Lecture 1: From LGA to LBE — A Historic Review

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Hierarchy of Physical "Scales"

Microscopic Scale

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}$$

$$H = \sum_{k=1}^{(D+K)N} p_k^2 + V$$

$$i\hbar\dot{\psi} = \mathcal{H}\psi$$

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N} \boldsymbol{\nabla}_j^2 + V$$

$h \approx 6.62 \cdot 10^{-34} (\mathrm{J \cdot s})$

$c \approx 2.99 \cdot 10^{8} (\mathrm{m/s})$

$a \approx 0.53(\text{Å}) \approx 5 \cdot 10^{-11} (\mathrm{m})$

$t_a \approx 2.41 \cdot 10^{-17} (\mathrm{s})$

$m = 1(\mathrm{amu}) \approx 10^{-27} (\mathrm{kg})$

$N \geq 1$

Mesoscopic Scale

$$\partial_t f + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f = \frac{1}{\varepsilon} Q(f, f)$$

$$f = f(\boldsymbol{x}, \boldsymbol{\xi}, t)$$

$$\varepsilon = \mathrm{Kn} = \frac{\ell}{L}, \quad \mathrm{Ma} = \frac{U}{c_s}$$

$k_B \approx 1.38 \cdot 10^{-23} (\mathrm{J/°K})$

$\ell \approx 10^2 – 10^3 \ (\text{Å})$

$\approx 10 – 100 \ (\mathrm{nm})$

$\tau \approx 10^{-10} (\mathrm{s})$

$c_s \approx 300 \ (\mathrm{m/s})$

$N \gg 1$

Macroscopic Scale

$$\rho D_t \boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}} \boldsymbol{\nabla} \cdot \sigma$$

$$D_t = \partial_t + \boldsymbol{u} \cdot \boldsymbol{\nabla}$$

$$\sigma = \mu[(\boldsymbol{\nabla u}) + (\boldsymbol{\nabla u})^{\dagger}] + \frac{2}{D}\eta \mathsf{I}(\boldsymbol{\nabla} \cdot \boldsymbol{u})$$

$$\mathrm{Re} = \frac{UL}{\nu} \sim \frac{\mathrm{Ma}}{\mathrm{Kn}}, \quad \nu = \frac{\mu}{\rho}$$

$\nu \approx 10^{-6} – 10^{-4} \ (\mathrm{m^2/s})$

$\mathrm{Kn} \approx 0 \qquad \mathrm{Ma} < 10^3$

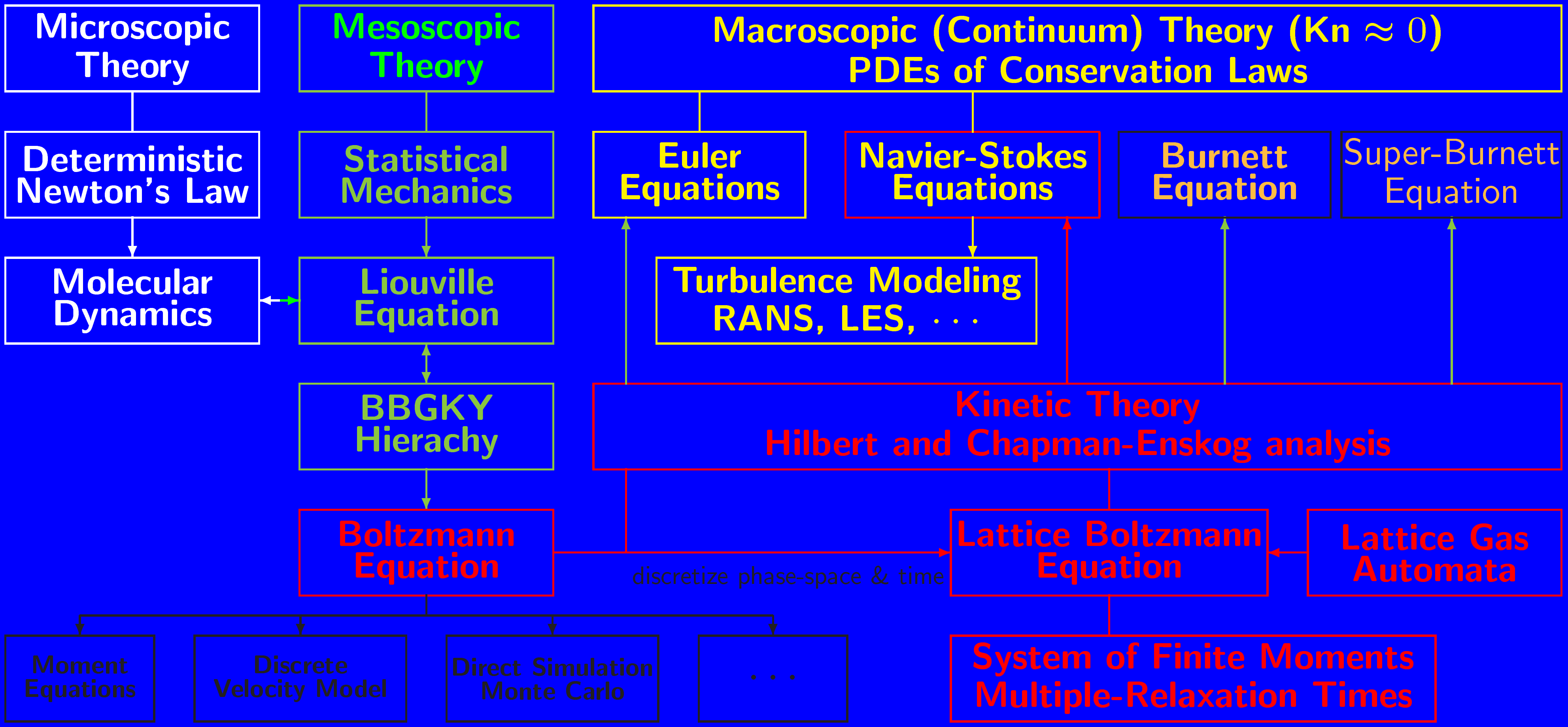
$L \geq 10^{-5} \ (\mathrm{m}) = 10 \ (\mu\mathrm{m})$

$T \geq 10^{-4} \ (\mathrm{s})$

$N \geq N_A \approx 6.02 \cdot 10^{23} \gg 1$

Microscopic, Mesoscopic, Macroscopic Descriptions of Fluids

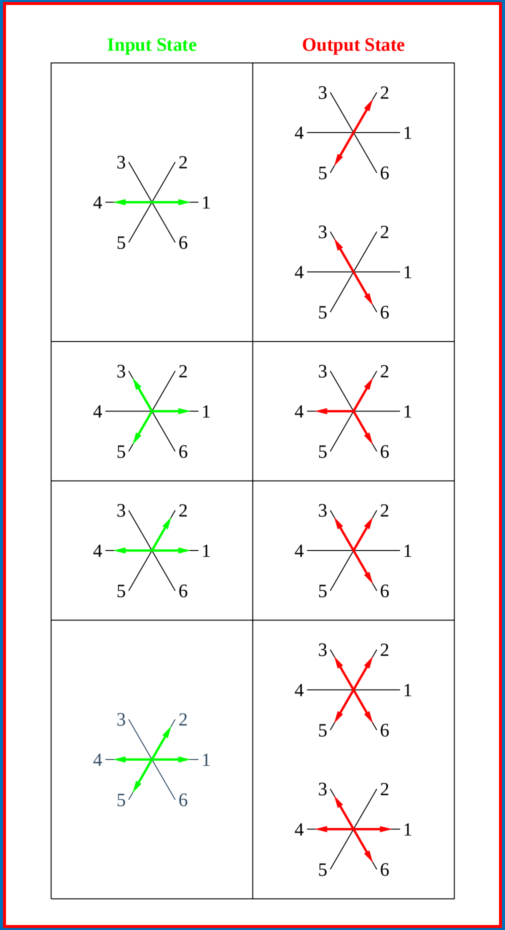
$$\text{Knudsen Number Kn} := \frac{\ell}{L} = \frac{\text{Mean Free Path}}{\text{Characteristic Hydrodynamic Length}}$$



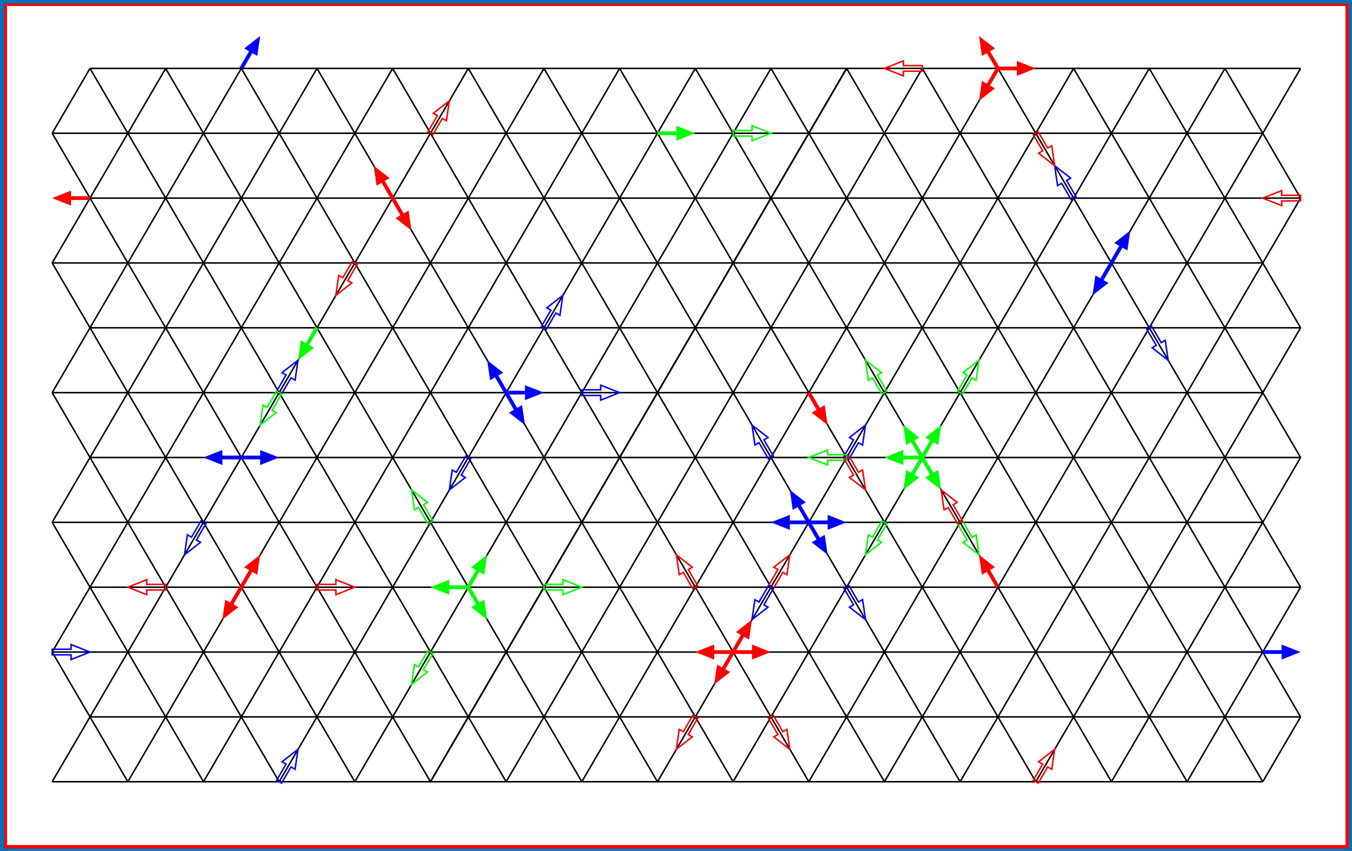
Evolution of LGA: Collision & Advection

$$n_\alpha(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1) = n_\alpha(\boldsymbol{x}_i,\, t) + C_\alpha(\{n_\beta\})$$

FHP LGA Collision Rules



Evolution from t (solid arrows) to $t+1$ (hollow arrows):



Background: Lattice-Gas Automata

The evolution equation of LGA:

$$\boxed{n_\alpha(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1) = n_\alpha(\boldsymbol{x}_i,\, t) + C_\alpha(\{n_\beta\})} \tag{1}$$

$$\rho(\boldsymbol{x}_i,\, t) = m \sum_\alpha n_\alpha(\boldsymbol{x}_i,\, t) \tag{2a}$$

$$\rho\boldsymbol{u}(\boldsymbol{x}_i,\, t) = m \sum_\alpha \boldsymbol{e}_\alpha n_\alpha(\boldsymbol{x}_i,\, t) \tag{2b}$$

α**,** β **:** Discrete velocity index; $\alpha,\ \beta \in \{1,\, 2,\, \cdots,\, b\}$;

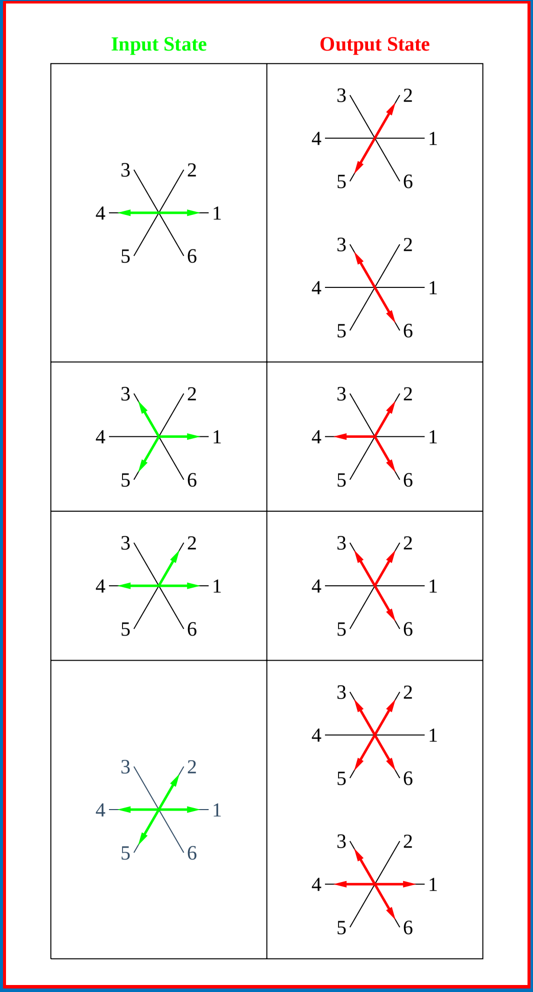
$n_\alpha(\boldsymbol{x}_i,\, t)$ **:** Particle (Boolean) number, with velocity $\boldsymbol{e}_\alpha$, $n_\alpha \in \{0,\, 1\}$.

$C_\alpha(n)$ **:** Collision operator, $C_\alpha \in \{-1,\, 0,\, 1\}$;

$\boldsymbol{e}_\alpha \equiv (\cos[(\alpha-1)\pi/3],\, \sin[(\alpha-1)\pi/3])$: discrete velocity.

Collision Table for 6-Bit FHP Model

FHP LGA Collision Rules



Binary Representation of FHP LGA Collision Rules

INPUT STATE	OUTPUT STATE
001001	010010 100100
010101	101010
001011	100110
011011	110110 101101

Collision Operator

For the FHP model:

$$\begin{aligned} C_\alpha(\{n_\alpha(\boldsymbol{x},\, t)\}) &= \sum_{\boldsymbol{s},\, \boldsymbol{s}'} (s'_\alpha - s_\alpha)\, \xi_{\boldsymbol{s}\boldsymbol{s}'} \prod_{\sigma=1}^{b} n_\sigma^{s_\sigma} (1 - n_\sigma)^{(1-s_\sigma)} \\ &= \sum_{\boldsymbol{s},\, \boldsymbol{s}'} (s'_\alpha - s_\alpha)\, \xi_{\boldsymbol{s}\boldsymbol{s}'} \prod_{\sigma=1}^{b} \delta_{n_\sigma s_\sigma} \qquad (3) \end{aligned}$$

where $\boldsymbol{s} \equiv \{s_1,\, s_2,\, \ldots,\, s_b\}$ and $\boldsymbol{s}' \equiv \{s'_1,\, s'_2,\, \ldots,\, s'_b\}$ are possible pre-collision and post-collision Boolean state, respectively. The Boolean random number satisfies:

Normalization: $$\sum_{\boldsymbol{s}'} \xi_{\boldsymbol{s}\boldsymbol{s}'} = 1\,, \qquad \forall\, \boldsymbol{s} \qquad (4a)$$

Semi-detailed Balance: $$\sum_{\boldsymbol{s}} \xi_{\boldsymbol{s}\boldsymbol{s}'} = 1\,, \qquad \forall\, \boldsymbol{s}' \qquad (4b)$$

Isotropy: $$\xi_{g(\boldsymbol{s})g(\boldsymbol{s}')} = \xi_{\boldsymbol{s}\boldsymbol{s}'}\,, \qquad \forall\, g \in \mathcal{G} \qquad (4c)$$

Collision Operator

Conservation laws:

$$\sum_{\alpha}(s_\alpha - s'_\alpha)\langle\xi_{\boldsymbol{s}\boldsymbol{s}'}\rangle = 0 \qquad \text{(mass)} \tag{5a}$$

$$\sum_{\alpha}(s_\alpha - s'_\alpha)\boldsymbol{e}_\alpha\langle\xi_{\boldsymbol{s}\boldsymbol{s}'}\rangle = 0 \qquad \text{(momentum)} \tag{5b}$$

$$\sum_{\alpha}(s_\alpha - s'_\alpha)\boldsymbol{e}^2_\alpha\langle\xi_{\boldsymbol{s}\boldsymbol{s}'}\rangle = 0 \qquad \text{(energy)} \tag{5c}$$

Example: two-body collision term in 6-velocity FHP model

$$\begin{aligned} C^{(2)}_\alpha \; = \; & +\xi^{(2)}_R\, n_{\alpha+1}n_{\alpha+4}\bar{n}_\alpha\bar{n}_{\alpha+2}\bar{n}_{\alpha+3}\bar{n}_{\alpha+5} \\ & +\xi^{(2)}_L\, n_{\alpha+2}n_{\alpha+5}\bar{n}_\alpha\bar{n}_{\alpha+1}\bar{n}_{\alpha+3}\bar{n}_{\alpha+4} \\ & -[\xi^{(2)}_R + \xi^{(2)}_L]\, n_\alpha n_{\alpha+3}\bar{n}_{\alpha+1}\bar{n}_{\alpha+2}\bar{n}_{\alpha+4}\bar{n}_{\alpha+5} \end{aligned} \tag{6}$$

where $\langle\xi^{(2)}_R\rangle = \langle\xi^{(2)}_L\rangle$, and $\bar{n}_\alpha \equiv (1 - n_\alpha)$.

Chapman-Enskog Analysis

The Boltzmann equation:

$$\partial_t f + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} f = \frac{1}{\varepsilon}\mathcal{C}(f,\, f), \qquad \varepsilon \equiv K_n = \frac{l}{L} \ \text{(Knudsen number)}\,, \tag{7}$$

with the ansatz (normal solution):

$$f(\boldsymbol{x},\, \boldsymbol{\xi},\, t) = f(\boldsymbol{x},\, \boldsymbol{\xi};\, \rho,\, \boldsymbol{u},\, T).$$

Expand

$$f = \sum_{n=0}^{\infty} \varepsilon^n f^{(n)}, \qquad \mathcal{C}(f,\, f) = \sum_{n=0}^{\infty} \varepsilon^n \mathcal{C}^{(n)} \tag{8}$$

with constraints

$$\int d\boldsymbol{\xi} f^{(0)} \begin{bmatrix} 1 \\ \boldsymbol{\xi} \\ (\boldsymbol{\xi}-\boldsymbol{u})^2 \end{bmatrix} = \rho \begin{bmatrix} 1 \\ \boldsymbol{u} \\ D\theta \end{bmatrix}, \tag{9}$$

$$\int d\boldsymbol{\xi} f^{(n)} \begin{bmatrix} 1 \\ \boldsymbol{\xi} \\ (\boldsymbol{\xi}-\boldsymbol{u})^2 \end{bmatrix} = 0\,, \qquad n \geq 1\,. \tag{10}$$

The Normal Solution of the Boltzmann Equation

Solve the ordered equations successively:

$$
\begin{aligned}
O(\epsilon^{-1}) : &\qquad \mathcal{C}(f^{(0)},\, f^{(0)}) = 0, && (11a)\\
O(\epsilon^{0}) : &\qquad \partial_t f^{(0)} + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} f^{(0)} = 2\mathcal{C}(f^{(0)},\, f^{(1)}), && (11b)
\end{aligned}
$$

to obtain the “normal” solution.
The $O(\epsilon^{-1})$ equation yields the Maxwellian equilibrium distribution function:

$$f^{(0)} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\theta}\right]. \qquad (12)$$

The hydrodynamic equations are obtained as follows:

$$\int d\boldsymbol{\xi}\, D_t f \begin{bmatrix} 1 \\ \boldsymbol{\xi} \\ (\boldsymbol{\xi}-\boldsymbol{u})^2 \end{bmatrix} = 0 \begin{cases} f = f^{(0)} & \Rightarrow \text{Euler Equations} \\ f = f^{(0)} + f^{(1)} & \Rightarrow \text{Navier-Stokes Equations} \end{cases}$$

where $D_t \equiv \partial_t + \boldsymbol{\xi}\cdot\boldsymbol{\nabla}$.

Lattice Boltzmann Equation

LBE $\equiv$ Ensemble Average of LGA evolution equation:[1]

$$\boxed{f_\alpha(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1) = f_\alpha(\boldsymbol{x}_i,\, t) + \Omega_\alpha(f)} \tag{13}$$

$$\rho(\boldsymbol{x}_i,\, t) = \sum_\alpha f_\alpha(\boldsymbol{x}_i,\, t) \tag{14a}$$

$$\rho\boldsymbol{u}(\boldsymbol{x}_i,\, t) = \sum_\alpha \boldsymbol{e}_\alpha f_\alpha(\boldsymbol{x}_i,\, t) \tag{14b}$$

$f_\alpha(\boldsymbol{x}_i,\, t)$ **:** Single particle distribution function, with discrete velocity $\boldsymbol{e}_\alpha$,
$f_\alpha = \langle n_\alpha \rangle \in [0,\, 1]$.

$\Omega_\alpha(f)$ **:** LBE Collision operator, $\Omega_\alpha(f) = \langle C_\alpha(n) \rangle \in [-1,\, 1]$.

$$\Omega_\alpha(f) = \sum_{\boldsymbol{s},\, \boldsymbol{s}'} (s'_\alpha - s_\alpha) \left\langle \xi_{\boldsymbol{s}\boldsymbol{s}'} \right\rangle \prod_{\sigma=1}^{b} f_\sigma^{s_\sigma} (1 - f_\sigma)^{(1-s_\sigma)} \tag{15}$$

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[1] G. McNamara and G. Zanetti, *Phys. Rev. Lett.* **61**:2332–2335 (1988)

Lattice Gas Automata Hydrodynamics

The macroscopic equation derived from the Frisch-Hasslacher-Pomeau (FHP) lattice-gas automaton model[2,3,4] through the Chapman-Enskog analysis in the hydrodynamic limit (long wave-length, low frequency):

$$\boxed{\partial_t(\rho\boldsymbol{u}) + \nabla\cdot[g(\rho)\rho\boldsymbol{u}\boldsymbol{u}] = -\nabla P + \nu\nabla^2(\rho\boldsymbol{u}) + \eta\nabla\nabla\cdot(\rho\boldsymbol{u})} \tag{16}$$

Drawbacks of FHP lattice-gas models:

- Simulations are intrinsically noisy due to large fluctuation;
- Lack of Galilean invariance due to $g(\rho) \neq 1$;
- Difficult to increase the Reynolds number Re due to the lower bound of ν;
- $P = c_s^2\rho\,[1 - g(\rho)\,\boldsymbol{u}^2/c^2]$ ($\boldsymbol{u}^2$ term unphysical);
- There exist (unphysical) spurious conserved quantities.

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[2] U. Frisch, B. Hasslacher, and Y. Pomeau, *Phys. Rev. Lett.* **56**:1505–1508 (1986).

[3] S. Wolfram, *J. Stat. Phys.* **45**:471–526 (1986).

[4] U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, *Complex Systems* **1**:649–707 (1987).

Linearized LBE Model

Due to the Boolean nature of the lattice-gas automata, the equilibrium distribution is a Fermi-Dirac distribution:

$$f_\alpha^{(0)} = \frac{1}{1 + \exp(a + \boldsymbol{b} \cdot \boldsymbol{e}_\alpha)} \tag{17}$$

where $a = a(\rho,\, \boldsymbol{u})$ and $\boldsymbol{b} = \boldsymbol{b}(\rho,\, \boldsymbol{u})$.
The collision operator can be linearized about the equilibrium:[5,6]

$$\mathcal{L}_{\alpha\beta} = \left.\frac{\partial \Omega_\beta}{\partial f_\alpha}\right|_{f=f^{(0)}} [f_\alpha - f_\alpha^{(0)}] \tag{18}$$

With the linearized collision operator, the LBE computation is greatly simplified.

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[5] F.J. Higuera and J. Jiménez, *Europhys. Lett.* **9**:663–668 (1989).

[6] F.J. Higuera, S. Succi, and R. Benzi, *Europhys. Lett.* **9**:345–349 (1989).

Bhatnagar-Gross-Krook Approximation

LBE collision operator: LGA ⇒ LBE ⇒ Linearized LBE ⇒ LBGK

$$\Omega_\alpha(f) = -\frac{1}{\tau}[f_\alpha - f_\alpha^{(\mathrm{eq})}]\,, \tag{19}$$

Equilibrium distribution function:

$$f_\alpha^{(\mathrm{eq})} = w_\alpha \rho \left[1 + A\,(\boldsymbol{e}_\alpha \cdot \boldsymbol{u}) + B\,(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})^2 + C\,\boldsymbol{u}^2\right]\,, \tag{20}$$

where w_α, A, B, and C are determined by conservation laws.
The lattice (BGK) Boltzmann Equation:[5,6]

$$\boxed{f_\alpha(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1) = f_\alpha(\boldsymbol{x}_i,\, t) - \frac{1}{\tau}\left[f_\alpha(\boldsymbol{x}_i,\, t) - f_\alpha^{(\mathrm{eq})}(\boldsymbol{x}_i,\, t)\right]} \tag{21}$$

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[6] Y.H. Qian, D. d'Humières, and P. Lallemand, *Europhys. Lett.* **17**:479–484 (1992).

[7] H. Chen, S. Chen, and W.H. Matthaeus, *Phys. Rev. A* **45**:R5339–R5342 (1992).

LBE Hydrodynamics

LBE $\Longrightarrow$ the Navier-Stokes equation ($K_n,\ \delta_x,\ \delta_t \to 0$):

$$\boxed{\rho\,\partial_t \boldsymbol{u} + \rho\,\boldsymbol{u}\nabla\cdot\boldsymbol{u} = -\nabla P + \rho\,\nu\nabla^2\boldsymbol{u}} \tag{22}$$

$$P = c_s^2\,\rho \tag{23a}$$

$$\nu = c_s^2\left(\tau - \frac{1}{2}\right) \tag{23b}$$

where $c_s \sim \sqrt{k_B T/m} = \sqrt{\theta}$ is the sound speed, depending on the discrete velocity set.

- LBE overcomes many shortcomings of LGA;
- Tradeoff: floating number calculations, roundoff error.

Features of the Lattice Boltzmann Equation

Key Features of the LBE method

- Derived from hyperbolic equation;
- Linear advection term $e_\alpha \cdot \nabla f_\alpha$;
- Intrinsically compressible and has correct acoustics;
- Preserve conservation laws and all the necessary symmetries;
- 1st order finite-difference in form,
  Accuracy: 2nd-order δ_x and 1st-order δ_t;
- Grid CFL $= 1$;
- Ability to include model interactions.

Computational Characteristics of the LBE method

- Usually use Cartesian grid;
- Use equation of state to obtain pressure;
- Intrinsic parallelism due to uniform, nearest neighbor data communications (streaming) and purely local calculations (collision);
- Ability to handle complex boundaries without losing computat. speed;
- Broad applications.

First-Order PDE's *vs.* Higher-Order PDE's

Possible advantages of using the PDE's of the lowest possible order (1st-order) as oppose to the traditional higher-order systems:[7]

- Require the smallest possible stencil for accurate discretization;
- Local stiffness *vs.* global stiffness;
- May be easier to derive to convergence than equivalent higher-order systems;
- First-order PDE's yield the highest potential discretization accuracy on non-smooth, adaptively refined grids;
- Better suited for functional decomposition;
- Can be used to describe extended hydrodynamics.

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[7] B. van Leer, *AIAA Tech. Paper 2001-2520* (2001).

Summary

The lattice-gas automata:

- Mimicking (simplified) molecular dynamics;
- Exactly preserving conservation laws;
- Processing basic symmetries;
- Spurious conserved quantities;
- Large fluctuations;
- Boolean nature (integer or logic or table-lookup algorithms).

The lattice Boltzmann equation:

- Simplified Boltzmann equation;
- Overcoming some defects of the lattice-gas automata;
- No fluctuations;
- Floating number algorithms;
- Enhance numerical efficiency.

Conclusion: The LGA and LBE methods can simulate hydrodynamics.