Lattice Boltzmann Equation
Its Mathematical Essence and Key Properties

Li-Shi Luo

Department of Mathematics and Statistics
Old Dominion University, Norfolk, Virginia 23529, USA
Computational Science Research Center, Beijing, China
Email: lluo@odu.edu, URL: http://www.lions.odu.edu/~lluo

Computational Aerosciences Branch
NASA Ames Research Center, Moffett Field, CA
Wednesday, March 13, 2019
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
1 Motivations
   • The Role of Kinetic Theory
   • Scales and Related Methods

2 LBE: Mathematical Derivation
   • Discretizing time $t$
   • Low-Mach-Number (Gauss-Hermite) Expansion
   • Discretize Velocity Space $\xi$
   • Discretize Space $x$
   • Treatment of Collision — Relaxation Models
   • Example: D3Q19
   • Other Models

3 Numerical Results
   • DNS of Homogeneous Isotropic Turbulence
   • DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Conservation laws of mass, momentum, and energy:

\[ \partial_t \rho + \nabla \cdot (\rho u) = 0 \]  
\[ \rho \partial_t u + \rho u \cdot \nabla u = -\nabla \cdot P \]  
\[ \rho \partial_t e + \rho u \cdot \nabla e = -P : \nabla u - \nabla \cdot q \]

\[ P = pI - S, \quad S_{\alpha\beta} = \mu (\partial_\alpha u_\beta + \partial_\beta u_\alpha) + \left( \zeta - \frac{2}{3} \mu \right) \delta_{\alpha\beta} \nabla \cdot u \]

\[ q = -\kappa \nabla T, \quad e = e(T), \quad p = p(\rho, T) \]

Dimensionless Navier-Stokes equations (similarity law):

\[ \rho \partial_t u + \rho u \cdot \nabla u = -\frac{1}{\gamma \text{Ma}^2} \nabla p + \frac{1}{\text{Re}} \nabla \cdot S \]  
\[ \rho \partial_t e + \rho u \cdot \nabla e = -\frac{1}{\gamma \text{Ma}^2} p \nabla \cdot u + \frac{1}{\alpha} \nabla^2 T + \frac{1}{\text{Re}} S : \nabla u \]

\[ \alpha = (\gamma - 1) \text{Pr Ma Re}, \quad \gamma := \frac{C_P}{C_V} \]
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Kinetic Equation

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

\[
\partial_t f + \nabla \cdot (\xi f) = Q, \quad f := f(x, \xi, t)
\]  

(3)

The Uehling-Uhlenbeck collision model:

\[
Q[f,f] = \int_{\mathbb{R}^3} d\xi_2 \int_{S^2} d\Omega K \left[ (1 + \eta_{f_1}) (1 + \eta_{f_2}) f'_1 f'_2 - (1 + \eta_{f'_1}) (1 + \eta_{f'_2}) f_1 f_2 \right]
\]  

(4)

where \( \Omega \) is the solid angle, \( K := K(\xi_1, \xi_2, \Omega) \) is the collision kernel,

\[
K(\xi_1, \xi_2, \Omega) = K(\xi_2, \xi_1, \Omega) = K(\xi'_1, \xi'_2, \Omega) \geq 0
\]  

(5)

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

(6)
Expansion of $f$ in terms of the Knudsen number $\varepsilon = Kn := \ell/L$:

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

(7)

Velocity moments of $f$ are hydrodynamic quantities and their fluxes:
Expansion of $f$ in terms of the Knudsen number $\varepsilon = \text{Kn} := \ell/L$:

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

Velocity moments of $f$ are hydrodynamic quantities and their fluxes:

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

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

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

$$ \xi^2: \quad P = \int ccf d\xi, \quad \xi^3: \quad q = \int \frac{1}{2} c^2 cf d\xi \quad (8d) $$
\[
\partial_t \langle \xi^n f \rangle + \nabla \cdot \langle \xi^{n+1} f \rangle = \langle \xi^n Q \rangle, \quad n = 1, 2, 3,
\]
\[ \partial_t \langle \xi^n f \rangle + \nabla \cdot \langle \xi^{n+1} f \rangle = \langle \xi^n Q \rangle, \quad n = 1, 2, 3, \]

\[
\begin{align*}
\partial_t \rho + \nabla \cdot \rho \mathbf{u} &= 0 \quad (9a) \\
\partial_t \rho \mathbf{u} + \nabla \cdot \rho (\mathbf{u} \mathbf{u} + \mathbf{P}) &= 0 \quad (9b) \\
\partial_t \rho E + \nabla \cdot \rho (\mathbf{u} E + \mathbf{u} \cdot \mathbf{P} + \mathbf{q}) &= 0, \quad E := \rho e + \frac{1}{2} \rho \mathbf{u}^2 \quad (9c) \\
\mathbf{P} &= \mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \cdots \quad \mathbf{q} = \mathbf{q}^{(0)} + \mathbf{q}^{(1)} + \mathbf{q}^{(2)} + \cdots \quad (9d)
\end{align*}
\]
\[ \partial_t \langle \xi^n f \rangle + \nabla \cdot \langle \xi^{n+1} f \rangle = \langle \xi^n Q \rangle, \quad n = 1, 2, 3, \]

\[ \partial_t \rho + \nabla \cdot \rho \mathbf{u} = 0 \quad (9a) \]
\[ \partial_t \rho \mathbf{u} + \nabla \cdot \rho (\mathbf{u} \mathbf{u} + \mathbf{P}) = 0 \quad (9b) \]
\[ \partial_t \rho E + \nabla \cdot \rho (uE + \mathbf{u} \cdot \mathbf{P} + q) = 0, \quad E := \rho e + \frac{1}{2} \rho u^2 \quad (9c) \]
\[ \mathbf{P} = \mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \cdots \quad q = q^{(0)} + q^{(1)} + q^{(2)} + \cdots \quad (9d) \]

\[ f = f^{(0)} \implies \begin{cases} \mathbf{P}^{(0)} = \frac{3}{2} \rho RT \mathbf{I} \\ q^{(0)} = 0 \end{cases} \implies \text{Euler Eqns (inviscid)} \]

\[ f = f^{(0)} + f^{(1)} \implies \begin{cases} \mathbf{P}^{(1)} = -\frac{1}{2} \mu [ (\nabla \mathbf{u}) + (\nabla \mathbf{u})^\dagger ] \\ q^{(1)} = -\kappa \nabla T \end{cases} \implies \text{NS Eqns} \]
Knudsen Number $\text{Kn} := \frac{\ell}{L} = \frac{\text{Mean Free Path}}{\text{Characteristic Hydrodynamic Length}}$

**Microscopic Theory**
- Deterministic Newton’s Law
- Molecular Dynamics

**Mesoscopic Theory**
- Statistical Mechanics
- Liouville Equation
- BBGKY Hierarchy
- Boltzmann Equation

**Macroscopic (Continuum) Theory ($\text{Kn} \approx 0$)**
- PDEs of Conservation Laws
  - Navier-Stokes Equations
  - Euler Equations
  - Turbulence Models
    - RANS, LES, · · ·

**Kinetic Theory**
- Hilbert and Chapman-Enskog analysis
- Gas-Kinetic Scheme
- Lattice Boltzmann Equation

**Linear Relaxation Models**
- System of Finite Moments
- Direct Simulation Monte Carlo
- Discrete Velocity Models
- Discrete Ordinance Method
- Moment Equations
- LBE for CFD
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
A Priori Derivation of Lattice Boltzmann Equation

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

\[
\partial_t f + \xi \cdot \nabla f = \int [f'_1 f'_2 - f_1 f_2] d\mu \approx \mathcal{L}(f, f) \approx -\frac{1}{\lambda}[f - f^{(0)}]
\]  

(10)

The Boltzmann-Maxwellian equilibrium distribution function:

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

(11)

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

\[
\rho \begin{pmatrix} 1 \\ u \\ e \end{pmatrix} = \int \begin{pmatrix} 1 \\ \xi \\ c \cdot c/2 \end{pmatrix} f d\xi = \int \begin{pmatrix} 1 \\ \xi \\ c \cdot c/2 \end{pmatrix} f^{(0)} d\xi, \quad c := \xi - u
\]  

(12)

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

\[
\int \begin{pmatrix} 1 \\ \xi \\ c \cdot c/2 \end{pmatrix} Q d\xi = \int \begin{pmatrix} 1 \\ \xi \\ \xi \cdot \xi/2 \end{pmatrix} Q d\xi = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
\]  

(13)
Rewrite the Boltzmann BGK Equation in the form of ODE:

\[ D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)}, \quad D_t := \partial_t + \xi \cdot \nabla \]  \hspace{1cm} (14)

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

\[ f(x + \xi \delta_t, \xi, t + \delta_t) = e^{-\delta_t/\lambda} f(x, \xi, t) \]

\[ + \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^{t'/\lambda} f^{(0)}(x + \xi t', \xi, t + t') \, dt' \]  \hspace{1cm} (15)

Remark: a fully compressible finite-volume scheme or higher-order schemes can also be formulated based upon the integral solution.\(^1\)

---

Rewrite the Boltzmann BGK Equation in the form of ODE:

\[ D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)}, \quad D_t := \partial_t + \xi \cdot \nabla \]  \hspace{1cm} (14)

Integrate Eq. (14) over a time step \( \delta t \) along characteristics:

\[ f(x + \xi \delta t, \xi, t + \delta t) = e^{-\delta t/\lambda} f(x, \xi, t) \]
\[ + \frac{1}{\lambda} e^{-\delta t/\lambda} \int_0^{\delta t} e^{t'/\lambda} f^{(0)}(x + \xi t', \xi, t + t') \, dt' \]  \hspace{1cm} (15)

Remark: a fully compressible finite-volume scheme or higher-order schemes can also be formulated based upon the integral solution.\(^1\)

The necessary steps to derive LBE:\textsuperscript{2}

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

Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
     - Low-Mach-Number (Gauss-Hermite) Expansion
     - Discretize Velocity Space $\xi$
     - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
     - Example: D3Q19
     - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

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

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

the integral solution (15) becomes:

$$f(x + \xi \delta_t, \xi, t + \delta_t) - f(x, \xi, t) = \left(e^{-\delta_t/\lambda} - 1\right) \left[f(x, \xi, t) - f^{(0)}(x, \xi, t)\right]$$

$$+ \left(1 + \frac{\delta_t}{\lambda} \left(e^{-\delta_t/\lambda} - 1\right)\right) \left[f^{(0)}(t + \delta_t) - f^{(0)}(t)\right] + O(\delta_t^2)$$

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

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

(16)
Outline

1 Motivations
   • The Role of Kinetic Theory
   • Scales and Related Methods

2 LBE: Mathematical Derivation
   • Discretizing time $t$
   • Low-Mach-Number (Gauss-Hermite) Expansion
     • Discretize Velocity Space $\xi$
     • Discretize Space $x$
     • Treatment of Collision — Relaxation Models
     • Example: D3Q19
     • Other Models

3 Numerical Results
   • DNS of Homogeneous Isotropic Turbulence
   • DNS of Flow past a Sphere — Drag Crisis

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

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

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

where $a^{(0)} = 1$, $a^{(1)} = u$, $a^{(2)} = uu - (\theta - 1)I$, and $\{H^{(n)}(\xi)\}$ are the tensorial Hermite polynomials.
Low Mach Number Expansion (Approximation)

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

\[
\begin{align}
\left(f^{(eq)}\right) &= \frac{\rho}{(2\pi \theta)^{D/2}} \exp \left[-\frac{\xi^2}{2\theta}\right]\left\{1 + \frac{\xi \cdot u}{\theta} + \frac{(\xi \cdot u)^2}{2\theta^2} - \frac{u^2}{2\theta}\right\} + O(u^3) \quad (17a) \\
f &= \frac{\rho}{(2\pi \theta)^{D/2}} \exp \left[-\frac{\xi^2}{2\theta}\right]\sum_{n=0}^{2} \frac{1}{n!} a^{(n)}(x, t) : H^{(n)}(\xi) \quad (17b)
\end{align}
\]

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

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

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
To compute conserved moments \((\rho, \rho u, \text{and } \rho e)\) and their fluxes, one must evaluate:

\[
I = \int \xi^m f^{(eq)} d\xi = \int \exp(-\xi^2/2\theta) \psi(\xi) d\xi,
\]

(18)

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

\[
I = \int \exp(-\xi^2/2\theta) \psi(\xi) d\xi = \sum_j W_j \exp(-\xi_j^2/2\theta) \psi(\xi_j)
\]

(19)

where \(\xi_j\) and \(W_j\) are the abscissas and the weights. Then

\[
\rho = \sum_i f_i^{(eq)} = \sum_i f_i,
\]

\[
\rho u = \sum_i \xi_i f_i^{(eq)} = \sum_i \xi_i f_i,
\]

(20)

where \(f_i := f_i(x, t) := W_i f(x, \xi_i, t)\), and \(f_i^{(eq)} := W_i f^{(eq)}(x, \xi_i, t)\).

The quadrature must preserve the conservation laws exactly!
In two-dimensional Cartesian (momentum) space, set

\[ \psi(\xi) = \xi^m_x \xi^n_y \]

the integral of the moments can be given by

\[ I = (\sqrt{2\theta})^{(m+n+2)} I_m I_n, \quad I_m = \int_{-\infty}^{+\infty} e^{-\frac{\zeta^2}{2}} \zeta^m d\zeta, \quad (21) \]

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 $\xi$-Space (9-bit Model)

The three abscissas in momentum space ($\zeta_j$) and the corresponding weights ($\omega_j$) are:

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

Then, the integral of moments becomes:

$$I = 2\theta \left[ \omega_2^2 \psi(0) + \sum_{i=1}^{4} \omega_1 \omega_2 \psi(\xi_i) + \sum_{i=5}^{8} \omega_1^2 \psi(\xi_i) \right],$$

where

$$\begin{align*}
\xi_i &= \begin{cases} 
(0, 0) & i = 0, \\
(\pm 1, 0)\sqrt{3}\theta, (0, \pm 1)\sqrt{3}\theta, & i = 1 - 4, \\
(\pm 1, \pm 1)\sqrt{3}\theta, & i = 5 - 8.
\end{cases}
\end{align*}$$
Identifying

\[ W_i = (2\pi \theta) \exp\left(\frac{\xi_i^2}{2\theta}\right)w_i, \quad (25) \]

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

\[
f^{(eq)}_i(x, t) = W_if^{(eq)}(x, \xi_i, t) = w_i \rho \left\{ 1 + \frac{3(c_i \cdot u)}{c^2} + \frac{9(c_i \cdot u)^2}{2c^4} - \frac{3u^2}{2c^2} \right\}, \quad (26)
\]

where weight coefficient \( w_i \) and discrete velocity \( c_i \) are:

\[
w_i = \begin{cases} 
4/9, & i = 0, \\
1/9, & i = 1 - 4, \\
1/36, & i = 5 - 8.
\end{cases}
\]

\[
c_i = \xi_i = \begin{cases} 
(0, 0), & i = 0, \\
(\pm1, 0) c, (0, \pm1) c, & i = 1 - 4, \\
(\pm1, \pm1) c, & i = 5 - 8.
\end{cases}
\]

With \( \{c_i|i = 0, 1, \ldots, 8\} \), a square lattice structure is constructed in the physical space.
Discretized 2D Velocity Space

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

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

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

Luo (ODU)  
LBE for CFD
Discretized 2D Velocity Space

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

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

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

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

\[
\mathbf{c}_i = (0, 0), \\
\mathbf{c}_{ix} = \cos[(i - 1)\pi/3]c, \quad i = 1 - 6, \\
\mathbf{c}_{iy} = \sin[(i - 1)\pi/3]c, \quad i = 1 - 6.
\]
Discrete velocities on a basic 3D cube:

\[ c_i = \begin{cases} 
(0, 0, 0), & 1 \text{ (Z)} \\
(\pm 1, 0, 0) c, (0, \pm 1, 0) c, (0, 0, \pm 1) c, & 6 \text{ (F)} \\
(\pm 1, \pm 1, 0) c, (0, \pm 1, \pm 1) c, (\pm 1, 0, \pm 1) c, & 12 \text{ (E)} \\
(\pm 1, \pm 1, \pm 1) c, & 8 \text{ (C)}
\end{cases} \]
Discretized 3D Velocity Space on a Basic Cube

Discrete velocities on a basic 3D cube:

\[
c_i = \begin{cases} 
(0, 0, 0), & 1 \text{ (Z)} \\
(\pm 1, 0, 0) c, (0, \pm 1, 0) c, (0, 0, \pm 1) c, & 6 \text{ (F)} \\
(\pm 1, \pm 1, 0) c, (0, \pm 1, \pm 1) c, (\pm 1, 0, \pm 1) c, & 12 \text{ (E)} \\
(\pm 1, \pm 1, \pm 1) c, & 8 \text{ (C)} 
\end{cases}
\]

Possible models with the discrete velocities on a basic cube:

<table>
<thead>
<tr>
<th>Model</th>
<th>Velocities</th>
<th>Speeds</th>
</tr>
</thead>
<tbody>
<tr>
<td>D3Q13</td>
<td>Z + E = 13</td>
<td>0 + \sqrt{2}c</td>
</tr>
<tr>
<td>D3Q15</td>
<td>Z + F + C = 15</td>
<td>0 + 1c + \sqrt{3}c</td>
</tr>
<tr>
<td>D3Q19</td>
<td>Z + F + E = 19</td>
<td>0 + 1c + \sqrt{2}c</td>
</tr>
<tr>
<td>D3Q27</td>
<td>Z + F + E + C = 27</td>
<td>0 + 1c + \sqrt{2}c + \sqrt{3}c</td>
</tr>
</tbody>
</table>
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
The “basic cell” defined by a discrete velocity set 
\[ \mathbb{V}_q := \{ \mathbf{c}_i | 0 \leq i \leq (q - 1) \} \] 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 \( \delta_x \) and periodic boundary conditions,

\[ \mathbf{x}_j + \mathbf{c}_i \delta_t \in \delta_x \mathbb{Z}_d, \quad \forall \mathbf{x}_j \in \delta_x \mathbb{Z}_d \text{ and } \forall \mathbf{c}_j \in \mathbb{V}_q \]

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

The \textbf{coherent discretization} is one of distinctive feature of the LBE.
Outline

1 Motivations
   • The Role of Kinetic Theory
   • Scales and Related Methods

2 LBE: Mathematical Derivation
   • Discretizing time $t$
   • Low-Mach-Number (Gauss-Hermite) Expansion
   • Discretize Velocity Space $\xi$
   • Discretize Space $x$
   • Treatment of Collision — Relaxation Models
     • Example: D3Q19
     • Other Models

3 Numerical Results
   • DNS of Homogeneous Isotropic Turbulence
   • DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Collision Term

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

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

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

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

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

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

$$\mathcal{L}[f_{ijk}] := \mathcal{L}[f(\xi_{ijk})] := F(\Xi)$$ is the Laplace transform of

$$f_{ijk} := f(\xi_{ijk}), \quad C_{000} = 0, \quad (C_{100}, C_{101}, C_{001}) = (u, v, w) := u.$$
Collision Term

- Based on the distribution functions $f_i$ and $f_i^{(eq)}(\rho, u)$:
  \[ Q = -\frac{1}{\tau} \left[ f - f^{(eq)}(\rho, u) \right] \]

- Based on the moments of the distributions $f_i$ and $f_i^{(eq)}(\rho, u)$:
  \[ Q = -MS \left[ m - m^{(eq)}(\rho, u) \right], \quad m := Mf, \quad f := M^{-1}m \]

- Based on the cumulants of the distributions $f_i$ and $f_i^{(eq)}(\rho, u)$:
  \[ Q = Q(C), \quad C_{lmn} := \frac{1}{c^{l+m+n}} \frac{\partial^l \partial^m \partial^n \ln \mathcal{L} [f_{ijk} + w_{ijk}(1 - \rho)]}{\partial \Xi_1^l \partial \Xi_2^m \partial \Xi_3^n} \bigg|_{\Xi = 0} \]
  \[ \mathcal{L}[f_{ijk}] := \mathcal{L}[f(\xi_{ijk})] := F(\Xi) \text{ is the Laplace transform of} \]
  \[ f_{ijk} := f(\xi_{ijk}), \quad C_{000} = 0, \quad (C_{100}, C_{101}, C_{001}) = (u, v, w) := u. \]
Collision Term

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

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

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

$$Q = -\text{MS} \left[ m - m^{(eq)}(\rho, u) \right], \quad m := Mf, \quad f := M^{-1}m$$

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

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

$$\mathcal{L}[f_{ijk}] := \mathcal{L}[f(\xi_{ijk})] := F(\Xi)$$ is the Laplace transform of

$$f_{ijk} := f(\xi_{ijk}), \quad C_{000} = 0, \quad (C_{100}, C_{101}, C_{001}) = (u, v, w) := u.$$
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
     - Example: D3Q19
     - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Example: D3Q19 MRT-LBE Model\textsuperscript{3}

\[
f(x_j + c\delta t, t_n + \delta t) = f(x_j, t_n) - M^{-1}S \left[ m - m^{(eq)}(\rho, \mathbf{u}) \right]
\] (28)

Example: D3Q19 MRT-LBE Model\textsuperscript{3}

\[
f(x_j + c\delta_t, t_n + \delta_t) = f(x_j, t_n) - M^{-1}S [m - m^{(eq)}(\rho, u)]
\]  

(28)

Conserved quantities:

\[
\rho = \sum_{i=0}^{Q-1} f_i, \quad j = \rho u = \sum_{i=0}^{Q-1} f_i c_i
\]

Transport coefficients and the speed of sound (\(c := \delta x/\delta t\)):

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

Example: D3Q19 MRT-LBE Model

\[
f(x_j + c\delta_t, t_n + \delta_t) = f(x_j, t_n) - M^{-1}S [m - m^{(eq)}(\rho, u)]
\]  (28)

Conserved quantities:

\[
\rho = \sum_{i=0}^{Q-1} f_i, \quad j = \rho u = \sum_{i=0}^{Q-1} f_i c_i
\]

Transport coefficients and the speed of sound \((c := \delta x / \delta t)\):

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

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

\[
m = Mf, \quad f = M^{-1}m
\]

Note \(\Lambda = MM^\dagger\) is diagonal, thus \(M^{-1} = M^\dagger \Lambda^{-1}\).

---

\[ e^{(eq)} = -11\rho + \frac{19}{\rho} \mathbf{j} \cdot \mathbf{j} \]  
\[ p_x^{(eq)} = \frac{1}{3\rho} \left[ 2j_x^2 - (j_y^2 + j_z^2) \right], \quad p_y^{(eq)} = \frac{1}{\rho} [j_y^2 - j_z^2] \]  
\[ p_x^{(eq)} = \frac{1}{\rho} j_x j_y, \quad p_y^{(eq)} = \frac{1}{\rho} j_y j_z, \quad p_z^{(eq)} = \frac{1}{\rho} j_x j_z \]  
\[ (q_x^{(eq)}, q_y^{(eq)}, q_z^{(eq)}) = -\frac{2}{3} (j_x, j_y, j_z) \]  
\[ m_x^{(eq)} = m_y^{(eq)} = m_z^{(eq)} = 0 \]  
\[ \epsilon^{(eq)} = 3\rho - \frac{11}{2\rho} \mathbf{j} \cdot \mathbf{j}, \quad \pi_x^{(eq)} = -\frac{1}{2} p_x^{(eq)}, \quad \pi_y^{(eq)} = -\frac{1}{2} p_y^{(eq)} \]
Outline

1 Motivations
   • The Role of Kinetic Theory
   • Scales and Related Methods

2 LBE: Mathematical Derivation
   • Discretizing time $t$
   • Low-Mach-Number (Gauss-Hermite) Expansion
   • Discretize Velocity Space $\xi$
   • Discretize Space $x$
   • Treatment of Collision — Relaxation Models
   • Example: D3Q19
   • Other Models

3 Numerical Results
   • DNS of Homogeneous Isotropic Turbulence
   • DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Other Models

- **D3Q39 Model:**

\[
c_{i} = \begin{cases} 
(0, 0, 0), (\pm 1, 0, 0) c, \ldots, (\pm 1, \pm 1, \pm 1) c, \ldots & 15 \\
(\pm 2, 0, 0) c, \ldots, (\pm 2, \pm 2, 0) c, \ldots & 18 \\
(\pm 3, 0, 0) c, \ldots & 6 
\end{cases}
\]

The energy equation is solved *separately*,\(^5\) \(k\)-\(\epsilon\) model, ...

- **Crystallographic LBE Model (RD3Q27):**\(^6\)

\[
c_{i} = \begin{cases} 
(0, 0, 0) & 1 (Z) \\
(\pm 1, 0, 0) c, (0, \pm 1, 0) c, (0, 0, \pm 1) c & 6 (F) \\
(\pm 1, \pm 1, 0) c, (0, \pm 1, \pm 1) c, (\pm 1, 0, \pm 1) c & 12 (E) \\
(\pm 1/2, \pm 1/2, \pm 1/2) c & 8 (C) 
\end{cases}
\]

---

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


Other Models

- D3Q39 Model: \(^4\)
  \[
  \mathbf{c}_i = \begin{cases} 
  (0, 0, 0), \ (\pm 1, 0, 0) \ c, \ldots, \ (\pm 1, \pm 1, \pm 1) \ c, \ldots & 15 \\
  (\pm 2, 0, 0) \ c, \ldots, \ (\pm 2, \pm 2, 0) \ c, \ldots & 18 \\
  (\pm 3, 0, 0) \ c, \ldots & 6 
  \end{cases}
  \]

  The energy equation is solved separately, \(^5\) \(k-\epsilon\) model, \ldots

- Crystallographic LBE Model (RD3Q27): \(^6\)
  \[
  \mathbf{c}_i = \begin{cases} 
  (0, 0, 0) & 1 \ (Z) \\
  (\pm 1, 0, 0) \ c, \ (0, \pm 1, 0) \ c, \ (0, 0, \pm 1) \ c & 6 \ (F) \\
  (\pm 1, \pm 1, 0) \ c, \ (0, \pm 1, \pm 1) \ c, \ (\pm 1, 0, \pm 1) \ c & 12 \ (E) \\
  (\pm 1/2, \pm 1/2, \pm 1/2) \ c & 8 \ (C) 
  \end{cases}
  \]

---

\(^4\) Y.B. Li et al. AIAA 2016-2312182 (2016).
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Decaying Homogeneous Isotropic Turbulence

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

\[
\partial_t u + u \cdot \nabla u = -\nabla p + \nu \nabla^2 u, \quad \nabla \cdot u = 0, \quad x \in [0, 2\pi]^3, \quad (30)
\]

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

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

The initial velocity \( u_0 \) can be given by Rogallo procedure:

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

where \( \alpha = \sqrt{E_0(k)/4\pi k^2} e^{i\theta_1} \cos \phi, \ \beta = \sqrt{E_0(k)/4\pi k^2} e^{i\theta_2} \sin \phi, \ \iota := \sqrt{-1}, \ \text{and} \ \theta_1, \ \theta_2, \ \phi \in [0, 2\pi] \) are uniform random variables.
Pseudo-Spectral Method

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

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

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

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

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

Use $N^3 = 128^3$ and $[k_a, k_b] = [3, 8]$.

In LBE: $\nu = 1/600 (c \delta x)$, $c := \delta x/\delta t = 1$, $Ma_{\text{max}} = \|u_0\|_{\text{max}}/c_s \leq 0.15$, $A = 1.4293 \cdot 10^{-4}$ 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 $u'_0 = \sqrt{2/3}$.

<table>
<thead>
<tr>
<th>Method</th>
<th>$L$</th>
<th>$\delta x$</th>
<th>$u'_0$</th>
<th>$\delta t$</th>
<th>$\nu$</th>
<th>$\delta t'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LBE</td>
<td>$2\pi$</td>
<td>$2\pi/N$</td>
<td>$\sqrt{2K_0/3}$</td>
<td>$2\pi/N$</td>
<td>$\nu$</td>
<td>$2\pi/Nt_0$</td>
</tr>
<tr>
<td>PS</td>
<td>$2\pi$</td>
<td>$2\pi/N$</td>
<td>$\sqrt{2/3}$</td>
<td>$2\pi\sqrt{K_0/N}$</td>
<td>$\nu/\sqrt{K_0}$</td>
<td>$2\pi/Nt_0$</td>
</tr>
</tbody>
</table>

The Taylor microscale Reynolds number:

$$Re_\lambda := \frac{u' \lambda}{\nu}, \quad \lambda := \sqrt{\frac{15}{2\Omega}} u' := \sqrt{\frac{15\nu}{\varepsilon}} u' \quad (33)$$

The resolution criterion:

SP: $N \sim 0.4Re_\lambda^{3/2}$, $\eta/\delta x \geq 1/2.1$, $N = 128 \rightarrow Re_\lambda = 46.78$

LBE: $\eta k_{\text{max}} = \eta/\delta x \geq 1$, $N = 128 \rightarrow Re_\lambda = 24.35$. 
Initial Conditions

For the pseudo-spectral method:

- Generate $\tilde{u}_0(k)$ in $k$-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 $k$-space.


- Use the initial velocity $u_0$ as in PS method except a scaling factor so that $Ma_{\text{max}} = 0.15$;  
- The pressure $p_0$ is obtained by an iterative procedure with a given $u_0$. 

Velocity Iso-surface in 3D, $Re_\lambda = 24.37$

LBE vs. PS1 (equal $\delta t$): $t' = 0.1348, 0.2359, 0.573$; $\|u(t')/u'\| = 2.0$
Vorticity Iso-surface in 3D, $Re_\lambda = 24.37$

LBE vs. PS1 (equal $\delta t$): $t' = 0.1348, 0.2359, 0.573$; $\|\omega(t')/u'\| = 13.0$
\[ \| \mathbf{u}(t')/u' \| \text{ and } \| \mathbf{\omega}(t')/u' \| \text{ at } Re_\lambda = 24.37, \ t' = 4.048 \]

LBE vs. PS1 (equal $\delta t$) and PS2 ($\delta t/3$), PS1 vs. PS2
\|u(t')/u'\| \text{ and } \|\omega(t')/u'\| \text{ at } \text{Re}_\lambda = 24.37, t' = 29.949

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

Luo (ODU)  LBE for CFD
$L^2 \| \delta u(t') \| \text{ and } \| \delta \omega(t') \|$

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

![Graphs showing comparison of LBE vs. PS1 and PS2 for different Re values.](image-url)
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
Flow past a Sphere: DNS of Drag Crisis

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
\(D = 640\delta_x\)

---

Flow past a Sphere: DNS of Drag Crisis

![Graph showing drag coefficient vs. Reynolds number for different simulations and flow conditions.](image)

- Prandtl
- Achenbach
- Bakic
- Morrison
- Almedeij

- Coarse
- Medium
- Fine

Re = 100000

Re = 240000
Outline

1 Motivations
   - The Role of Kinetic Theory
   - Scales and Related Methods

2 LBE: Mathematical Derivation
   - Discretizing time $t$
   - Low-Mach-Number (Gauss-Hermite) Expansion
   - Discretize Velocity Space $\xi$
   - Discretize Space $x$
   - Treatment of Collision — Relaxation Models
   - Example: D3Q19
   - Other Models

3 Numerical Results
   - DNS of Homogeneous Isotropic Turbulence
   - DNS of Flow past a Sphere — Drag Crisis

4 Conclusions
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
- Accuracy: 2nd-order for both velocity $u$ and the stress $\sigma$, 1st-order for pressure $p$
- Valid for variable viscosity models, e.g., $\nu = \nu(\sigma(x))$.

---

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
- Accuracy: 2nd-order for both velocity $u$ and the stress $\sigma$, 1st-order for pressure $p$
- Valid for variable viscosity models, e.g., $\nu = \nu(\sigma(x))$.

Some other Features:

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

---

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:

- 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.

---

For CFD, hyperbolic or elliptic PDEs?

For an $n$-th order scheme, how to guarantee that the operators $\nabla$ and $\nabla^2$ 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?
Food for Thought

- For CFD, hyperbolic or elliptic PDEs?
- For an $n$-th order scheme, how to guarantee that the operators $\nabla$ and $\nabla^2$ 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?
For CFD, hyperbolic or elliptic PDEs?

For an \( n \)-th order scheme, how to guarantee that the operators \( \nabla \) and \( \nabla^2 \) 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?
Food for Thought

- For CFD, hyperbolic or elliptic PDEs?
- For an $n$-th order scheme, how to guarantee that the operators $\nabla$ and $\nabla^2$ 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?
Other Applications (Animations)

- **Free-Surface Flow (Krafczyk et al., TUB):**
  - Water-Tunnel: $384 \times 64 \times 48$, $\delta_x = 10\text{cm}$, LES, $Re = 3 \cdot 10^6$
  - Flow past a bridge
  - Tsumani over S. Manhatten: $512 \times 512 \times 80$, $\delta_x = 2.35\text{m}$

- **Computational Steering (Krafczyk et al., TUB):**
  - Digital Wind Tunnel, $64 \times 64 \times 320$, $\delta_x = 10\text{cm}$, $Re = 4 \cdot 10^3$

- **Ladd (UFL):** Cluster of 1812 particles, $Re = 0.3$

- **Flow through Porous Media (Krafczyk et al., TUB):**
  - Air through fluids in a packed-sphere bio-filter
  - Multi-component flow past porous media: Imbibe-Drain-Reimbibe

- **Droplet collision (Frohn et al., Univ. Stuttgart):**
  - Merge, Separate, and Extra-One; LBE vs. Experiment.

- **More (Thüry et al., Univ. Erlangen):**
  - Bubbles rising in water tank
  - Metal foams
“You want proof? I’ll give you proof!”