

Lecture 2: Derivation of LBE Models

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A *Priori* Derivation of Lattice Boltzmann Equation

The Boltzmann Equation with BGK approximation:

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = -\frac{1}{\lambda} [f - f^{(0)}], \quad f \equiv f(x, \boldsymbol{\xi}, t). \quad (1)$$

The Boltzmann-Maxwellian equilibrium distribution function:

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

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

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

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

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

Integral Solution of Continuous Boltzmann Equation

Rewrite the Boltzmann BGK Equation in the form of ODE:

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

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

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

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

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

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

Passage to Lattice Boltzmann Equation

Necessary steps to obtain LBE:^{1,2}

1. Low Mach number expansion of the equilibrium distribution function;
2. Discretization of velocity space ξ to obtain necessary and minimum number of ξ_α ;
3. Discretization of x space according to $\{\xi_\alpha\}$.

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

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

It should be noted that many defects of the lattice Boltzmann method are related to the above “low Mach number expansion of the equilibrium function. However, this expansion is necessary to make the lattice Boltzmann method a simple and explicit scheme.

¹X. He and L.-S. Luo, *Phys. Rev. E* **55**:R6333 (1997); *ibid* **56**:6811 (1997).

²T. Abe, *J. Comp. Phys.* **131**:241 (1997).

Luo, NIA: LBE Method for CFD, CAB-TUB, Aug. 7-12, 2003

Discretization and Conservation Laws

The **conservation laws** are preserved **exactly**, if the hydrodynamic moments (ρ , ρu , and $\rho \epsilon$) are evaluated **exactly**:

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

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

$$I = \int \exp(-\xi^2/2\theta) \psi(\xi) d\xi = \sum_j W_j \exp(-\xi_j^2/2\theta) \psi(\xi_j) \quad (9)$$

where ξ_j and W_j are the abscissas and the weights. Then

$$\rho = \sum_{\alpha} f_{\alpha}^{(\text{eq})} = \sum_{\alpha} f_{\alpha}, \quad \rho u = \sum_{\alpha} \xi_{\alpha} f_{\alpha}^{(\text{eq})} = \sum_{\alpha} \xi_{\alpha} f_{\alpha}, \quad (10)$$

where $f_{\alpha} \equiv f_{\alpha}(\mathbf{x}, t) \equiv W_{\alpha} f(\mathbf{x}, \xi_{\alpha}, t)$, and $f_{\alpha}^{(\text{eq})} \equiv W_{\alpha} f^{(\text{eq})}(\mathbf{x}, \xi_{\alpha}, t)$.

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

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

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 ξ -Space (9-bit Model)

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

$$\begin{aligned} \zeta_1 &= -\sqrt{3}/2, & \zeta_2 &= 0, & \zeta_3 &= \sqrt{3}/2, \\ \omega_1 &= \sqrt{\pi}/6, & \omega_2 &= 2\sqrt{\pi}/3, & \omega_3 &= \sqrt{\pi}/6. \end{aligned} \quad (12)$$

Then, the integral of moments becomes:

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

where

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

Discretization of Velocity ξ -Space (9-bit Model)

Identifying

$$W_\alpha = (2\pi\theta) \exp(\xi_\alpha^2/2\theta) w_\alpha, \quad (15)$$

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:

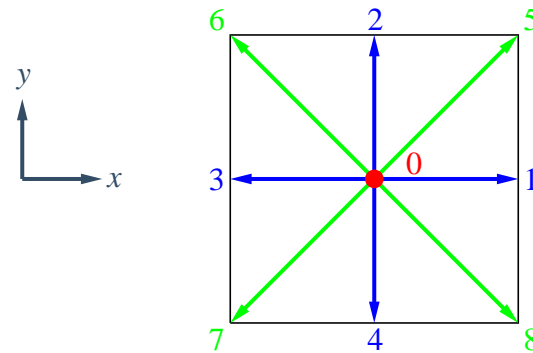
$$\begin{aligned} f_\alpha^{(\text{eq})}(\mathbf{x}, t) &= W_\alpha f^{(\text{eq})}(\mathbf{x}, \xi_\alpha, t) \\ &= w_\alpha \rho \left\{ 1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u})}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c^4} - \frac{3u^2}{2c^2} \right\}, \end{aligned} \quad (16)$$

where weight coefficient w_α and discrete velocity \mathbf{e}_α are:

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

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

Discretized 2D Velocity Space (9-bit)



$$e_{\alpha} = \begin{cases} (0, 0), & \alpha = 0, \\ (\pm 1, 0) c, (0, \pm 1) c, & \alpha = 1 - 4, \\ (\pm 1, \pm 1) c, & \alpha = 5 - 8. \end{cases}$$

Boltzmann Theory for Rarefied Gases (1890')

The Boltzmann equation

$$\partial_t f + \xi \cdot \nabla f + a \cdot \nabla_{\xi} f = \int d\mu_1 [f' f'_1 - f f_1] \quad (18)$$

is valid in the Boltzmann Gas Limit (BGL):

$$\text{Particle Number} \quad N \rightarrow \infty, \quad (19a)$$

$$\text{Interaction Range} \quad r_0 \rightarrow 0, \quad (19b)$$

$$\text{Mean-Free-Path} \quad l \sim (Nr_0^2)^{-1} \rightarrow \text{Constant}, \quad (19c)$$

$$\text{Interaction Volume} \quad Nr_0^3 \rightarrow 0. \quad (19d)$$

Because of $Nr_0^3 \rightarrow 0$, the Boltzmann equation can *only* retain the thermodynamics of *ideal* gases.

Enskog's Theory for Dense Gases (1917)

For hard spheres of radius r_0 , the Boltzmann equation is modified dense gases as follows (by Enskog):

$$\partial_t f + \xi \cdot \nabla f + \mathbf{a} \cdot \nabla_\xi f = J, \quad (20)$$

$$\begin{aligned} J &= \int d\mu_1 [g(\mathbf{x} + r_0 \hat{\mathbf{r}}) f' f'_1(\mathbf{x} + 2r_0 \hat{\mathbf{r}}) - g(\mathbf{x} - r_0 \hat{\mathbf{r}}) f f_1(\mathbf{x} - 2r_0 \hat{\mathbf{r}})] \\ &= J^{(0)} + J^{(1)} + J^{(2)} + \dots, \end{aligned} \quad (21a)$$

$$J^{(0)} = g \int d\mu_1 [f' f'_1 - f f_1], \quad (21b)$$

$$J^{(1)} = r_0 \int d\mu_1 \hat{\mathbf{r}} \cdot \nabla [f' f'_1 + f f_1], \quad (21c)$$

$$J^{(2)} = 2r_0 g \int d\mu_1 \hat{\mathbf{r}} \cdot [f' \nabla f'_1 + f \nabla f_1], \quad (21d)$$

Enskog Closure of f_2 (1917)

The essential assumption is the factorization of the two particle distribution function — the Enskog closure:

$$f_2(\boldsymbol{x}_1, \boldsymbol{\xi}_1, \boldsymbol{x}_2, \boldsymbol{\xi}_2, t) = g(|\boldsymbol{x}_1 - \boldsymbol{x}_2|) f_1(\boldsymbol{x}_1, \boldsymbol{\xi}_1, t) f_1(\boldsymbol{x}_2, \boldsymbol{\xi}_2, t), \quad (22)$$

where g is the radial distribution function (pairwise correlation).

The Boltzmann closure:

$$f_2(\boldsymbol{x}_1, \boldsymbol{\xi}_1, \boldsymbol{x}_2, \boldsymbol{\xi}_2, t) = f_1(\boldsymbol{x}_1, \boldsymbol{\xi}_1, t) f_1(\boldsymbol{x}_2, \boldsymbol{\xi}_2, t)$$

Non-Local Collision Terms in the Enskog Equation

With the approximation $f \approx f^{(0)}$, which is consistent with the Chapman-Enskog analysis:

$$J^{(1)} = -f^{(0)} b \rho \xi_0 \cdot \nabla g, \quad (23a)$$

$$\begin{aligned} J^{(2)} = & -f^{(0)} b \rho g \left[2\xi_0 \cdot \nabla \ln \rho + \frac{2}{(D+2)} \frac{\xi_{0i} \xi_{0j} \partial_i u_j}{\theta} \right. \\ & + \left. \left(\frac{1}{(D+2)} \frac{\xi_0^2}{\theta} - 1 \right) \nabla \cdot u \right. \\ & \left. + \frac{1}{2} \left(\frac{D}{(D+2)} \frac{\xi_0^2}{\theta} - 1 \right) \xi_0 \cdot \nabla \ln \theta \right], \end{aligned} \quad (23b)$$

$$f^{(0)}(\rho, \mathbf{u}, \theta) = \rho (2\pi\theta)^{-D/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2\theta} \right], \quad (24)$$

where $\boldsymbol{\xi}_0 = (\boldsymbol{\xi} - \mathbf{u})$ is the peculiar velocity, $\theta = k_B T/m$ is the normalized temperature, and $b = V_0/m = 4\pi r_0^3/3m$ is the second virial coefficient.

Normal Solutions of the Enskog Equation (1917)

The first and second order normal solution of the Enskog equation, obtained via Chapman-Enskog analysis, are:

$$f^{(0)} = \rho (2\pi\theta)^{-D/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2\theta} \right], \quad (25)$$

$$f^{(1)} = -f^{(0)} \frac{1}{g} \left[\left(1 + \frac{2}{(D+2)} b\rho g \right) \mathbf{A} \cdot \nabla \ln \theta \right. \\ \left. + \left(1 + \frac{4}{D(D+2)} b\rho g \right) B_{ij} \partial_i u_j \right]. \quad (26)$$

With $b = 0$ and $g = 1$, the solutions reduce to that of the Boltzmann equation.

Note that $\nabla \rho$ does *NOT* appear in $f^{(1)}$, it appears in $f^{(2)}$ — the Burnett solution (1935). This is consistent with the dimensional analysis of the Navier-Stokes equation, $\nabla \rho$ is in the order of $O(K_n^2)$, where K_n is the Knudsen number, which is also the small expansion parameter in the Chapman-Enskog analysis.

The Navier-Stokes Equations

The Navier-Stokes equations derived from the Enskog equation:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (27a)$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla P + \mathbf{a}, \quad (27b)$$

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = -\frac{1}{\rho} \nabla \cdot \mathbf{q} - \frac{1}{\rho} \mathbf{P}_{ij} \partial_i u_j + \mathbf{a} \cdot \mathbf{u}, \quad (27c)$$

where

$$\begin{aligned} \mathbf{P}_{ij} = \int d\xi \xi_0 i \xi_0 j f = & [\rho \theta (1 + b\rho g) - \eta_2 \nabla \cdot \mathbf{u}] \delta_{ij} \\ & - \left[\frac{2}{g} \left(1 + \frac{4}{D(D+2)} b\rho g \right)^2 \eta_1 + \frac{2D}{(D+2)} \eta_2 \right] S_{ij}, \end{aligned} \quad (28a)$$

$$S_{ij} = \frac{1}{2} [\partial_i u_j + \partial_j u_i] - \frac{1}{D} \nabla \cdot \mathbf{u} \delta_{ij}, \quad (28b)$$

$$\mathbf{q} = \int d\xi \frac{1}{2} \xi_0^2 \xi_0 f = - \left[\frac{1}{g} (1 + b\rho g)^2 \kappa + \frac{D}{2} \eta_2 \right] \nabla \theta. \quad (28c)$$

Incompressible and Isothermal Fluids

Because $\nabla \cdot \mathbf{u} = 0$ and $\nabla \theta = 0$:

$$\begin{aligned} J^{(1)} + J^{(2)} &\approx -f^{(0)} b \rho (\boldsymbol{\xi} - \mathbf{u}) \cdot [\nabla g + g \nabla \ln \rho^2] \\ &= -f^{(0)} b \rho g (\boldsymbol{\xi} - \mathbf{u}) \cdot \nabla \ln(\rho^2 g) = J' . \end{aligned} \quad (29)$$

The modified Boltzmann equation, with BGK approximation:

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f + \mathbf{a} \cdot \nabla_{\boldsymbol{\xi}} f = -\frac{g}{\lambda} [f - f^{(0)}] - f^{(0)} b \rho g (\boldsymbol{\xi} - \mathbf{u}) \cdot \nabla \ln(\rho^2 g) . \quad (30)$$

The equation of state derived from the above modified Boltzmann equation (by computing the first moment of the non-local collision term):

$$P = \rho \theta [1 + b \rho g] , \quad g = g(b \rho) . \quad (31)$$

Physics: The non-ideal gas effects come from the non-local collision term, which is the manifestation of the volume exclusion effect, or other inter-particle interactions. It cannot be a result of body force.

Integral Solution of Continuous Enskog Equation

Rewrite the Enskog BGK Equation in the form of ODE:

$$\frac{df}{dt} + \frac{g}{\lambda} f = \frac{g}{\lambda} f^{(0)} + J', \quad \frac{d}{dt} \equiv \frac{\partial}{\partial t} + \boldsymbol{\xi} \cdot \nabla + \mathbf{a} \cdot \nabla_{\boldsymbol{\xi}}. \quad (32)$$

Integrate Eq. (32) over a time step δ_t along characteristic line:

$$f(\mathbf{x} + \boldsymbol{\xi} \delta_t + \frac{1}{2} \mathbf{a} \delta_t^2, \boldsymbol{\xi} + \mathbf{a} \delta_t, t + \delta_t) = e^{-\delta_t g / \lambda} f(\mathbf{x}, \boldsymbol{\xi}, t) \\ + e^{-\delta_t g / \lambda} \int_0^{\delta_t} dt' e^{t' g / \lambda} \left[\frac{g}{\lambda} f^{(0)} + J' \right]_{(\mathbf{x} + \boldsymbol{\xi} t' + \frac{1}{2} \mathbf{a} t'^2, \boldsymbol{\xi} + \mathbf{a} t', t + t')}. \quad (33)$$

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

$$f(\mathbf{x} + \boldsymbol{\xi} \delta_t, \boldsymbol{\xi}, t + \delta_t) - f(\mathbf{x}, \boldsymbol{\xi}, t) = -\frac{g}{\tau} [f(\mathbf{x}, \boldsymbol{\xi}, t) - f^{(0)}(\mathbf{x}, \boldsymbol{\xi}, t)] \\ + [J' - \mathbf{a} \cdot \nabla_{\boldsymbol{\xi}} f] \delta_t + \mathcal{O}(\delta_t^2). \quad (34)$$

Temporal discretization is completed.

The External Forcing

The forcing term must satisfy the following moment constraints:

$$\int d\xi \mathbf{a} \cdot \nabla_{\xi} f = 0, \quad (35a)$$

$$\int d\xi \xi \mathbf{a} \cdot \nabla_{\xi} f = -\rho \mathbf{a}, \quad (35b)$$

$$\int d\xi \xi_i \xi_j \mathbf{a} \cdot \nabla_{\xi} f = -\rho (a_i u_j + a_j u_i). \quad (35c)$$

Similar to the equilibrium, the forcing term is expanded in term of \mathbf{u} , and we obtain

$$\mathbf{a} \cdot \nabla_{\xi} f = -\rho \exp(-\xi^2/2\theta) \left[\frac{1}{\theta} (\xi - \mathbf{u}) + \frac{(\xi \cdot \mathbf{u})}{\theta^2} \xi \right] \cdot \mathbf{a}. \quad (36)$$

Note that in the above expansion, only the terms up to the first order in \mathbf{u} have been retained, because there is an overall factor of δ_{τ} in the forcing term. If the second-order moment constraint Eq. (35) is ignored:

$$\mathbf{a} \cdot \nabla_{\xi} f = -\rho \exp(-\xi^2/2\theta) \frac{1}{\theta} \xi \cdot \mathbf{a}. \quad (37)$$

Discretized Enskog Equation: LBE Nonideal Gas Model

The LBE model for non-ideal gases with external forcing:

$$f_{\alpha}(\boldsymbol{x} + \boldsymbol{e}_{\alpha}\delta t, t + \delta t) = -\frac{g}{\tau}[f_{\alpha} - f_{\alpha}^{(\text{eq})}] + (J'_{\alpha} + F_{\alpha})\delta t \quad (38)$$

$$J'_{\alpha} = -f_{\alpha}^{(\text{eq})}b\rho g(\boldsymbol{e}_{\alpha} - \boldsymbol{u}) \cdot \nabla \ln(\rho^2 g) \quad (39a)$$

$$F_{\alpha} = w_{\alpha}\rho \left[\frac{3}{c^2}(\boldsymbol{e}_{\alpha} - \boldsymbol{u}) + \frac{g}{c^4}(\boldsymbol{e}_{\alpha} \cdot \boldsymbol{u})\boldsymbol{e}_{\alpha} \right] \cdot \boldsymbol{a} \quad (39b)$$

For hard-spheres:

$$g = 1 + \frac{5}{8}b\rho + 0.2869(b\rho)^2 + \dots$$

The Enskog equation has an H -Theorem and a consistent thermodynamics.

Equation of State and Viscosity

The equation of state:

$$P = \rho\theta[1 + b\rho g]$$

Viscosity:

$$\nu = \frac{1}{3} \left(\frac{\tau}{g} - \frac{1}{2} \right) c\delta_x = \left(\frac{\tau}{g} - \frac{1}{3} \right) \theta\delta_t$$

The g -dependence in ν can be eliminated by setting the relaxation parameter to $1/\tau$.

Summary

- Lattice Boltzmann equation can be derived (**without referenced to LGA**);
- Lattice Boltzmann equation is a finite difference scheme;
- LBE preserves conservation laws rigorously (conservative form);
- LBE can use Interpolations (with care);
- LBE models for multi-phase and multi-component fluids can also be derived from kinetic equations.