{\star(1)} + n_i^{(1)}\right) = h^{-1} \Delta_i^{(2)}$$

Zeroth order

$$0 = \Delta_i^{(0)} = \Delta_i(\{n_i^{(0)}\})$$

- $\{n_i^{(0)}\}$ collisional invariant, $\{n_i^{(0)}\} = n_i^{eq}$
- no spurious conservation laws $\Rightarrow$
- $n_i^{(0)} = n_i^{(0)}(\rho, \vec{j})$
- $\rho^{(0)} = \rho$, $\vec{j}^{(0)} = \vec{j}$
- $$\sum_i n_i^{eq} = \rho$$
- $$\sum_i n_i^{eq} \vec{c}_i = \vec{j}$$

higher orders: take moments $\sum_i \ldots$, $\sum_i \vec{c}_i \ldots$

Zeroth moment: Mass conservation

$$\partial_{t_1}\rho + \partial_{1\alpha} j_\alpha = 0$$

$$\partial_{t_2}\rho = 0$$

Now,

$$\partial_\alpha = \varepsilon \partial_{1\alpha}$$

$$\partial_t = \varepsilon \partial_{t_1} + \varepsilon^2 \partial_{t_2}$$

Hence,

👍 continuity equation OK!!!

First moment: Momentum conservation

$$\partial_{t_1} j_\alpha + \partial_{1\beta} \Pi^{(0)}_{\alpha\beta} = 0$$

$$\partial_{t_2} j_\alpha + \frac{1}{2} \partial_{1\beta} \left(\Pi^{\star(1)}_{\alpha\beta} + \Pi^{(1)}_{\alpha\beta} \right) = 0$$

with

$$\Pi_{\alpha\beta} = \sum_i n_i c_{i\alpha} c_{i\beta}$$

together:

$$\partial_t j_\alpha + \partial_\beta \Pi^{eq}_{\alpha\beta} + \frac{1}{2} \partial_\beta \left(\Pi^{\star neq}_{\alpha\beta} + \Pi^{neq}_{\alpha\beta} \right) = 0$$

with

$$n_i^{neq} = \varepsilon n_i^{(1)}$$

comparison with Navier–Stokes:

$\Pi^{eq}_{\alpha\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$ $\qquad$ $\frac{1}{2} \left(\Pi^{\star neq}_{\alpha\beta} + \Pi^{neq}_{\alpha\beta} \right) = -\sigma_{\alpha\beta}$

Second moment: A useful relation

$$\partial_{t_1}\Pi^{(0)}_{\alpha\beta} + \partial_{1\gamma}\Phi^{(0)}_{\alpha\beta\gamma} = h^{-1}\left(\Pi^{\star(1)}_{\alpha\beta} - \Pi^{(1)}_{\alpha\beta}\right)$$

with

$$\Phi_{\alpha\beta\gamma} = \sum_i n_i c_{i\alpha} c_{i\beta} c_{i\gamma}$$

or

$$\Pi^{\star neq}_{\alpha\beta} - \Pi^{neq}_{\alpha\beta} = h\left(\partial_t \Pi^{eq}_{\alpha\beta} + \partial_\gamma \Phi^{eq}_{\alpha\beta\gamma}\right)$$

later (from explicit form of n_i^{eq}):

$$\Phi^{eq}_{\alpha\beta\gamma} = \rho c_s^2 \left(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}\right)$$

use continuity and Euler (∂_{t_1} !!!) for

$$\partial_t \Pi^{eq}_{\alpha\beta} = \partial_t(\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta)$$

result (neglecting terms $O(u^3)$):

$$\Pi^{\star neq}_{\alpha\beta} - \Pi^{neq}_{\alpha\beta} = h\rho c_s^2 \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha\right)$$

Linear stress relaxation

$$\Pi_{\alpha\beta} = \bar{\Pi}_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta}\Pi_{\gamma\gamma}$$

later:

$$\bar{\Pi}^{\star neq}_{\alpha\beta} = \gamma_s \bar{\Pi}^{neq}_{\alpha\beta}$$
$$\Pi^{\star neq}_{\alpha\alpha} = \gamma_b \Pi^{neq}_{\alpha\alpha}$$

together with

$$\Pi^{\star neq}_{\alpha\beta} - \Pi^{neq}_{\alpha\beta} = h\rho c_s^2 \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha\right)$$

two equations with two unknowns Π^{neq}, $\Pi^{\star neq}$
result:

$$\frac{1}{2}\left(\Pi^{\star neq}_{\alpha\beta} + \Pi^{neq}_{\alpha\beta}\right) = -\sigma_{\alpha\beta}$$

with

$$\eta = \frac{h\rho c_s^2}{2}\frac{1+\gamma_s}{1-\gamma_s} \qquad \zeta = \frac{h\rho c_s^2}{3}\frac{1+\gamma_b}{1-\gamma_b}$$

So, what do we need?

1. n_i^{eq} such that:
   - $$\sum_i n_i^{eq} = \rho \qquad \sum_i n_i^{eq} \vec{c}_i = \vec{j}$$
   - $$\sum_i n_i^{eq} c_{i\alpha} c_{i\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$
   - (and hopefully)
   $$\sum_i n_i^{eq} c_{i\alpha} c_{i\beta} c_{i\gamma} = \rho c_s^2 \left(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta} \right)$$
2. Δ_i such that n_i^{eq} invariant, and
   - $$\sum_i \Delta_i = 0 \qquad \sum_i \Delta_i \vec{c}_i = 0$$
   - $$\bar{\Pi}_{\alpha\beta}^{\star neq} = \gamma_s \bar{\Pi}_{\alpha\beta}^{neq} \qquad \Pi_{\alpha\alpha}^{\star neq} = \gamma_b \Pi_{\alpha\alpha}^{neq}$$

D3Q19 model I: Equilibrium populations

ansatz:

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho \left(1 + A\vec{u} \cdot \vec{c}_i + B(\vec{u} \cdot \vec{c}_i)^2 + Cu^2\right)$$

cubic symmetry:

$$\sum_i w_i = 1$$

$$\sum_i w_i c_{i\alpha} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} = \sigma_2 \, \delta_{\alpha\beta}$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = \kappa_4 \, \delta_{\alpha\beta\gamma\delta}$$

$$= \begin{cases} 1 & \text{all indices equal} \\ 0 & \text{else} \end{cases}$$

$$+\sigma_4 \left(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}\right)$$

$$\overset{4\,q/}{\Lambda} = \frac{1}{\rho} \sum_i n_i^{eq} = \sum_i w_i + A u_\alpha \sum_i w_i c_{i\alpha}$$

$$+ B u_\alpha u_\beta \sum_i w_i c_{i\alpha} c_{i\beta} + C u^2 \sum_i w_i =$$

$$= 1 + B u_\alpha u_\beta \sigma_2 \delta_{\alpha\beta} + C u^2 =$$

$$= 1 + B \sigma_2 u^2 + C u^2 \Rightarrow \underbrace{B\sigma_2 + C = 0}$$

$$\overset{\leftrightarrow}{\Pi} \Rightarrow \sigma_2 = c_s^2 \,, \quad 2B\sigma_4 = 1$$

$$B\sigma_4 + C\sigma_2 = 0$$

$$B x_4 = 0$$

$$\overset{\leftrightarrow}{j} \Rightarrow \underbrace{A\sigma_2 = 1}$$

$$c_s^2 \, \delta_{\alpha\beta} + u_\alpha u_\beta =$$

$$= \underbrace{\sigma_2 \, \delta_{\alpha\beta} + 2B \, \sigma_4 \, u_\alpha u_\beta}$$

$$+ (B\sigma_4 + C\sigma_2)\, \delta_{\alpha\beta} \, u^2$$

$$\cancel{+ B \, \kappa_4 \, \delta_{\alpha\beta\gamma\delta} \, u_\gamma u_\delta}$$

$$\Rightarrow A = \frac{1}{c_s^2}, \quad B = \frac{1}{2c_s^4}, \quad C = -\frac{1}{2c_s^2}$$

$$\sigma_2 = c_s^2 \qquad \sigma_4 = c_s^4, \quad \kappa_4 = 0$$

ρ, $\vec{j}$, $\overleftrightarrow{\Pi}$:

$$n_i^{eq}(\rho, \vec{u}) = w_i \rho \left(1 + \frac{\vec{u} \cdot \vec{c}_i}{c_s^2} + \frac{(\vec{u} \cdot \vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right)$$

- $$c_s^2 = \sigma_2$$
- $$\sum_i w_i = 1 \qquad \sigma_4 = \sigma_2^2 \qquad \kappa_4 = 0$$

solution:

- $w_i = 1/3$ (zero velocity)
- $w_i = 1/18$ (6 nearest neighbors)
- $w_i = 1/36$ (12 next–nearest neighbors)
- $c_s^2 = (1/3)(a/h)^2$
- 3rd moment OK

D3Q19 model II: Linear collision operator

ansatz (n_i^{eq} invariant):

$$n_i^{\star neq} = \sum_j \Gamma_{ij} n_j^{neq}$$

"modes" $\Rightarrow$ diagonal representation:

$$m_k = \sum_i e_{ki} n_i \qquad\qquad m_k^{\star neq} = \gamma_k m_k^{neq}$$

- $m_0 \propto \rho$
- $(m_1, m_2, m_3) \propto \vec{j}$
- $m_4 \in \mathrm{span}(\rho, \Pi_{\alpha\alpha})$
- $\mathrm{span}(m_5, \ldots, m_9) = \mathrm{span}(\bar{\Pi}_{\alpha\beta})$
- kinetic modes $m_{10}, \ldots, m_{19}$

- conserved modes: eigenvalue irrelevant: $\gamma_0 = \ldots = \gamma_3 = 1$
- bulk stress: $\gamma_4 = \gamma_b$
- shear stresses: $\gamma_5 = \ldots \gamma_9 = \gamma_s$
- kinetic modes: $\gamma_k = 0$ (easiest choice)

Statistical mechanics: Theory of fluctuations

B. D., U. Schiller, A. J. C. Ladd, PRE 76, 036704 (2007)

$\mu = m_p/a^3$, $\nu_i = n_i/\mu$, $\bar{\nu}_i = w_i\rho/\mu$

$$P(\{\nu_i\}) \propto \prod_i \frac{\bar{\nu}_i^{\nu_i}}{\nu_i!} e^{-\bar{\nu}_i} \delta\left(\mu \sum_i \nu_i - \rho\right) \delta\left(\mu \sum_i \nu_i \vec{c}_i - \vec{j}\right)$$

Stirling:

$$S(\{\nu_i\}) = -\sum_i \left(\nu_i \ln \nu_i - \nu_i - \nu_i \ln \bar{\nu}_i + \bar{\nu}_i\right)$$

$$P \propto \exp\left[S(\{\nu_i\})\right] \delta\left(\mu \sum_i \nu_i - \rho\right) \delta\left(\mu \sum_i \nu_i \vec{c}_i - \vec{j}\right)$$

- $P = max \Rightarrow S = max$ with constraints
- solution (neglecting terms $O(u^3)$): n_i^{eq} as before

Fluctuation statistics

Gaussian approximation around the mean:

$$P \propto \exp\left(-\sum_i \frac{\left(n_i^{neq}\right)^2}{2\mu n_i^{eq}}\right) \delta\left(\sum_i n_i^{neq}\right) \delta\left(\sum_i \vec{c}_i\, n_i^{neq}\right)$$

$n_i^{eq} \approx \rho w_i \Rightarrow$

$$P \propto \exp\left(-\sum_i \frac{\left(n_i^{neq}\right)^2}{2\mu\rho w_i}\right) \delta\left(\sum_i n_i^{neq}\right) \delta\left(\sum_i \vec{c}_i\, n_i^{neq}\right)$$

recall: unnormalized modes:

$$m_k = \sum_i e_{ki} n_i$$

normalized modes $\hat{m}_k \propto m_k$:

$$\hat{m}_k = \sum_i \hat{e}_{ki} \frac{n_i}{\sqrt{w_i \mu \rho}}$$

with orthogonal matrix $\hat{e}_{ki}$

Fluctuation statistics in mode space, Monte Carlo

$$P\left(\left\{\hat{m}_k^{neq}\right\}\right) \propto \exp\left(-\frac{1}{2}\sum_{k\geq 4}\hat{m}_k^{neq\,2}\right)$$

$$\hat{m}_k^{\star neq} = \gamma_k \hat{m}_k^{neq} + \varphi_k r_k$$

r_k Gaussian with

$$\langle r_k \rangle = 0 \qquad \langle r_k^2 \rangle = 1$$

detailed balance holds for

$$\varphi_k = \left(1-\gamma_k^2\right)^{1/2}$$

Fluctuating hydrodynamics

Chapman–Enskog applied to the stochastic term ⇒ equations of fluctuating hydrodynamics (Landau / Lifshitz 1957)

$$\begin{aligned} \partial_t \rho + \partial_\alpha j_\alpha &= 0 \\ \partial_t j_\alpha + \partial_\beta \left(\rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta \right) &= \partial_\beta \eta_{\alpha\beta\gamma\delta} \partial_\gamma u_\delta + \partial_\beta Q_{\alpha\beta} \end{aligned}$$

$$\begin{aligned} \langle Q_{\alpha\beta} \rangle &= 0 \\ \left\langle Q_{\alpha\beta}(\vec{r}, t)\, Q_{\gamma\delta}\left(\vec{r}', t'\right) \right\rangle &= 2 k_B T \eta_{\alpha\beta\gamma\delta} \delta\left(\vec{r} - \vec{r}'\right) \delta\left(t - t'\right) \end{aligned}$$