Lattice Boltzmann Equation
Its Mathematical Essence and Key Properties

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Outline

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1. Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods
2. LBE: Mathematical Derivation
   - Discretizing time t
   - Low-Mach-Number Expansion
   - Discretize Velocity Space ξ
   - Discretize Space x
   - Treatment of Collision
   - Example: D3Q19
   - Other Models
3. Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis
4. Conclusions

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Navier-Stokes Equations: Continuum Theory

Conservation laws of mass, momentum, and energy:

$$\partial_t \rho + \boldsymbol{\nabla}\cdot \rho \boldsymbol{u} = 0 \tag{1a}$$

$$\rho \partial_t \boldsymbol{u} + \rho \boldsymbol{u}\cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla}\cdot \mathsf{P} \tag{1b}$$

$$\rho \partial_t e + \rho \boldsymbol{u}\cdot \boldsymbol{\nabla} e = -\mathsf{P} : \boldsymbol{\nabla} \boldsymbol{u} - \boldsymbol{\nabla}\cdot \boldsymbol{q} \tag{1c}$$

$$\mathsf{P} = p\mathsf{I} - \mathsf{S}, \quad \mathsf{S}_{\alpha\beta} = \mu \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha\right) + \left(\zeta - \frac{2}{3}\mu\right) \delta_{\alpha\beta} \boldsymbol{\nabla}\cdot \boldsymbol{u} \tag{1d}$$

$$\boldsymbol{q} = -\kappa \boldsymbol{\nabla} T, \quad e = e(T), \quad p = p(\rho, T) \tag{1e}$$

Dimensionless Navier-Stokes equations (similarity law):

$$\rho \partial_t \boldsymbol{u} + \rho \boldsymbol{u}\cdot \boldsymbol{\nabla} \boldsymbol{u} = -\frac{1}{\gamma \mathrm{Ma}^2} \boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}} \boldsymbol{\nabla}\cdot \mathsf{S} \tag{2a}$$

$$\rho \partial_t e + \rho \boldsymbol{u}\cdot \boldsymbol{\nabla} e = -\frac{1}{\gamma \mathrm{Ma}^2} p \boldsymbol{\nabla}\cdot \boldsymbol{u} + \frac{1}{\alpha} \nabla^2 T + \frac{1}{\mathrm{Re}} \mathsf{S} : \boldsymbol{\nabla} \boldsymbol{u} \tag{2b}$$

$$\alpha = (\gamma - 1)\, \mathrm{Pr}\, \mathrm{Ma}\, \mathrm{Re}, \quad \gamma := C_P / C_V$$

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Kinetic Equation

The kinetic equation for the single particle distribution function f in phase space $\boldsymbol{\Gamma} := (\boldsymbol{x}, \boldsymbol{\xi})$:

$$\partial_t f + \boldsymbol{\nabla} \cdot (\boldsymbol{\xi} f) = Q, \qquad f := f(\boldsymbol{x}, \boldsymbol{\xi}, t) \tag{3}$$

The Uehling-Uhlenbeck collision model:

$$Q[f, f] = \int d\boldsymbol{\xi}_2 \int d\Omega \, K \left[(1 + \eta f_1)(1 + \eta f_2) f_1' f_2' - \left(1 + \eta f_1'\right)\left(1 + \eta f_2'\right) f_1 f_2 \right] \tag{4}$$

where Ω is the solid angle, $K := K(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \Omega)$ is the collision kernel,

$$K(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \Omega) = K(\boldsymbol{\xi}_2, \boldsymbol{\xi}_1, \Omega) = K(\boldsymbol{\xi}_1', \boldsymbol{\xi}_2', \Omega) \geq 0 \tag{5}$$

$$\eta = \begin{cases} +1 & \text{Bose-Einstein} \\ 0 & \text{Maxwell-Boltzmann} \\ -1 & \text{Fermi-Dirac} \end{cases} \tag{6}$$

From KE to Hydrodynamics Equations

Expansion of f in terms of the Knudsen number $\varepsilon = \mathrm{Kn} := \ell/L$:

$$f = f^{(0)} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \cdots, \qquad f^{(0)} = \frac{\rho}{(2\pi RT)^{D/2}} e^{-(\boldsymbol{\xi}-\boldsymbol{u})^2/2RT} \tag{7}$$

Velocity moments of f are hydrodynamic quantities and their fluxes:

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Velocity moments of f are hydrodynamic quantities and their fluxes:

$$\boldsymbol{\xi}^0: \quad \rho = \int f \mathrm{d}\boldsymbol{\xi} = \int f^{(0)} \mathrm{d}\boldsymbol{\xi} \tag{8a}$$

$$\boldsymbol{\xi}^1: \quad \rho\boldsymbol{u} = \int f \boldsymbol{\xi} \mathrm{d}\boldsymbol{\xi} = \int f^{(0)} \boldsymbol{\xi} \mathrm{d}\boldsymbol{\xi} \tag{8b}$$

$$\boldsymbol{\xi}^2: \quad \rho e = \frac{D}{2}\rho RT = \int \frac{1}{2} c^2 \boldsymbol{c} f \, \mathrm{d}\boldsymbol{\xi} = \int \frac{1}{2} c^2 \boldsymbol{c} f^{(0)} \, \mathrm{d}\boldsymbol{\xi}, \quad \boldsymbol{c} := \boldsymbol{\xi} - \boldsymbol{u} \tag{8c}$$

$$\boldsymbol{\xi}^2: \quad \mathsf{P} = \int \boldsymbol{c}\boldsymbol{c} f \, \mathrm{d}\boldsymbol{\xi}, \qquad \boldsymbol{\xi}^3: \quad \boldsymbol{q} = \int \frac{1}{2} c^2 \boldsymbol{c} f \, \mathrm{d}\boldsymbol{\xi} \tag{8d}$$

Multiscale Formalism

$$\partial_t \rho + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u} = 0 \tag{9a}$$

$$\partial_t \rho \boldsymbol{u} + \boldsymbol{\nabla} \cdot \rho \left(\boldsymbol{u}\boldsymbol{u} + \mathsf{\mathbf{P}} \right) = 0 \tag{9b}$$

$$\partial_t \rho E + \boldsymbol{\nabla} \cdot \rho \left(\boldsymbol{u} E + \boldsymbol{u} \cdot \mathsf{\mathbf{P}} + \boldsymbol{q} \right) = 0, \quad E := \rho e + \frac{1}{2} \rho u^2 \tag{9c}$$

$$\mathsf{\mathbf{P}} = \mathsf{P}^{(0)} + \mathsf{P}^{(1)} + \mathsf{P}^{(2)} + \cdots \tag{9d}$$

$$\boldsymbol{q} = \boldsymbol{q}^{(0)} + \boldsymbol{q}^{(1)} + \boldsymbol{q}^{(2)} + \cdots \tag{9e}$$

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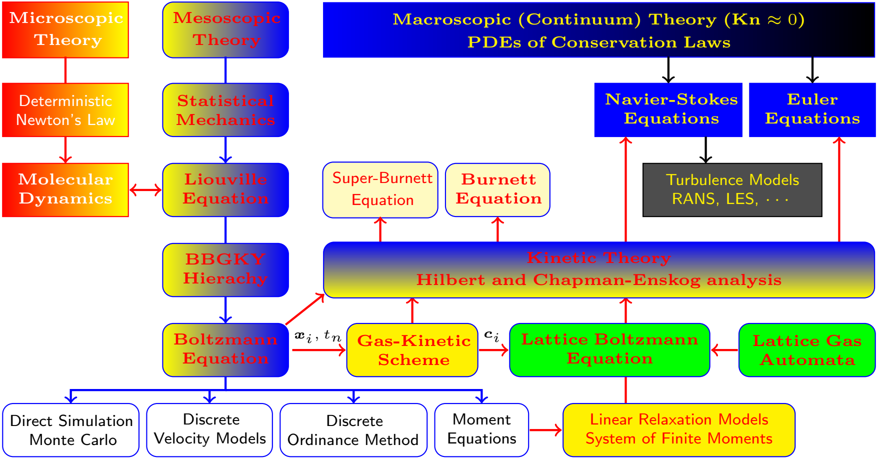
$$f = f^{(0)} \implies \left\{ \begin{array}{l} \mathsf{P}^{(0)} = \dfrac{3}{2} \rho R T \mathsf{I} \\ \boldsymbol{q}^{(0)} = \boldsymbol{0} \end{array} \right\} \implies \text{Euler Eqns (inviscid)}$$

$$f = f^{(0)} + f^{(1)} \implies \left\{ \begin{array}{l} \mathsf{P}^{(1)} = -\dfrac{1}{2} \mu [(\boldsymbol{\nabla} \boldsymbol{u}) + (\boldsymbol{\nabla} \boldsymbol{u})^{\dagger}] \\ \boldsymbol{q}^{(1)} = -\kappa \boldsymbol{\nabla} T \end{array} \right\} \implies \text{NS Eqns}$$

$\dots$

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



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A Priori Derivation of Lattice Boltzmann Equation

The Boltzmann Equation for $f := f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ with BGK approximation:

$$\partial_t f + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f = \int [f_1' f_2' - f_1 f_2] \mathrm{d}\boldsymbol{\mu} \approx \mathcal{L}(f, f) \approx -\frac{1}{\lambda}[f - f^{(0)}] \tag{10}$$

The Boltzmann-Maxwellian equilibrium distribution function:

$$f^{(0)} = \rho \, (2\pi\theta)^{-D/2} \exp\left[-\frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2\theta}\right], \quad \theta := RT \tag{11}$$

The macroscopic variables are the first few $(d+2)$ moments of f or $f^{(0)}$:

$$\rho \begin{pmatrix} 1 \\ \boldsymbol{u} \\ e \end{pmatrix} = \int \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \boldsymbol{c} \cdot \boldsymbol{c}/2 \end{pmatrix} f \mathrm{d}\boldsymbol{\xi} = \int \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \boldsymbol{c} \cdot \boldsymbol{c}/2 \end{pmatrix} f^{(0)} \mathrm{d}\boldsymbol{\xi}, \quad \boldsymbol{c} := \boldsymbol{\xi} - \boldsymbol{u} \tag{12}$$

The *invariants* of the collision Q manifest the microscopic conservation laws, which are the physical basis of the macroscopic conservation laws:

$$\int \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \boldsymbol{c} \cdot \boldsymbol{c}/2 \end{pmatrix} Q \, \mathrm{d}\boldsymbol{\xi} = \int \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \boldsymbol{\xi} \cdot \boldsymbol{\xi}/2 \end{pmatrix} Q \, \mathrm{d}\boldsymbol{\xi} = \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \end{pmatrix} \tag{13}$$

Integral Solution of Continuous Boltzmann Equation

Rewrite the Boltzmann BGK Equation in the form of ODE:

$$D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)}, \qquad D_t := \partial_t + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} \tag{14}$$

Integrate Eq. (14) over a time step δ_t along characteristics:

$$\begin{aligned} f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) = {} & e^{-\delta_t/\lambda} f(\boldsymbol{x}, \boldsymbol{\xi}, t) \\ & + \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^{t'/\lambda} f^{(0)}(\boldsymbol{x} + \boldsymbol{\xi} t', \boldsymbol{\xi}, t + t')\, \mathrm{d}t' \end{aligned} \tag{15}$$

Remark: a fully compressible *finite-volume* scheme or higher-order schemes can also be formulated based upon the integral solution.[1]

[1] K. Xu and K. Prendergast. *J. Comput. Phys.* **114**9 (1994); K. Xu *ibid* **171** 289–335 (2001)

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Passage to Lattice Boltzmann Equation

The necessary steps to derive LBE:[2]

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

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

Outline

LBE: Discretizing t

Linear approximation of $f^{(0)}$ in the integral solution (15):

$$f^{(0)}(\boldsymbol{x}+\boldsymbol{\xi}t',\,\boldsymbol{\xi},\,t+t') = \left(1-\frac{t'}{\delta_t}\right)f^{(0)}(t) + \frac{t'}{\delta_t}f^{(0)}(t+\delta_t) + O(\delta_t^2)$$

the integral solution (15) becomes:

$$\begin{aligned} f(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\,\boldsymbol{\xi},\,t+\delta_t) - f(\boldsymbol{x},\,\boldsymbol{\xi},\,t) &= \left(e^{-\delta_t/\lambda}-1\right)\left[f(\boldsymbol{x},\,\boldsymbol{\xi},\,t) - f^{(0)}(\boldsymbol{x},\,\boldsymbol{\xi},\,t)\right] \\ &+ \underbrace{\left(1+\frac{\delta_t}{\lambda}\left(e^{-\delta_t/\lambda}-1\right)\right)\left[f^{(0)}(t+\delta_t) - f^{(0)}(t)\right]}_{O(\delta_t^2)} + O(\delta_t^2) \end{aligned}$$

With the Taylor expansion in δ_t, and $\tau := \lambda/\delta_t$,

$$f(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\,\boldsymbol{\xi},\,t+\delta_t) - f(\boldsymbol{x},\,\boldsymbol{\xi},\,t) = -\frac{1}{\tau}\left[f(\boldsymbol{x},\,\boldsymbol{\xi},\,t) - f^{(0)}(\boldsymbol{x},\,\boldsymbol{\xi},\,t)\right] + O(\delta_t^2) \tag{16}$$

Outline

Low Mach Number Expansion (Approximation)

The low-Mach-number ($\boldsymbol{u} \approx 0$) expansion of the distribution functions $f^{(0)}$ and f up to $O(\boldsymbol{u}^2)$ is sufficient to derive the Navier-Stokes equations:

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \left\{1 + \frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{\theta} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2\theta^2} - \frac{\boldsymbol{u}^2}{2\theta}\right\} + O(\boldsymbol{u}^3) \tag{17a}$$

$$f = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \sum_{n=0}^{2} \frac{1}{n!} \mathbf{a}^{(n)}(\boldsymbol{x},\, t) : \mathbf{H}^{(n)}(\boldsymbol{\xi}) \tag{17b}$$

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

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$$f = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \sum_{n=0}^{2} \frac{1}{n!} \mathsf{a}^{(n)}(\boldsymbol{x},\, t) : \mathsf{H}^{(n)}(\boldsymbol{\xi}) \quad \text{(17b)}$$

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It should be noted that some defects of the lattice Boltzmann method are related to the low-Mach-number expansion of the distribution functions. However, this expansion is necessary to make the lattice Boltzmann method a simple and explicit scheme.

Outline

Discretize $\boldsymbol{\xi}$ and Preserve Conservation Laws

To compute conserved moments (ρ, $\rho\boldsymbol{u}$, and ρe) and their fluxes, one must evalute:

$$I = \int \boldsymbol{\xi}^m f^{(\mathrm{eq})} d\boldsymbol{\xi} = \int \exp(-\boldsymbol{\xi}^2/2\theta)\psi(\boldsymbol{\xi})d\boldsymbol{\xi}, \tag{18}$$

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

$$I = \int \exp(-\boldsymbol{\xi}^2/2\theta)\psi(\boldsymbol{\xi})d\boldsymbol{\xi} = \sum_j W_j \exp(-\boldsymbol{\xi}_j^2/2\theta)\psi(\boldsymbol{\xi}_j) \tag{19}$$

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

$$\rho = \sum_i f_i^{(\mathrm{eq})} = \sum_i f_i, \qquad \rho\boldsymbol{u} = \sum_i \boldsymbol{\xi}_i f_i^{(\mathrm{eq})} = \sum_i \boldsymbol{\xi}_i f_i, \tag{20}$$

where $f_i := f_i(\boldsymbol{x}, t) := W_i f(\boldsymbol{x}, \boldsymbol{\xi}_i, t)$, and $f_i^{(\mathrm{eq})} := W_i f^{(\mathrm{eq})}(\boldsymbol{x}, \boldsymbol{\xi}_i, t)$.

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

$$I = (\sqrt{2\theta})^{(m+n+2)} I_m I_n, \qquad I_m = \int_{-\infty}^{+\infty} e^{-\zeta^2} \zeta^m d\zeta, \tag{21}$$

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:

$$\begin{array}{lll} \zeta_1 = -\sqrt{3/2}\,, & \zeta_2 = 0\,, & \zeta_3 = \sqrt{3/2}\,, \\ \omega_1 = \sqrt{\pi}/6\,, & \omega_2 = 2\sqrt{\pi}/3\,, & \omega_3 = \sqrt{\pi}/6\,. \end{array} \tag{22}$$

Then, the integral of moments becomes:

$$I = 2\theta\left[\omega_2^2\psi(\mathbf{0}) + \sum_{i=1}^{4}\omega_1\omega_2\psi(\boldsymbol{\xi}_i) + \sum_{i=5}^{8}\omega_1^2\psi(\boldsymbol{\xi}_i)\right], \tag{23}$$

where

$$\boldsymbol{\xi}_i = \begin{cases} (0,\,0) & i = 0, \\ (\pm 1,\,0)\sqrt{3\theta},\ (0,\,\pm 1)\sqrt{3\theta}, & i = 1-4, \\ (\pm 1,\,\pm 1)\sqrt{3\theta}, & i = 5-8. \end{cases} \tag{24}$$

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

Identifying

$$W_i = (2\pi\,\theta)\,\exp(\boldsymbol{\xi}_i^2/2\theta)\,w_i\,, \tag{25}$$

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

$$\begin{aligned} f_i^{(\mathrm{eq})}(\boldsymbol{x},\,t) &= W_i\, f^{(\mathrm{eq})}(\boldsymbol{x},\,\boldsymbol{\xi}_i,\,t) \\ &= w_i\,\rho\left\{1 + \frac{3(\boldsymbol{c}_i\cdot\boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c^4} - \frac{3\boldsymbol{u}^2}{2c^2}\right\}, \end{aligned} \tag{26}$$

where weight coefficient w_i and discrete velocity $\boldsymbol{c}_i$ are:

$$w_i = \begin{cases} 4/9, \\ 1/9, \\ 1/36, \end{cases} \quad \boldsymbol{c}_i = \boldsymbol{\xi}_i = \begin{cases} (0,\,0), & i = 0\,, \\ (\pm 1,\,0)\,c,\ (0,\,\pm 1)\,c, & i = 1-4, \\ (\pm 1,\,\pm 1)\,c, & i = 5-8. \end{cases} \tag{27}$$

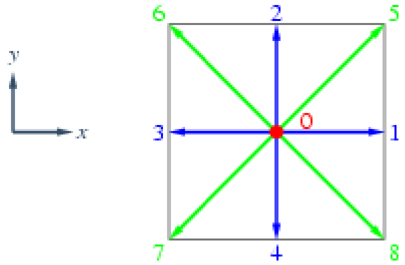
With $\{\boldsymbol{c}_i | i = 0,\,1,\,\ldots,\,8\}$, a square lattice structure is constructed in the physical space.

Discretized 2D Velocity Space

Cartesian coordinates in $\boldsymbol{\xi}$ lead to a 2D square lattice:

$$\boldsymbol{c}_i = \begin{cases} (0,\ 0), & i = 0\,, \\ (\pm 1,\ 0)\,c,\ (0,\ \pm 1)\,c, & i = 1-4, \\ (\pm 1,\ \pm 1)\,c, & i = 5-8, \end{cases}$$

where $c := \delta_x/\delta_t$.



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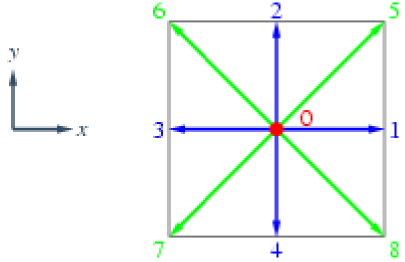
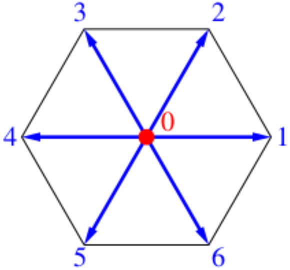
where $c := \delta_x / \delta_t$.



Polar coordinates $(r,\ \theta)$ lead to a 2D triangular lattice:

$$\boldsymbol{c}_i = (0,\ 0), \qquad 1 = 0,$$
$$\boldsymbol{c}_{ix} = \cos[(i-1)\pi/3]c, \quad i = 1-6,$$
$$\boldsymbol{c}_{iy} = \sin[(i-1)\pi/3]c, \quad i = 1-6.$$



Discretized 3D Velocity Space on a Basic Cube

Discrete velocities on a basic 3D cube:

$$\boldsymbol{c}_i = \begin{cases} (0,\,0,\,0), & 1\ (\mathrm{Z}) \\ (\pm1,\,0,\,0)\,c,\ \ (0,\,\pm1,\,0)\,c,\ \ (0,\,0,\,\pm1)\,c, & 6\ (\mathrm{F}) \\ (\pm1,\,\pm1,\,0)\,c,\ \ (0,\,\pm1,\,\pm1)\,c,\ \ (\pm1,\,0,\,\pm1)\,c, & 12\ (\mathrm{E}) \\ (\pm1,\,\pm1,\,\pm1)\,c, & 8\ (\mathrm{C}) \end{cases}$$

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Possible models with the discrete velocities on a basic cube:

Model	Velocities	Speeds
D3Q13	Z + E = 13	$0 + \sqrt{2}c$
D3Q15	Z + F + C = 15	$0 + 1c + \sqrt{3}c$
D3Q19	Z + F + E = 19	$0 + 1c + \sqrt{2}c$
D3Q27	Z + F + E + C = 27	$0 + 1c + \sqrt{2}c + \sqrt{3}c$

Outline

LBE: Discretizing $\boldsymbol{x}$

- The "basic cell" defined by a discrete velocity set $\mathbb{V}_q := \{\boldsymbol{c}_i | 0 \leq i \leq (q-1)\}$ is space-filling, *e.g.*, square and equilateral triangle in 2D, and cube in 3D;
- In the d-dimensional lattice space $\delta_x \mathbb{Z}_d$ with the lattice constant δ_x and periodic boundary conditions,

$$\boldsymbol{x}_j + \boldsymbol{c}_i \delta_t \in \delta_x \mathbb{Z}_d, \qquad \forall \boldsymbol{x}_j \in \delta_x \mathbb{Z}_d \text{ and } \forall \boldsymbol{c}_j \in \mathbb{V}_q$$

Coherent discretization: Phase space $(\boldsymbol{x}, \boldsymbol{\xi})$ and the time t are discretized *coherently* such that $\delta_x = \|\boldsymbol{c}_i\| \delta_t$ (for some $\boldsymbol{c}_i$).

The coherent discretization is one of distinctive feature of the LBE.

Outline

Collision Term

- Based on the distribution functions f_i and $f_i^{(\mathrm{eq})}(\rho, \boldsymbol{u})$:

$$\mathbf{Q} = -\frac{1}{\tau}\left[\mathbf{f} - \mathbf{f}^{(\mathrm{eq})}(\rho, \boldsymbol{u})\right]$$

- Based on the moments of the distributions f_i and $f_i^{(\mathrm{eq})}(\rho, \boldsymbol{u})$:

$$\mathbf{Q} = -\mathsf{MS}\left[\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}(\rho, \boldsymbol{u})\right], \qquad \mathbf{m} := \mathsf{M}\mathbf{f}, \quad \mathbf{f} := \mathsf{M}^{-1}\mathbf{m}$$

- Based on the cumulants of the distributions f_i and $f_i^{(\mathrm{eq})}(\rho, \boldsymbol{u})$:

$$\mathbf{Q} = \mathbf{Q}(\mathbf{C}), \;\; C_{lmn} := \frac{1}{c^{(l+m+n)}} \frac{\partial^l \partial^m \partial^n \ln \mathcal{L}\left[f_{ijk} + w_{ijk}(1-\rho)\right]}{\partial \Xi_1^l \partial \Xi_2^m \partial \Xi_3^n}\Bigg|_{\boldsymbol{\Xi}=\mathbf{0}}$$

$\mathcal{L}[f_{ijk}] := \mathcal{L}[f(\boldsymbol{\xi}_{ijk})] := F(\boldsymbol{\Xi})$ is the Laplace transform of $f_{ijk} := f(\boldsymbol{\xi}_{ijk})$, $C_{000} = 0$, $(C_{100}, C_{101}, C_{001}) = (u, v, w) := \boldsymbol{u}$.

Collision Term

- Based on the distribution functions f_i and $f_i^{(\mathrm{eq})}(\rho,\,\boldsymbol{u})$:

$$\mathbf{Q} = -\frac{1}{\tau}\left[\mathbf{f} - \mathbf{f}^{(\mathrm{eq})}(\rho,\,\boldsymbol{u})\right]$$

- Based on the moments of the distributions f_i and $f_i^{(\mathrm{eq})}(\rho,\,\boldsymbol{u})$:

$$\mathbf{Q} = -\mathsf{MS}\left[\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}(\rho,\,\boldsymbol{u})\right], \qquad \mathbf{m} := \mathsf{M}\mathbf{f}, \quad \mathbf{f} := \mathsf{M}^{-1}\mathbf{m}$$

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Outline

Example: D3Q19 MRT-LBE Model[3]

$$\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\delta_t,\, t_n + \delta_t) = \mathbf{f}(\boldsymbol{x}_j,\, t_n) - \mathsf{M}^{-1}\mathsf{S}\left[\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}(\rho,\, \boldsymbol{u})\right] \tag{28}$$

[3] D. d'Humières, I. Ginzburg, M. Krafczyk, P. Lallemand, and L.-S. Luo, *Philos. Trans. R. Soc. London A* **360**(1792):437–451 (2002).

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Conserved quantities:

$$\rho = \sum_{i=0}^{Q-1} f_i, \quad \boldsymbol{j} = \rho\boldsymbol{u} = \sum_{i=0}^{Q-1} f_i \boldsymbol{c}_i$$

Transport coefficients and the speed of sound ($c := \delta_x/\delta_t$):

$$\nu = \frac{1}{3}\left(\frac{1}{s_\nu} - \frac{1}{2}\right)c\delta_x, \quad \zeta = \frac{(5 - 9c_s^2)}{9}\left(\frac{1}{s_e} - \frac{1}{2}\right)c\delta_x, \quad c_s^2 = \frac{1}{3}c^2$$

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The transform between the discrete distribution functions $\mathbf{f} \in \mathbb{V} = \mathbb{R}^Q$ and the moments $\mathbf{m} \in \mathbb{M} = \mathbb{R}^Q$:

$$\mathbf{m} = \mathsf{M}\mathbf{f}, \qquad \mathbf{f} = \mathsf{M}^{-1}\mathbf{m}$$

Note $\boldsymbol{\Lambda} = \mathsf{M}\mathsf{M}^\dagger$ is diagonal, thus $\mathsf{M}^{-1} = \mathsf{M}^\dagger\boldsymbol{\Lambda}^{-1}$.

[3] D. d'Humières, I. Ginzburg, M. Krafczyk, P. Lallemand, and L.-S. Luo, *Philos. Trans. R. Soc. London A* **360**(1792):437–451 (2002).

D3Q19: Equilibria

$$e^{(\mathrm{eq})} = -11\rho + \frac{19}{\rho}\boldsymbol{j}\cdot\boldsymbol{j} \tag{29a}$$

$$p_{xx}^{(\mathrm{eq})} = \frac{1}{3\rho}\left[2j_x^2 - (j_y^2 + j_z^2)\right], \quad p_{ww}^{(\mathrm{eq})} = \frac{1}{\rho}\left[j_y^2 - j_z^2\right] \tag{29b}$$

$$p_{xy}^{(\mathrm{eq})} = \frac{1}{\rho}j_x j_y, \quad p_{yz}^{(\mathrm{eq})} = \frac{1}{\rho}j_y j_z, \quad p_{xz}^{(\mathrm{eq})} = \frac{1}{\rho}j_x j_z \tag{29c}$$

$$(q_x^{(\mathrm{eq})}, q_y^{(\mathrm{eq})}, q_z^{(\mathrm{eq})}) = -\frac{2}{3}(j_x, j_y, j_z) \tag{29d}$$

$$m_x^{(\mathrm{eq})} = m_y^{(\mathrm{eq})} = m_z^{(\mathrm{eq})} = 0 \tag{29e}$$

$$\epsilon^{(\mathrm{eq})} = 3\rho - \frac{11}{2\rho}\boldsymbol{j}\cdot\boldsymbol{j}, \quad \pi_{xx}^{(\mathrm{eq})} = -\frac{1}{2}p_{xx}^{(\mathrm{eq})}, \quad \pi_{ww}^{(\mathrm{eq})} = -\frac{1}{2}p_{ww}^{(\mathrm{eq})} \tag{29f}$$

Outline

Other Models

- D3Q39 Model:[4]

$$\boldsymbol{c}_i = \begin{cases} (0,\,0,\,0),\ (\pm1,\,0,\,0)\,c,\ \ldots,\ (\pm1,\,\pm1,\,\pm1)\,c,\ \ldots & 15 \\ (\pm2,\,0,\,0)\,c,\ \ldots,\ (\pm2,\,\pm2,\,0)\,c,\ \ldots & 18 \\ (\pm3,\,0,\,0)\,c,\ \ldots & 6 \end{cases}$$

  The energy equation is solved *separately*,[5] k-ϵ model, ...

- Crystallographic LBE Model (RD3Q27):[6]

$$\boldsymbol{c}_i = \begin{cases} (0,\,0,\,0) & 1\ (\mathrm{Z}) \\ (\pm1,\,0,\,0)\,c,\ \ (0,\,\pm1,\,0)\,c,\ \ (0,\,0,\,\pm1)\,c & 6\ (\mathrm{F}) \\ (\pm1,\,\pm1,\,0)\,c,\ \ (0,\,\pm1,\,\pm1)\,c,\ \ (\pm1,\,0,\,\pm1)\,c & 12\ (\mathrm{E}) \\ (\pm1/2,\,\pm1/2,\,\pm1/2)\,c & 8\ (\mathrm{C}) \end{cases}$$

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4 Y.B. Li *et al.* AIAA 2016-2312182 (2016).

5 P. Lallemand and L.-S. Luo. *Phys. Rev. E* **68**(3):036706 (2003).

6 M. Namburi, S. Krithivasan, S. Ansumali, *Sci. Rep.* 27172 (2017).

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Outline

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Decaying Homogeneous Isotropic Turbulence

The decaying homogeneous isotropic turbulence is the solution of the *incompressible* Navier-Stokes equation

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} p + \nu \nabla^2 \boldsymbol{u}, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \quad \boldsymbol{x} \in [0,\, 2\pi]^3, \tag{30}$$

with periodic boundary conditions. The initial velocity satisfies a given initial energy spectrum $E_0(k)$

$$E_0(k) := E(k,\, t = 0) = A k^4 e^{-0.14 k^4}, \quad k \in [k_a,\, k_b] \tag{31}$$

The initial velocity $\boldsymbol{u}_0$ can be given by Rogallo procedure:

$$\tilde{\boldsymbol{u}}_0(\boldsymbol{k}) = \frac{\alpha k k_2 + \beta k_1 k_3}{k\sqrt{k_1^2 + k_2^2}} \hat{\boldsymbol{k}}_1 + \frac{\beta k_2 k_3 - \alpha k_1 k}{k\sqrt{k_1^2 + k_2^2}} \hat{\boldsymbol{k}}_2 - \frac{\beta\sqrt{k_1^2 + k_2^2}}{k} \hat{\boldsymbol{k}}_3, \tag{32}$$

where $\alpha = \sqrt{E_0(k)/4\pi k^2} e^{\imath\theta_1} \cos\phi$, $\beta = \sqrt{E_0(k)/4\pi k^2} e^{\imath\theta_2} \sin\phi$, $\imath := \sqrt{-1}$, and θ_1, θ_2, $\phi \in [0,\, 2\pi]$ are uniform random variables.

Pseudo-Spectral Method

The pseudo-spectral (PS) method solve the Navier-Stokes equation in the Fourier space $\boldsymbol{k}$, i.e.,

$$\boldsymbol{u}(\boldsymbol{x}, t) = \sum_{\boldsymbol{k}} \tilde{\boldsymbol{u}}(\boldsymbol{k}, t) e^{\imath \boldsymbol{k} \cdot \boldsymbol{x}}, \quad -N/2 + 1 \leq k_\alpha \leq N/2.$$

- The nonlinear term $\boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u}$ computed in physical space $\boldsymbol{x}$ by inverse Fourier-transform $\tilde{\boldsymbol{u}}$ and $\boldsymbol{k}\tilde{\boldsymbol{u}}$ to $\boldsymbol{x}$ for form the nonlinear term; and it is transformed back to $\boldsymbol{k}$ space;
- De-aliasing: $\tilde{\boldsymbol{u}}(\boldsymbol{k}, t) = \boldsymbol{0} \; \forall \|\boldsymbol{k}\| \geq N/6$;
- Time matching: second-order Adams-Bashforth scheme:

$$\frac{\tilde{\boldsymbol{u}}(t + \delta t) - \tilde{\boldsymbol{u}}(t)}{\delta t} = -\frac{3}{2}\tilde{T}(t) + \frac{1}{2}\tilde{T}(t - \delta t) e^{-\nu k^2 \delta t},$$

where $\tilde{T} := \mathcal{F}[\boldsymbol{\omega} \times \boldsymbol{u}] - (\mathcal{F}[\boldsymbol{\omega} \times \boldsymbol{u}] \cdot \hat{\boldsymbol{k}})\hat{\boldsymbol{k}}$.

Parameters in DNS

Use $N^3 = 128^3$ and $[k_a, k_b] = [3, 8]$.
In LBE: $\nu = 1/600\,(c\delta x)$, $c := \delta x/\delta t = 1$, $\mathrm{Ma}_{\max} = \|\boldsymbol{u}_0\|_{\max}/c_s \le 0.15$, $A = 1.4293 \cdot 10^{-4}$ in $E_0(k)$, and $K_0 \approx 1.0130 \cdot 10^{-2}$, $u_0' \approx 8.2181 \cdot 10^{-2}$.
The time t is normalized by the turbulence turn-over time $t_0 = K_0/\varepsilon_0$.
In SP method, $K_0 = 1$ and $u_0' = \sqrt{2/3}$.

Method	L	δx	u_0'	δt	ν	$\delta t'$
LBE	2π	$2\pi/N$	$\sqrt{2K_0/3}$	$2\pi/N$	ν	$2\pi/Nt_0$
PS	2π	$2\pi/N$	$\sqrt{2/3}$	$2\pi\sqrt{K_0}/N$	$\nu/\sqrt{K_0}$	$2\pi/Nt_0$

The Taylor microscale Reynolds number:

$$\mathrm{Re}_\lambda := \frac{u'\lambda}{\nu}, \quad \lambda := \sqrt{\frac{15}{2\Omega}}u' := \sqrt{\frac{15\nu}{\varepsilon}}u' \tag{33}$$

The resolution criterion:

$$\text{SP: } N \sim 0.4\mathrm{Re}_\lambda^{3/2}, \quad \eta/\delta x \ge 1/2.1, \quad N = 128 \to \mathrm{Re}_\lambda = 46.78$$

$$\text{LBE: } \eta k_{\max} = \eta/\delta x \ge 1, \quad N = 128 \to \mathrm{Re}_\lambda = 24.35.$$

Initial Conditions

For the pseudo-spectral method:

- Generate $\tilde{\boldsymbol{u}}_0(\boldsymbol{k})$ in $\boldsymbol{k}$-space with a given $E_0(k)$ (Rogallo's procedure) with $K_0 = 1$ and $u' = \sqrt{3/2}$;
- The initial pressure p_0 is obtained by solving the Poisson equation in $\boldsymbol{k}$-space.

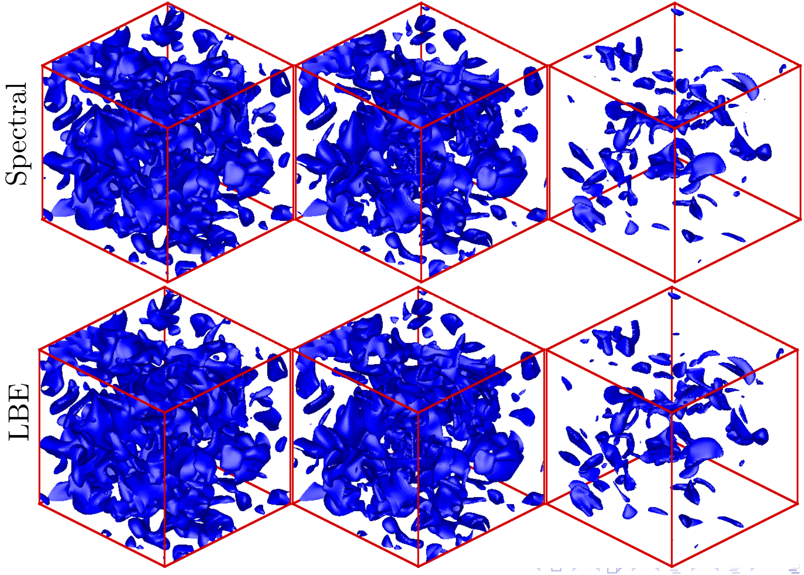
For the LBE method:[7]

- Use the initial velocity $\boldsymbol{u}_0$ as in PS method except a scaling factor so that $\mathrm{Ma}_{\max} = 0.15$;
- The pressure p_0 is obtained by an iterative procedure with a given $\boldsymbol{u}_0$.

[7] R. Mei, L.-S. Luo, P. Lallemand, and D. d'Humières. Computers & Fluids **35**(8/9):855–862 (2006).

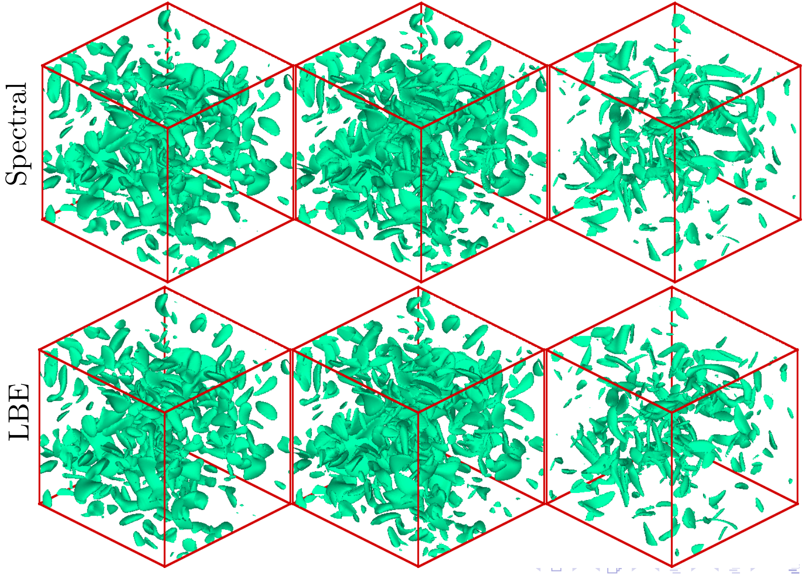
Velocity Iso-surface in 3D, $\mathrm{Re}_\lambda = 24.37$

LBE vs. PS1 (equal δt): $t' = 0.1348, 0.2359, 0.573$; $\|\boldsymbol{u}(t')/u'\| = 2.0$



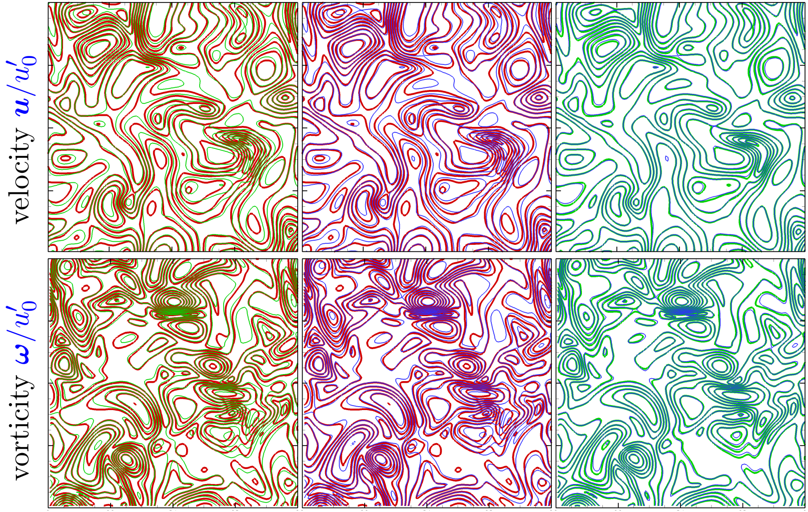
Vorticity Iso-surface in 3D, $\mathrm{Re}_\lambda = 24.37$

LBE vs. PS1 (equal δt): $t' = 0.1348$, 0.2359, 0.573; $\|\boldsymbol{\omega}(t')/u'\| = 13.0$



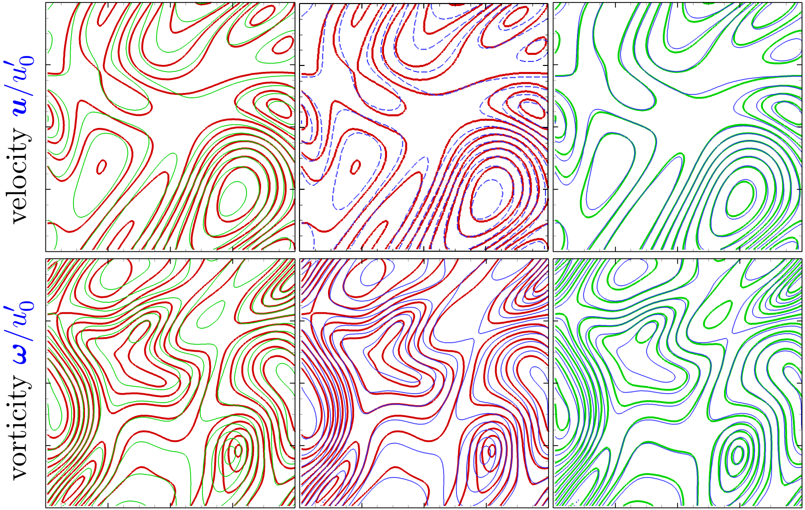
$\|\boldsymbol{u}(t')/u'\|$ and $\|\boldsymbol{\omega}(t')/u'\|$ at $\mathrm{Re}_\lambda = 24.37$, $t' = 4.048$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2



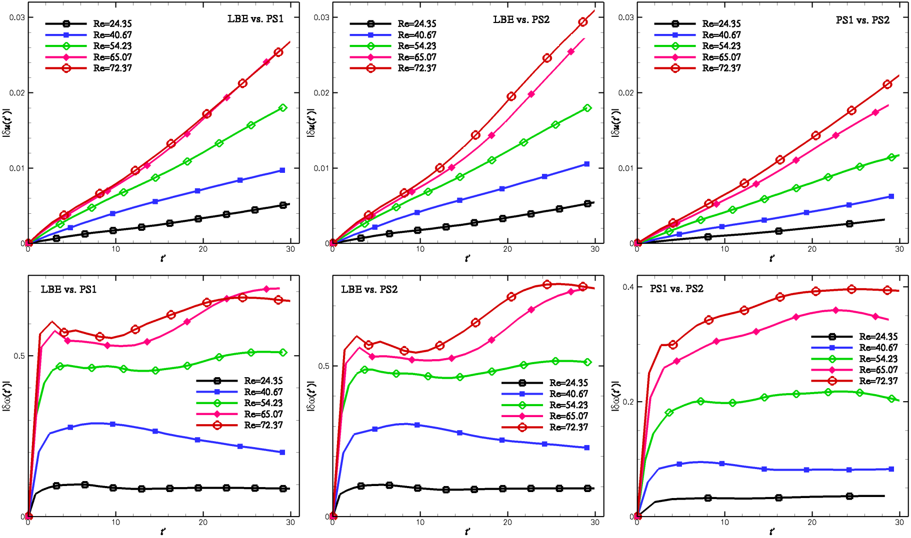
$\|\boldsymbol{u}(t')/u'\|$ and $\|\boldsymbol{\omega}(t')/u'\|$ at $\mathrm{Re}_\lambda = 24.37$, $t' = 29.949$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2



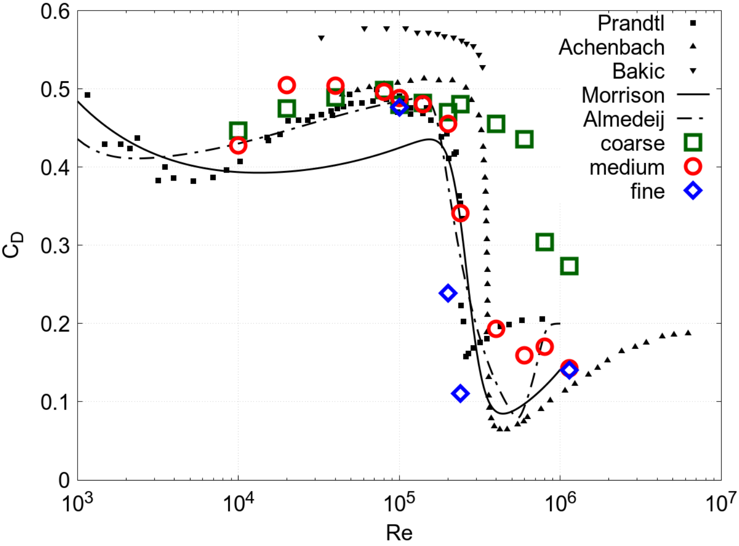
L^2 $\|\delta\boldsymbol{u}(t')\|$ and $\|\delta\boldsymbol{\omega}(t')\|$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2.



Outline

Flow past a Sphere: DNS of Drag Crisis[8]



6 refinement levels

3 resolutions:

coarse 40,769,886 $D = 410\delta_x$

medium 73,855,027 $D = 512\delta_x$

fine 133,438,032 $D = 640\delta_x$

[8] M. Geier, A. Pasquali, M. Schönherr. *J. Comput. Phys.* **348**:862–888 (2017); *ibid* **348**:889–898 (2017).

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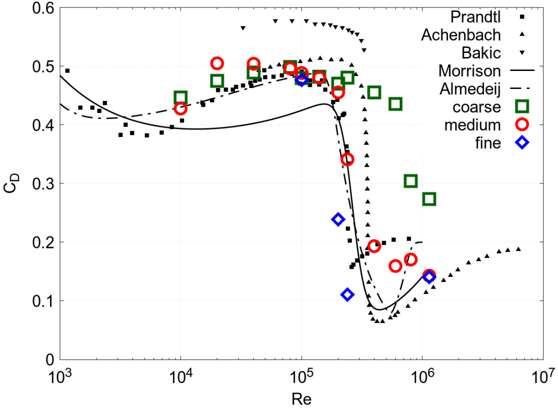

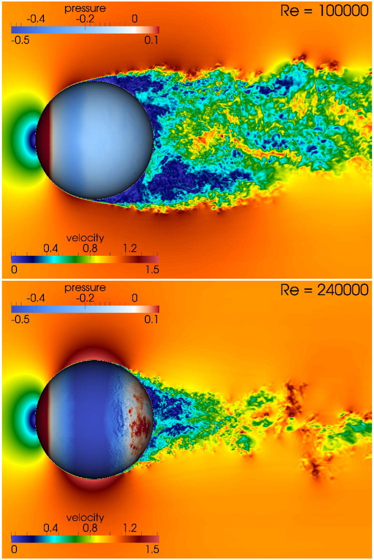

Outline

Characteristics and Features of LBE

It can be shown:

- Related to (central) finite-difference scheme — stencil defined by the discrete velocities
- Related to artificial compressibility model
- Conservative — Galilean invariant, isotropic[9]
- Accuracy: 2nd-order for both velocity $\boldsymbol{u}$ and the stress $\boldsymbol{\sigma}$,[10] 1st-order for pressure p
- Valid for variable viscosity models, *e.g.*, $\nu = \nu(\sigma(\boldsymbol{x}))$.[11]

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[9] P. Lallemand and L.-S. Luo. Phys. Rev. E **61**:6546–6562 (2000).
[10] W.-A. Yong and L.-S. Luo. Phys. Rev. E **86**(6):065701(R) (2012).
[11] Z. Yang and W.-A. Yong. Multiscale Model. Simul. **12**(3):1028 (2014).

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Some other Features:

- Simple and easy?!
- Cartesian cubic mesh, 2^{-n} refinement, cut-cell, ...
- low FLOP counts, memory/communication bound, ...

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Why Kinetic Methods?

The Boltzmann equation is a 1st-order *semi-linear* PDE (in phase space), the Navier-Stokes equation is a 2nd-order *nonlinear* PDE (in space). Features of kinetic schemes based on 1st-order PDEs include:[12]

- Requires the smallest possible stencil for accurate discretization, thus least need for inter-nodal data communication;
- Nonlinearity is in *local* collision term, stiffness of which can be overcome by *local* techniques.
- Discretized 1st-order systems may be easier to converge than equivalent higher-order systems.
- 1st-order PDE's yield the highest potential discretization accuracy on non-smooth, adaptively refined grids.
- The systems of 1st-order PDE's are better suited for functional decomposition, thus easier to parallelize.
- The Boltzmann equation is valid for nonequilibrium flows which cannot be modeled by the Navier-Stokes equations.

[12] B. van Leer, AIAA Paper 2001-2520 (2001).

Food for Thought

- For CFD, hyperbolic or elliptic PDEs?
- For an n-th order scheme, how to guarantee that the operators ∇ and ∇^2 are *isotropic* to the order consistent/comparable with n?
- How to construct *physics-based* numerics beyond upwind, (approximated) multi-dimensional Riemann solver, artificial dissipation, and limiters?
- How to construct accurate and simple(?) algorithms amendable to MIC/GPU technology, or any future hardware technologies?

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Thanks! Questions?