



Research Centre
for Gas Innovation

Lattice Boltzmann Method: An Introductory Overview

Adriano Grigolo
(adriano.grigolo@usp.br)

PME-5429 | Multiscale Methods (2020)

PME-5429 - Lattice Boltzmann Method

Summary of topics

- 20/10: Introduction & Kinetic Theory
- 27/10: Lattice Boltzmann & Hands-On
- 03/11: Dense Fluids & Hands-On

The logo consists of a square frame containing abstract shapes. A light green shape is in the top-left corner. A large white shape, resembling a stylized 'G' or a leaf, is the central element. A light blue shape is in the bottom-right corner, and another light blue shape is in the bottom-left corner.

Brief review

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$

$$g = f_0 \times \left(1 + \tau_c ((\boldsymbol{\xi} - \mathbf{u})/R T) \cdot \mathbf{g} \right)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$

$$g = f_0 \times \left(1 + \tau_c ((\boldsymbol{\xi} - \mathbf{u})/R T) \cdot \mathbf{g} \right)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$

$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$
$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$
$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$

$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$
$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$

$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$

$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Review

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c} (f - g)$$

$$f_0 = \frac{\rho}{m} (2\pi R T)^{-3/2} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R T} \right]$$
$$g = f_0(\mathbf{u} + \tau_c \mathbf{g}, \rho, T)$$

- τ_c : relaxation time (BGK collision model)
- f_0 : equilibrium distribution function
- $\mathbf{g}(\mathbf{r}, t)$: external force per unit mass
- equation of state: $p = \rho R T$ (ideal gas)
- transport coefficients: $\mu = \rho R T \tau_c$ and $\lambda = \frac{5}{3} c_v \rho R T \tau_c$
- multiscale modeling approach

Next steps

PHYSICAL REVIEW E

VOLUME 56, NUMBER 6

DECEMBER 1997

Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation

Xiaoyi He^{1,2,*} and Li-Shi Luo^{2,3,†}

¹*Center for Nonlinear Studies, MS-B258, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*

²*Complex Systems Group T-13, MS-B213, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*

³*ICASE, MS 403, NASA Langley Research Center, 6 North Dryden Street, Building 1298, Hampton, Virginia 23681-0001*

(Received 29 April 1997; revised manuscript received 26 August 1997)

- Design time-marching scheme
- Introduce discrete velocity space

Part 2:

The Lattice Boltzmann method

- 1 Time-marching scheme
- 2 Lattice scheme
- 3 The Lattice Boltzmann Equation
- 4 Boundary conditions
- 5 Hands-on tutorial

A stylized logo consisting of a light green square in the top-left corner, a light blue square in the bottom-left corner, and a light blue square in the bottom-right corner. A white, curved shape resembling a stylized 'G' or a leaf is centered within the composition.

Time-marching scheme

Time-marching – velocity characteristics

The left-hand side of the transport equation is an *exact differential along constant velocity lines*

$$f(\mathbf{r}(t), \boldsymbol{\xi}, t) \quad \text{with} \quad \dot{\mathbf{r}}(t) = \boldsymbol{\xi}$$

that is:

$$\frac{df(\mathbf{r}(t), \boldsymbol{\xi}, t)}{dt} = \frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}}$$

In the LB scheme, the transport equation is integrated along these constant velocity lines

$$\frac{df(t)}{dt} = \Omega_g(t)$$

Time-marching – velocity characteristics

The left-hand side of the transport equation is an *exact differential along constant velocity lines*

$$f(\mathbf{r}(t), \boldsymbol{\xi}, t) \quad \text{with} \quad \dot{\mathbf{r}}(t) = \boldsymbol{\xi}$$

that is:

$$\frac{df(\mathbf{r}(t), \boldsymbol{\xi}, t)}{dt} = \frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}}$$

In the LB scheme, the transport equation is integrated along these constant velocity lines

$$\frac{df(t)}{dt} = \Omega_g(t)$$

Time marching

Integrating over a small time interval δt we get

$$f(\mathbf{r} + \boldsymbol{\xi}\delta t, \boldsymbol{\xi}, t + \delta t) - f(\mathbf{r}, \boldsymbol{\xi}, t) = \int_t^{t+\delta t} \Omega_g(s) ds$$

The right-hand side must be approximated somehow...

$$\int_t^{t+\delta t} \Omega_g(s) ds \approx \delta t \Omega_g(t)$$

simple first-order scheme (too crude)

Time marching

Integrating over a small time interval δt we get

$$f(\mathbf{r} + \boldsymbol{\xi}\delta t, \boldsymbol{\xi}, t + \delta t) - f(\mathbf{r}, \boldsymbol{\xi}, t) = \int_t^{t+\delta t} \Omega_g(s) ds$$

The right-hand side must be approximated somehow...

$$\int_t^{t+\delta t} \Omega_g(s) ds \approx \delta t \Omega_g(t)$$

simple first-order scheme (too crude)

Time marching

Integrating over a small time interval δt we get

$$f(\mathbf{r} + \boldsymbol{\xi}\delta t, \boldsymbol{\xi}, t + \delta t) - f(\mathbf{r}, \boldsymbol{\xi}, t) = \int_t^{t+\delta t} \Omega_g(s) ds$$

The right-hand side must be approximated somehow...

$$\int_t^{t+\delta t} \Omega_g(s) ds \approx \frac{\delta t}{2} [\Omega_g(t + \delta t) + \Omega_g(t)]$$

✓ second-order scheme (OK!)

Avoiding implicit scheme

... but this leads to an implicit scheme:

$$f(t + \delta t) - f(t) = \frac{\delta t}{2} [\Omega_g(t + \delta t) + \Omega_g(t)]$$

Introduce new dynamic variable

$$\tilde{f}(t) \equiv f(t) - \frac{\delta t}{2} \Omega_g(t)$$

Then, after a few manipulations,

$$\tilde{f}(t + \delta t) - \tilde{f}(t) = -\frac{1}{\tau} (\tilde{f}(t) - g(t))$$

with the new (dimensionless) relaxation time

$$\tau = (\tau_c / \delta t) + \frac{1}{2}, \quad (\tau > 0.50)$$

Avoiding implicit scheme

... but this leads to an implicit scheme:

$$f(t + \delta t) - f(t) = \frac{\delta t}{2} [\Omega_g(t + \delta t) + \Omega_g(t)]$$

Introduce new dynamic variable

$$\tilde{f}(t) \equiv f(t) - \frac{\delta t}{2} \Omega_g(t)$$

Then, after a few manipulations,

$$\tilde{f}(t + \delta t) - \tilde{f}(t) = -\frac{1}{\tau} (\tilde{f}(t) - g(t))$$

with the new (dimensionless) relaxation time

$$\tau = (\tau_c / \delta t) + \frac{1}{2}, \quad (\tau > 0.50)$$

Avoiding implicit scheme

... but this leads to an implicit scheme:

$$f(t + \delta t) - f(t) = \frac{\delta t}{2} [\Omega_g(t + \delta t) + \Omega_g(t)]$$

Introduce new dynamic variable

$$\tilde{f}(t) \equiv \left(1 + \frac{\delta t}{2\tau_c}\right) f(t) - \frac{\delta t}{2\tau_c} g(t)$$

Then, after a few manipulations,

$$\tilde{f}(t + \delta t) - \tilde{f}(t) = -\frac{1}{\tau} (\tilde{f}(t) - g(t))$$

with the new (dimensionless) relaxation time

$$\tau = (\tau_c/\delta t) + \frac{1}{2}, \quad (\tau > 0.50)$$

Avoiding implicit scheme

... but this leads to an implicit scheme:

$$f(t + \delta t) - f(t) = \frac{\delta t}{2} [\Omega_g(t + \delta t) + \Omega_g(t)]$$

Introduce new dynamic variable

$$\tilde{f}(t) \equiv \left(1 + \frac{\delta t}{2\tau_c}\right) f(t) - \frac{\delta t}{2\tau_c} g(t)$$

Then, after a few manipulations,

$$\tilde{f}(t + \delta t) - \tilde{f}(t) = -\frac{1}{\tau} (\tilde{f}(t) - g(t))$$

with the new (dimensionless) relaxation time

$$\tau = (\tau_c/\delta t) + \frac{1}{2}, \quad (\tau > 0.50)$$

Time-marching scheme

The time propagation is conducted as

$$\tilde{f}(t + \delta t) = \tilde{f}(t) - \frac{1}{\tau}(\tilde{f}(t) - g(t))$$
$$g = f_0 \left[1 + \delta t \left(\tau - \frac{1}{2} \right) \frac{(\boldsymbol{\xi} - \mathbf{u})}{RT} \cdot \mathbf{g} \right]$$

In terms of \tilde{f} the flow fields are computed as

$$\rho = \int m \tilde{f} d\xi$$

$$\rho \mathbf{u} = \int m \boldsymbol{\xi} \tilde{f} d\xi + \frac{\delta t}{2} \rho \mathbf{g}$$

$$\rho e = \int \frac{1}{2} m \xi^2 \tilde{f} d\xi + \frac{\delta t}{2} \rho \mathbf{g} \cdot \mathbf{u}$$

Time-marching scheme

The time propagation is conducted as

$$\tilde{f}(t + \delta t) = \tilde{f}(t) - \frac{1}{\tau}(\tilde{f}(t) - g(t))$$
$$g = f_0 \left[1 + \delta t \left(\tau - \frac{1}{2} \right) \frac{(\boldsymbol{\xi} - \mathbf{u})}{RT} \cdot \mathbf{g} \right]$$

In terms of \tilde{f} the flow fields are computed as

$$\rho = \int m \tilde{f} d\boldsymbol{\xi}$$

$$\rho \mathbf{u} = \int m \boldsymbol{\xi} \tilde{f} d\boldsymbol{\xi} + \frac{\delta t}{2} \rho \mathbf{g}$$

$$\rho e = \int \frac{1}{2} m \boldsymbol{\xi}^2 \tilde{f} d\boldsymbol{\xi} + \frac{\delta t}{2} \rho \mathbf{g} \cdot \mathbf{u}$$

Time-marching scheme

The time propagation is conducted as

$$\begin{aligned}\tilde{f}(\mathbf{r} + \boldsymbol{\xi}\delta t, \boldsymbol{\xi}, t + \delta t) &= \tilde{f}(\mathbf{r}, \boldsymbol{\xi}, t) - \tilde{\Omega}_g(\mathbf{r}, \boldsymbol{\xi}, t) \\ \tilde{\Omega}_g &\equiv -\frac{1}{\tau}(\tilde{f} - g)\end{aligned}$$

In terms of \tilde{f} the flow fields are computed as

$$\rho = \int m\tilde{f}d\boldsymbol{\xi}$$

$$\rho\mathbf{u} = \int m\boldsymbol{\xi}\tilde{f}d\boldsymbol{\xi} + \frac{\delta t}{2}\rho\mathbf{g}$$

$$\rho e = \int \frac{1}{2}m\xi^2\tilde{f}d\boldsymbol{\xi} + \frac{\delta t}{2}\rho\mathbf{g} \cdot \mathbf{u}$$

A stylized logo consisting of overlapping shapes in light green, white, and light blue. The green shape is in the top-left corner. The white shape is a large, curved, leaf-like form in the center. The blue shape is a curved, leaf-like form overlapping the white one. The text "Lattice scheme" is centered over the white shape.

Lattice scheme

Discrete velocity space

Basic idea: introduce a discrete velocity space,

$$f(\mathbf{r}, \boldsymbol{\xi}, t) \rightarrow f(\mathbf{r}, \mathbf{e}_\alpha, t) \quad \alpha = 0, \dots, M$$

so that flow-field integrals can be replaced by some quadrature rule :

$$\rho = \int m f d\boldsymbol{\xi}$$

$$\rho \mathbf{u} = \int m \boldsymbol{\xi} f d\boldsymbol{\xi}$$

$$\rho e = \int \frac{1}{2} m \boldsymbol{\xi}^2 f d\boldsymbol{\xi}$$

Discrete velocity space

Basic idea: introduce a discrete velocity space,

$$f(\mathbf{r}, \boldsymbol{\xi}, t) \rightarrow f(\mathbf{r}, \mathbf{e}_\alpha, t) \quad \alpha = 0, \dots, M$$

so that flow-field integrals can be replaced by some quadrature rule :

$$\rho = \int m f d\boldsymbol{\xi} \approx \sum_{\alpha} W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho \mathbf{u} = \int m \boldsymbol{\xi} f d\boldsymbol{\xi} \approx \sum_{\alpha} m \mathbf{e}_{\alpha} W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho e = \int \frac{1}{2} m \boldsymbol{\xi}^2 f d\boldsymbol{\xi} \approx \sum_{\alpha} \frac{1}{2} m |\mathbf{e}_{\alpha}|^2 W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$\mathbf{e}_{\alpha} = \text{nodes}$, $W_{\alpha} = \text{weight factors}$, $M = \text{order}$

Discrete velocity space

Basic idea: introduce a discrete velocity space,

$$f(\mathbf{r}, \boldsymbol{\xi}, t) \rightarrow f(\mathbf{r}, \mathbf{e}_\alpha, t) \quad \alpha = 0, \dots, M$$

so that flow-field integrals can be replaced by some quadrature rule (**Chapman-Enskog assumptions**):

$$\rho = \int m f_0 d\boldsymbol{\xi} = \sum_{\alpha} W_{\alpha} f_0(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho \mathbf{u} = \int m \boldsymbol{\xi} f_0 d\boldsymbol{\xi} = \sum_{\alpha} m \mathbf{e}_{\alpha} W_{\alpha} f_0(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho e = \int \frac{1}{2} m \boldsymbol{\xi}^2 f_0 d\boldsymbol{\xi} = \sum_{\alpha} \frac{1}{2} m |\mathbf{e}_{\alpha}|^2 W_{\alpha} f_0(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

- *exact* under suitable conditions ...

Discrete velocity space

Basic idea: introduce a discrete velocity space,

$$f(\mathbf{r}, \boldsymbol{\xi}, t) \rightarrow f(\mathbf{r}, \mathbf{e}_\alpha, t) \quad \alpha = 0, \dots, M$$

so that flow-field integrals can be replaced by some quadrature rule (**Chapman-Enskog assumptions**):

$$\rho = \int m f d\boldsymbol{\xi} = \sum_{\alpha} W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho \mathbf{u} = \int m \boldsymbol{\xi} f d\boldsymbol{\xi} = \sum_{\alpha} m \mathbf{e}_{\alpha} W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho e = \int \frac{1}{2} m \boldsymbol{\xi}^2 f d\boldsymbol{\xi} = \sum_{\alpha} \frac{1}{2} m |\mathbf{e}_{\alpha}|^2 W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

- *exact* under suitable conditions ...

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f_0 = \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2RT} \right]$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\iint d\xi_x d\xi_y (\xi_x)^{m_1} (\xi_y)^{m_2} e^{-\frac{\xi^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{\max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f_0 = \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \exp \left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2RT} \right]$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\iint d\xi_x d\xi_y (\xi_x)^{m_1} (\xi_y)^{m_2} e^{-\frac{\xi^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{\max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f_0 \approx \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \left[1 + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{RT} + \frac{1}{2} \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{(RT)^2} - \frac{u^2}{2RT} \right] e^{-\frac{\xi^2}{2RT}}$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\iint d\xi_x d\xi_y (\xi_x)^{m_1} (\xi_y)^{m_2} e^{-\frac{\xi^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{\max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f^{eq} \equiv \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \left[1 + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{RT} + \frac{1}{2} \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{(RT)^2} - \frac{u^2}{2RT} \right] e^{-\frac{\xi^2}{2RT}}$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\iint d\xi_x d\xi_y (\xi_x)^{m_1} (\xi_y)^{m_2} e^{-\frac{\xi^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f^{eq} \equiv \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \left[1 + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{RT} + \frac{1}{2} \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{(RT)^2} - \frac{u^2}{2RT} \right] e^{-\frac{\xi^2}{2RT}}$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\iint d\xi_x d\xi_y (\xi_x)^{m_1} (\xi_y)^{m_2} e^{-\frac{\xi^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f^{eq} \equiv \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \left[1 + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{RT} + \frac{1}{2} \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{(RT)^2} - \frac{u^2}{2RT} \right] e^{-\frac{\xi^2}{2RT}}$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\iint d\xi_x d\xi_y (\xi_x)^{m_1} (\xi_y)^{m_2} e^{-\frac{\xi^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{\max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f^{eq} \equiv \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \left[1 + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{RT} + \frac{1}{2} \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{(RT)^2} - \frac{u^2}{2RT} \right] e^{-\frac{\xi^2}{2RT}}$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\int d\xi_x (\xi_x)^{m_1} e^{-\frac{\xi_x^2}{2RT}} \times \int d\xi_y (\xi_y)^{m_2} e^{-\frac{\xi_y^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{max} \leq (2M - 1)$

Low Mach number approximation

If we assume

$$(u^2/RT) \ll 1 \quad (\sqrt{RT} \propto \text{sound speed})$$

$$f^{eq} \equiv \frac{\rho/m}{(2\pi RT)^{\frac{D}{2}}} \left[1 + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{RT} + \frac{1}{2} \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{(RT)^2} - \frac{u^2}{2RT} \right] e^{-\frac{\xi^2}{2RT}}$$

(from now on we consider $D = 2$)

... evaluation of flow variables will involve integrals of the form:

$$\int d\xi_x (\xi_x)^{m_1} e^{-\frac{\xi_x^2}{2RT}} \times \int d\xi_y (\xi_y)^{m_2} e^{-\frac{\xi_y^2}{2RT}}$$

Gauss-Hermite quadratures exact if $m_{max} \leq (2M - 1)$

Gauss-Hermite quadratures

General M -th order formula (one dimension):

$$\int_{-\infty}^{+\infty} \psi(x) e^{-x^2} dx \approx \sum_{\alpha} w_{\alpha} \psi(x_{\alpha})$$

with node points and weight factors determined by

$$w_{\alpha} = \frac{2^{M-1} M! \sqrt{\pi}}{M^2 [H_{M-1}(x_{\alpha})]^2} \quad \text{with} \quad H_M(x_{\alpha}) = 0$$

$H_M(x)$ = M -th degree Hermite polynomial

ex: $M = 2$:
$$\begin{array}{l} x_{\alpha} = -1/\sqrt{2} \quad +1/\sqrt{2} \\ w_{\alpha} = \sqrt{\pi}/2 \quad \sqrt{\pi}/2 \end{array}$$

Gauss-Hermite quadratures

General M -th order formula (one dimension):

$$\int_{-\infty}^{+\infty} \psi(x) e^{-x^2} dx \approx \sum_{\alpha} w_{\alpha} \psi(x_{\alpha})$$

with node points and weight factors determined by

$$w_{\alpha} = \frac{2^{M-1} M! \sqrt{\pi}}{M^2 [H_{M-1}(x_{\alpha})]^2} \quad \text{with} \quad H_M(x_{\alpha}) = 0$$

$H_M(x)$ = M -th degree Hermite polynomial

$$\text{ex: } M = 2: \quad \begin{array}{l} x_{\alpha} = \quad -1/\sqrt{2} \quad +1/\sqrt{2} \\ w_{\alpha} = \quad \sqrt{\pi}/2 \quad \sqrt{\pi}/2 \end{array}$$

Gauss-Hermite quadratures

General M -th order formula (one dimension):

$$\int_{-\infty}^{+\infty} \psi(x) e^{-x^2} dx \approx \sum_{\alpha} w_{\alpha} \psi(x_{\alpha})$$

with node points and weight factors determined by

$$w_{\alpha} = \frac{2^{M-1} M! \sqrt{\pi}}{M^2 [H_{M-1}(x_{\alpha})]^2} \quad \text{with} \quad H_M(x_{\alpha}) = 0$$

$H_M(x)$ = M -th degree Hermite polynomial

ex: $M = 3$:

$$\begin{array}{l} x_{\alpha} = \quad -\sqrt{6}/2 \quad \quad 0 \quad \quad \sqrt{6}/2 \\ w_{\alpha} = \quad \sqrt{\pi}/6 \quad 2\sqrt{\pi}/3 \quad \sqrt{\pi}/6 \end{array}$$

Gauss-Hermite quadratures

General M -th order formula (one dimension):

$$\int_{-\infty}^{+\infty} \psi(x) e^{-x^2} dx \approx \sum_{\alpha} w_{\alpha} \psi(x_{\alpha})$$

with node points and weight factors determined by

$$w_{\alpha} = \frac{2^{M-1} M! \sqrt{\pi}}{M^2 [H_{M-1}(x_{\alpha})]^2} \quad \text{with} \quad H_M(x_{\alpha}) = 0$$

$H_M(x)$ = M -th degree Hermite polynomial

$$\int_{-\infty}^{+\infty} x^m e^{-x^2} dx = \sum_{\alpha} w_{\alpha} x_{\alpha}^m$$

if $m \leq 2M - 1$

Exact evaluation of flow variables

What is the minimum quadrature order needed?

$$\rho \mathbf{u} = \int d\xi \overbrace{m\xi}^{(1)} \cdot \overbrace{f^{eq}(\xi)}^{(2)} \quad (\text{isothermal})$$

$$\rho e = \int d\xi \overbrace{\frac{1}{2}m\xi^2}^{(2)} \cdot \overbrace{f^{eq}(\xi)}^{(2)} \quad (\text{thermal})$$

But this is not enough: the relations

$$\int d\xi m\xi \delta f = 0; \quad \int d\xi \frac{1}{2}m\xi^2 \delta f = 0$$

must also be preserved with $\delta f = \phi f^{eq}$ with $\phi(\xi)$ being of second-order in (ξ_x, ξ_y) [He-Luo (1997)].

Exact evaluation of flow variables

What is the minimum quadrature order needed?

$$\rho \mathbf{u} = \int d\boldsymbol{\xi} \overbrace{m\boldsymbol{\xi}}^{(1)} \cdot \overbrace{f^{eq}(\boldsymbol{\xi})}^{(2)} \quad (\text{isothermal})$$

$$\rho e = \int d\boldsymbol{\xi} \overbrace{\frac{1}{2}m\xi^2}^{(2)} \cdot \overbrace{f^{eq}(\boldsymbol{\xi})}^{(2)} \quad (\text{thermal})$$

But this is not enough: the relations

$$\int d\boldsymbol{\xi} m\boldsymbol{\xi} \delta f = 0; \quad \int d\boldsymbol{\xi} \frac{1}{2}m\xi^2 \delta f = 0$$

must also be preserved with $\delta f = \phi f^{eq}$ with $\phi(\boldsymbol{\xi})$ being of second-order in (ξ_x, ξ_y) [He-Luo (1997)].

Exact evaluation of flow variables

$$0 = \int d\xi \overbrace{m\xi}^{(1)} \cdot \overbrace{\phi(\xi)}^{(2)} \cdot \overbrace{f^{eq}(\xi)}^{(2)} \quad (\text{isothermal})$$

$$0 = \int d\xi \overbrace{\frac{1}{2}m\xi^2}^{(2)} \cdot \overbrace{\phi(\xi)}^{(2)} \cdot \overbrace{f^{eq}(\xi)}^{(2)} \quad (\text{thermal})$$

Thus, the minimum quadrature order for each velocity component (ξ_x, ξ_y) is

$$5 \leq 2M - 1 \Rightarrow M_{\min} = 3 \quad (\text{isothermal})$$

$$6 \leq 2M - 1 \Rightarrow M_{\min} = 4 \quad (\text{thermal})$$

Exact evaluation of flow variables

$$0 = \int d\boldsymbol{\xi} \overbrace{m\boldsymbol{\xi}}^{(1)} \cdot \overbrace{\phi(\boldsymbol{\xi})}^{(2)} \cdot \overbrace{f^{eq}(\boldsymbol{\xi})}^{(2)} \quad (\text{isothermal})$$

$$0 = \int d\boldsymbol{\xi} \overbrace{\frac{1}{2}m\xi^2}^{(2)} \cdot \overbrace{\phi(\boldsymbol{\xi})}^{(2)} \cdot \overbrace{f^{eq}(\boldsymbol{\xi})}^{(2)} \quad (\text{thermal})$$

Thus, the minimum quadrature order for each velocity component (ξ_x, ξ_y) is

$$5 \leq 2M - 1 \Rightarrow M_{\min} = 3 \quad (\text{isothermal})$$

$$6 \leq 2M - 1 \Rightarrow M_{\min} = 4 \quad (\text{thermal})$$

Exact evaluation of flow variables

$$0 = \int d\xi \overbrace{m\xi}^{(1)} \cdot \overbrace{\phi(\xi)}^{(2)} \cdot \overbrace{f^{eq}(\xi)}^{(2)} \quad (\text{isothermal})$$

$$0 = \int d\xi \overbrace{\frac{1}{2}m\xi^2}^{(2)} \cdot \overbrace{\phi(\xi)}^{(2)} \cdot \overbrace{f^{eq}(\xi)}^{(2)} \quad (\text{thermal})$$

... and the minimum number of nodes in two-dimensional velocity space for each case is

$$3 \times 3 = 9 \quad \text{nodes} \quad (\text{isothermal})$$

$$4 \times 4 = 16 \quad \text{nodes} \quad (\text{thermal})$$

Isothermal vs. thermal models

Difficulties involved in thermal models:

- Not really compatible with simple BGK model (recall: $\lambda/\mu c_v \neq 2.5$ for ideal gases)
- Finer lattices are required
- Nodal positions depend on temperature (weight function involves T)
- Second-order low Mach number approximation not really adequate (thermal models should account for high compressibility)
- Generally more unstable

Isothermal lattice models

From now on we consider only *isothermal models*

Hydrodynamic moments:

$$\rho = \int m \tilde{f} d\xi, \quad \rho \mathbf{u} = \int m \xi \tilde{f} d\xi + \frac{\delta t}{2} \rho \mathbf{g}$$

Equation of state (*ideal gas for now*):

$$p = \rho R T = \rho c_s^2$$

$$c_s \equiv \sqrt{(\partial p / \partial \rho)_T} = \sqrt{R T} \quad (\text{isothermal sound speed})$$

Transport coefficient:

$$\mu = \rho R T \tau_c \Rightarrow \nu \equiv \mu / \rho = c_s^2 \tau_c \quad (\text{kinematic viscosity})$$

Isothermal lattice models

From now on we consider only *isothermal models*

Hydrodynamic moments:

$$\rho = \int m \tilde{f} d\xi, \quad \rho \mathbf{u} = \int m \xi \tilde{f} d\xi + \frac{\delta t}{2} \rho \mathbf{g}$$

Equation of state (*ideal gas for now*):

$$p = \rho RT = \rho c_s^2$$

$$c_s \equiv \sqrt{(\partial p / \partial \rho)_T} = \sqrt{RT} \quad (\text{isothermal sound speed})$$

Transport coefficient:

$$\mu = \rho RT \tau_c \Rightarrow \nu \equiv \mu / \rho = c_s^2 \tau_c \quad (\text{kinematic viscosity})$$

Isothermal lattice models

From now on we consider only *isothermal models*

Hydrodynamic moments:

$$\rho = \int m \tilde{f} d\xi, \quad \rho \mathbf{u} = \int m \xi \tilde{f} d\xi + \frac{\delta t}{2} \rho \mathbf{g}$$

Equation of state (*ideal gas for now*):

$$p = \rho R T = \rho c_s^2$$

$$c_s \equiv \sqrt{(\partial p / \partial \rho)_T} = \sqrt{R T} \quad (\text{isothermal sound speed})$$

Transport coefficient:

$$\mu = \rho R T \tau_c \Rightarrow \nu \equiv \mu / \rho = c_s^2 \tau_c \quad (\text{kinematic viscosity})$$

Isothermal lattice models

From now on we consider only *isothermal models*

Hydrodynamic moments:

$$\rho = \int m \tilde{f} d\xi, \quad \rho \mathbf{u} = \int m \xi \tilde{f} d\xi + \frac{\delta t}{2} \rho \mathbf{g}$$

Equation of state (*ideal gas for now*):

$$p = \rho R T = \rho c_s^2$$

$$c_s \equiv \sqrt{(\partial p / \partial \rho)_T} = \sqrt{R T} \quad (\text{isothermal sound speed})$$

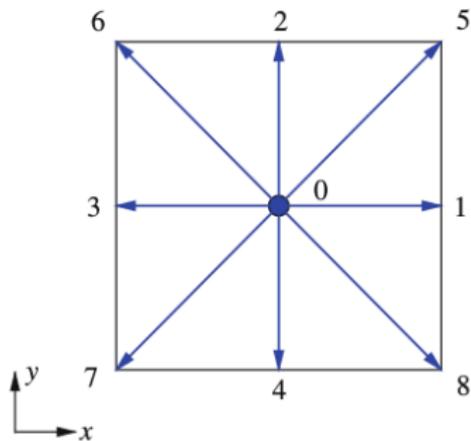
Transport coefficient:

$$\mu = \rho R T \tau_c \Rightarrow \nu \equiv \mu / \rho = c_s^2 \tau_c \quad (\text{kinematic viscosity})$$

D2Q9 isothermal lattice model

Evaluation of flow variables with 3×3 quadrature:

$$\rho = \sum_{\alpha} W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t), \quad \rho \mathbf{u} = \sum_{\alpha} m \mathbf{e}_{\alpha} W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$



$c = \sqrt{3RT}$: 'lattice speed'

$$\mathbf{e}_0 = (0, 0)$$

$$\mathbf{e}_1 = (+c, 0)$$

$$\mathbf{e}_2 = (0, +c)$$

$$\mathbf{e}_3 = (-c, 0)$$

$$\mathbf{e}_4 = (0, -c)$$

$$\mathbf{e}_5 = (+c, +c)$$

$$\mathbf{e}_6 = (-c, +c)$$

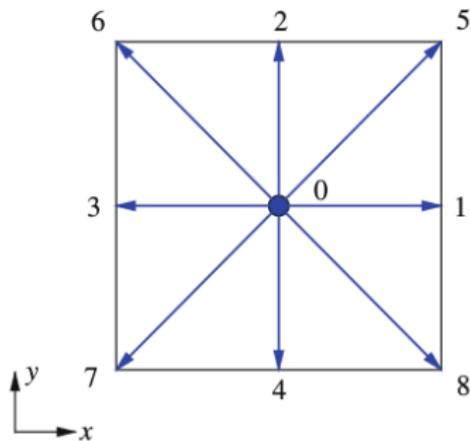
$$\mathbf{e}_7 = (-c, -c)$$

$$\mathbf{e}_8 = (+c, -c)$$

D2Q9 isothermal lattice model

Evaluation of flow variables with 3×3 quadrature:

$$\rho = \sum_{\alpha} W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t), \quad \rho \mathbf{u} = \sum_{\alpha} m \mathbf{e}_{\alpha} W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$



$c = \sqrt{3RT}$: 'lattice speed'

$$\mathbf{e}_0 = (0, 0)$$

$$\mathbf{e}_1 = (+c, 0)$$

$$\mathbf{e}_2 = (0, +c)$$

$$\mathbf{e}_3 = (-c, 0)$$

$$\mathbf{e}_4 = (0, -c)$$

$$\mathbf{e}_5 = (+c, +c)$$

$$\mathbf{e}_6 = (-c, +c)$$

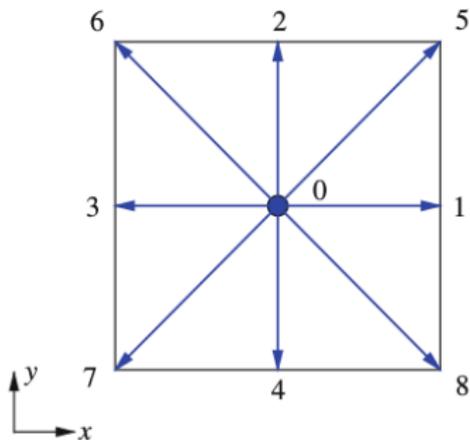
$$\mathbf{e}_7 = (-c, -c)$$

$$\mathbf{e}_8 = (+c, -c)$$

D2Q9 isothermal lattice model

Evaluation of flow variables with 3×3 quadrature:

$$\rho = \sum_{\alpha} W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t), \quad \rho \mathbf{u} = \sum_{\alpha} m \mathbf{e}_{\alpha} W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$



weights:

$$W_{\alpha} = \omega_{\alpha} \cdot (2\pi R T)^{\frac{D}{2}} \cdot e^{\frac{\xi_{\alpha}^2}{2RT}}$$

$$\omega_0 = \frac{4}{9}$$

$$\omega_1 = \omega_2 = \omega_3 = \omega_4 = \frac{1}{9}$$

$$\omega_5 = \omega_6 = \omega_7 = \omega_8 = \frac{1}{36}$$

(obs: $\sum_{\alpha} \omega_{\alpha} = 1$)

D2Q9: Lattice equilibrium distribution

Then:

$$\rho = \sum_{\alpha=0}^8 m \times W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} \times W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t) = \frac{\rho \omega_{\alpha}}{m} \left[1 + \frac{\mathbf{e}_{\alpha} \cdot \mathbf{u}}{RT} + \frac{(\mathbf{e}_{\alpha} \cdot \mathbf{u})^2}{2RT} - \frac{u^2}{2RT} \right]$$

D2Q9: Lattice equilibrium distribution

Then:

$$\rho = \sum_{\alpha=0}^8 m \times W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} \times W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)$$

$$W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t) = \frac{\rho \omega_{\alpha}}{m} \left[1 + \frac{\mathbf{e}_{\alpha} \cdot \mathbf{u}}{RT} + \frac{(\mathbf{e}_{\alpha} \cdot \mathbf{u})^2}{2RT} - \frac{u^2}{2RT} \right]$$

D2Q9: Lattice equilibrium distribution

Then:

$$\rho = \sum_{\alpha=0}^8 m n_{\alpha}^{eq}(\mathbf{r}, t)$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} n_{\alpha}^{eq}(\mathbf{r}, t)$$

$$n_{\alpha}^{eq}(\mathbf{r}, t) \equiv \frac{\rho \omega_{\alpha}}{m} \left[1 + \frac{3 \mathbf{e}_{\alpha} \cdot \mathbf{u}}{c^2} + \frac{9 (\mathbf{e}_{\alpha} \cdot \mathbf{u})^2}{2c^4} - \frac{3u^2}{2c^2} \right]$$

(D2Q9 lattice equilibrium distribution)

Fractional populations

D2Q9 lattice quadrature:

$$\rho = \sum_{\alpha=0}^8 m [W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} [W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

$$\rho = \sum_{\alpha=0}^8 m [W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} [W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

Fractional populations

D2Q9 lattice quadrature:

$$\rho = \sum_{\alpha=0}^8 m [W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} [W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

Same formulas apply to the dynamic variables f :

$$\rho = \sum_{\alpha=0}^8 m [W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} [W_{\alpha} f(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

Fractional populations

D2Q9 lattice quadrature:

$$\rho = \sum_{\alpha=0}^8 m [W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$
$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} [W_{\alpha} f^{eq}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$

And also to the time-marching variables \tilde{f} :

$$\rho = \sum_{\alpha=0}^8 m [W_{\alpha} \tilde{f}(\mathbf{r}, \mathbf{e}_{\alpha}, t)]$$
$$\rho \mathbf{u} = \sum_{\alpha=0}^8 m \mathbf{e}_{\alpha} [W_{\alpha} \tilde{f}(\mathbf{r}, \mathbf{e}_{\alpha}, t)] + \frac{\delta t}{2} \rho \mathbf{g}$$

Fractional populations

New dynamic variables:

$$n_\alpha(\mathbf{r}, t) \equiv W_\alpha \tilde{f}(\mathbf{r}, \mathbf{e}_\alpha, t) \quad (\text{obs: } [W_\alpha] = [d\xi])$$

Time-marching scheme translates to

$$n_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta t, t + \delta t) - n_\alpha(\mathbf{r}, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}, t) - g_\alpha(\mathbf{r}, t))$$

$$g_\alpha(\mathbf{r}, t) = n_\alpha^{eq}(\mathbf{r}, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}) \cdot \mathbf{g} \right]$$

Evaluation of flow fields

$$\rho(\mathbf{r}, t) = \sum_\alpha m n_\alpha(\mathbf{r}, t)$$

$$\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) = \sum_\alpha m \mathbf{e}_\alpha n_\alpha(\mathbf{r}, t) + (\delta t/2) \rho(\mathbf{r}, t) \mathbf{g}(\mathbf{r}, t)$$

just one step away from the LBE ...

Fractional populations

New dynamic variables:

$$n_\alpha(\mathbf{r}, t) \equiv W_\alpha \tilde{f}(\mathbf{r}, \mathbf{e}_\alpha, t) \quad (\text{obs: } [W_\alpha] = [d\xi])$$

Time-marching scheme translates to

$$n_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta t, t + \delta t) - n_\alpha(\mathbf{r}, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}, t) - g_\alpha(\mathbf{r}, t))$$

$$g_\alpha(\mathbf{r}, t) = n_\alpha^{eq}(\mathbf{r}, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}) \cdot \mathbf{g} \right]$$

Evaluation of flow fields

$$\rho(\mathbf{r}, t) = \sum_\alpha m n_\alpha(\mathbf{r}, t)$$

$$\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) = \sum_\alpha m \mathbf{e}_\alpha n_\alpha(\mathbf{r}, t) + (\delta t/2) \rho(\mathbf{r}, t) \mathbf{g}(\mathbf{r}, t)$$

just one step away from the LBE ...

Fractional populations

New dynamic variables:

$$n_\alpha(\mathbf{r}, t) \equiv W_\alpha \tilde{f}(\mathbf{r}, \mathbf{e}_\alpha, t) \quad (\text{obs: } [W_\alpha] = [d\xi])$$

Time-marching scheme translates to

$$n_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta t, t + \delta t) - n_\alpha(\mathbf{r}, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}, t) - g_\alpha(\mathbf{r}, t))$$

$$g_\alpha(\mathbf{r}, t) = n_\alpha^{eq}(\mathbf{r}, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}) \cdot \mathbf{g} \right]$$

Evaluation of flow fields

$$\rho(\mathbf{r}, t) = \sum_\alpha m n_\alpha(\mathbf{r}, t)$$

$$\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) = \sum_\alpha m \mathbf{e}_\alpha n_\alpha(\mathbf{r}, t) + (\delta t/2) \rho(\mathbf{r}, t) \mathbf{g}(\mathbf{r}, t)$$

just one step away from the LBE ...

Fractional populations

New dynamic variables:

$$n_\alpha(\mathbf{r}, t) \equiv W_\alpha \tilde{f}(\mathbf{r}, \mathbf{e}_\alpha, t) \quad (\text{obs: } [W_\alpha] = [d\xi])$$

Time-marching scheme translates to

$$n_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta t, t + \delta t) - n_\alpha(\mathbf{r}, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}, t) - g_\alpha(\mathbf{r}, t))$$

$$g_\alpha(\mathbf{r}, t) = n_\alpha^{eq}(\mathbf{r}, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}) \cdot \mathbf{g} \right]$$

Evaluation of flow fields

$$\rho(\mathbf{r}, t) = \sum_\alpha m n_\alpha(\mathbf{r}, t)$$

$$\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) = \sum_\alpha m \mathbf{e}_\alpha n_\alpha(\mathbf{r}, t) + (\delta t/2) \rho(\mathbf{r}, t) \mathbf{g}(\mathbf{r}, t)$$

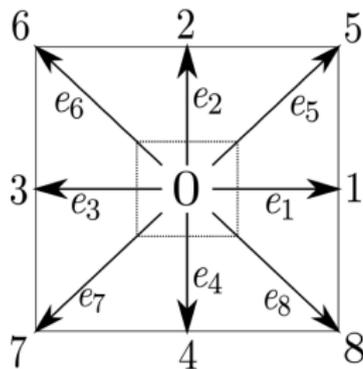
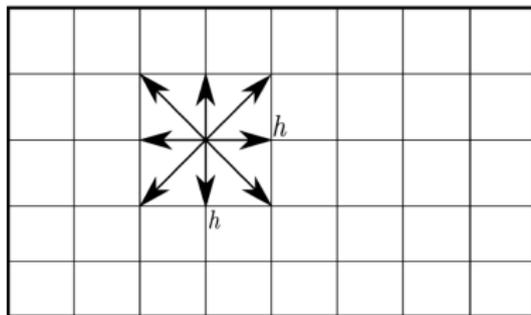
just one step away from the LBE ...

A stylized logo consisting of a square frame. The top-left corner is a light green triangle. The bottom-left and bottom-right corners are light blue triangles. The center of the square is a white area containing a large, light blue, stylized letter 'G' or a similar shape.

The Lattice Boltzmann Equation

Adjusting the spatial grid

Final step: spatial grid is chosen so that *updated populations are mapped to a new site* (instead of ending up in an arbitrary point)



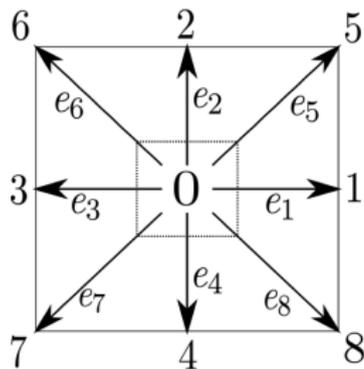
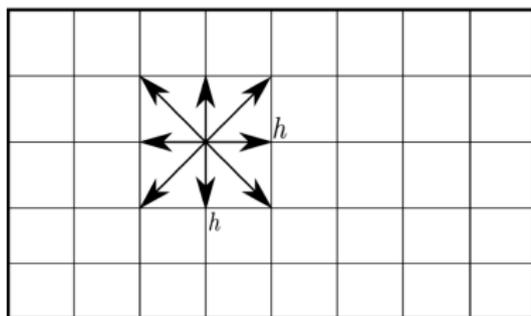
(image downloaded from Krishna Kumar's site: kks32-slides.github.io)

The grid becomes a regular lattice with parameter

$$\delta x = c \cdot \delta t = \sqrt{3RT} \cdot \delta t$$

Adjusting the spatial grid

Final step: spatial grid is chosen so that *updated populations are mapped to a new site* (instead of ending up in an arbitrary point)



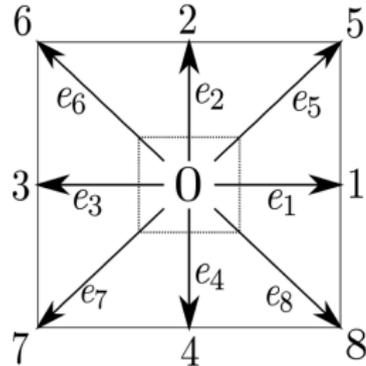
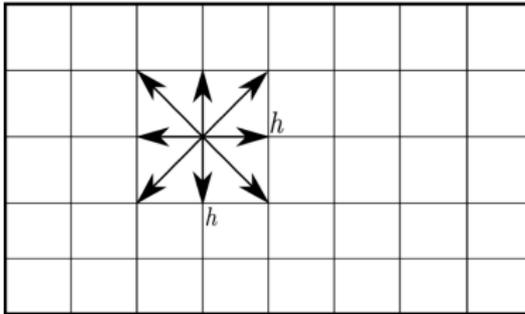
(image downloaded from Krishna Kumar's site: kks32-slides.github.io)

The grid becomes a regular lattice with parameter

$$\delta x = c \cdot \delta t = \sqrt{3RT} \cdot \delta t$$

Adjusting the spatial grid

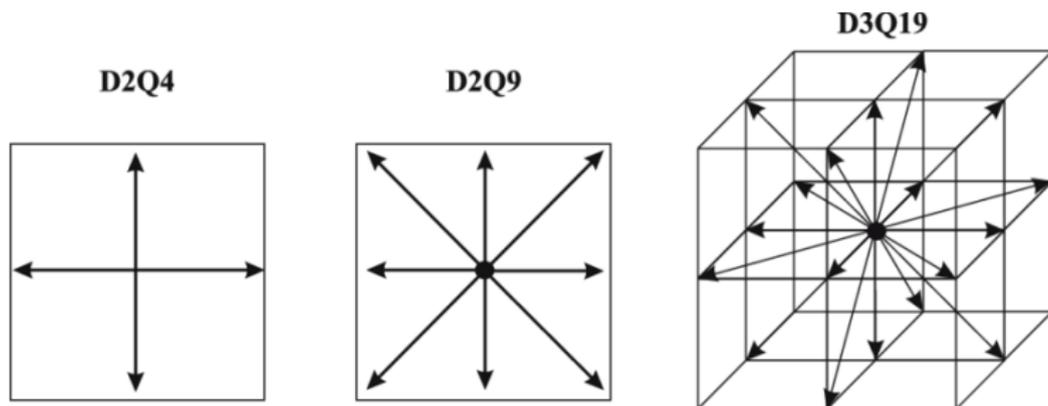
Final step: spatial grid is chosen so that *updated populations are mapped to a new site* (instead of ending up in an arbitrary point)



(image downloaded from Krishna Kumar's site: kks32-slides.github.io)

(spatial labels: \mathbf{r}_k , functions: $\psi_k = \psi(\mathbf{r}_k)$)

Other lattices



from: C. Körner *et. al.*, J. Stat. Phys, 121, 179-196 (2005)

- Not all lattices are physically acceptable
- Rotational properties of the Navier-Stokes equations must be preserved

The Lattice Boltzmann Equation

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t))$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \frac{\omega_\alpha \rho_k}{m} \left[1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u}_k)}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2}{2c^4} - \frac{3u_k^2}{2c^2} \right]$
- $\nu = \frac{1}{3} c^2 \delta t \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} c^2 \rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

The Lattice Boltzmann Equation

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t))$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \frac{\omega_\alpha \rho_k}{m} \left[1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u}_k)}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2}{2c^4} - \frac{3u_k^2}{2c^2} \right]$
- $\nu = \frac{1}{3} c^2 \delta t \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} c^2 \rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

The Lattice Boltzmann Equation

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t))$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \frac{\omega_\alpha \rho_k}{m} \left[1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u}_k)}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2}{2c^4} - \frac{3u_k^2}{2c^2} \right]$
- $\nu = \frac{1}{3} c^2 \delta t \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} c^2 \rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

The Lattice Boltzmann Equation

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t))$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \frac{\omega_\alpha \rho_k}{m} \left[1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u}_k)}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2}{2c^4} - \frac{3u_k^2}{2c^2} \right]$
- $\nu = \frac{1}{3} c^2 \delta t \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} c^2 \rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

The Lattice Boltzmann Equation

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t))$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \frac{\omega_\alpha \rho_k}{m} \left[1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u}_k)}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2}{2c^4} - \frac{3u_k^2}{2c^2} \right]$
- $\nu = \frac{1}{3} c^2 \delta t \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} c^2 \rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

The Lattice Boltzmann Equation

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} (n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t))$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3(\delta t/c^2) \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \frac{\omega_\alpha \rho_k}{m} \left[1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u}_k)}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2}{2c^4} - \frac{3u_k^2}{2c^2} \right]$
- $\nu = \frac{1}{3} c^2 \delta t \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} c^2 \rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

Lattice units

The formulas can be put in dimensionless form by employing *lattice units*:

$$\mathbf{r} = (\delta x) \bar{\mathbf{r}}, \quad t = (\delta t) \bar{t}, \quad \mathbf{u} = (\delta x / \delta t) \bar{\mathbf{u}}, \quad m = (m) \bar{m}$$

(obs: in these units: $\bar{c} = 1$ and $\bar{m} = 1$)

Other quantities:

$$n_\alpha = \bar{n}_\alpha \times (1 / \delta x^3)$$

$$\rho = \bar{\rho} \times (m / \delta x^3)$$

$$\mathbf{g} = \bar{\mathbf{g}} \times (\delta x / \delta t^2)$$

$$\nu = \bar{\nu} \times (\delta x^2 / \delta t)$$

etc.

LBE - dimensionless form

In lattice units (dimensionless form, bars omitted):

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} \left(n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t) \right)$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3 \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \omega_\alpha \rho_k \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}_k) + \frac{9}{2} (\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2 - \frac{3}{2} u_k^2 \right]$
- $\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} \rho$ (ideal gas), $c_s = 1/\sqrt{3}$
- $\rho = \sum_\alpha n_\alpha, \quad \rho \mathbf{u} = \sum_\alpha n_\alpha \mathbf{e}_\alpha + \frac{1}{2} \rho \mathbf{g}$

LBE - dimensionless form

In lattice units (dimensionless form, bars omitted):

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} \left(n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t) \right)$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3 \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \omega_\alpha \rho_k \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}_k) + \frac{9}{2} (\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2 - \frac{3}{2} u_k^2 \right]$
- $\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} \rho$ (ideal gas), $c_s = 1/\sqrt{3}$
- $\rho = \sum_\alpha n_\alpha, \quad \rho \mathbf{u} = \sum_\alpha n_\alpha \mathbf{e}_\alpha + \frac{1}{2} \rho \mathbf{g}$

LBE - dimensionless form

In lattice units (dimensionless form, bars omitted):

$$n_{\alpha}(\mathbf{r}_k + \mathbf{e}_{\alpha}, t + 1) = n_{\alpha}(\mathbf{r}_k, t) + \Omega_{\alpha}(\mathbf{r}_k, t)$$

- $\Omega_{\alpha}(\mathbf{r}_k, t) = -\frac{1}{\tau} \left(n_{\alpha}(\mathbf{r}_k, t) - g_{\alpha}(\mathbf{r}_k, t) \right)$
- $g_{\alpha}(\mathbf{r}_k, t) = n_{\alpha}^{eq}(\mathbf{r}_k, t) \left[1 + 3 \left(\tau - \frac{1}{2} \right) (\mathbf{e}_{\alpha} - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_{\alpha}^{eq}(\mathbf{r}_k, t) = \omega_{\alpha} \rho_k \left[1 + 3(\mathbf{e}_{\alpha} \cdot \mathbf{u}_k) + \frac{9}{2} (\mathbf{e}_{\alpha} \cdot \mathbf{u}_k)^2 - \frac{3}{2} u_k^2 \right]$
- $\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} \rho$ (ideal gas), $c_s = 1/\sqrt{3}$
- $\rho = \sum_{\alpha} n_{\alpha}, \quad \rho \mathbf{u} = \sum_{\alpha} n_{\alpha} \mathbf{e}_{\alpha} + \frac{1}{2} \rho \mathbf{g}$

LBE - dimensionless form

In lattice units (dimensionless form, bars omitted):

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} \left(n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t) \right)$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3 \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \omega_\alpha \rho_k \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}_k) + \frac{9}{2} (\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2 - \frac{3}{2} u_k^2 \right]$
- $\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} \rho$ (ideal gas), $c_s = 1/\sqrt{3}$
- $\rho = \sum_\alpha n_\alpha, \quad \rho \mathbf{u} = \sum_\alpha n_\alpha \mathbf{e}_\alpha + \frac{1}{2} \rho \mathbf{g}$

LBE - dimensionless form

In lattice units (dimensionless form, bars omitted):

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} \left(n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t) \right)$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3 \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \omega_\alpha \rho_k \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}_k) + \frac{9}{2} (\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2 - \frac{3}{2} u_k^2 \right]$
- $\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} \rho \text{ (ideal gas),} \quad c_s = 1/\sqrt{3}$
- $\rho = \sum_\alpha n_\alpha, \quad \rho \mathbf{u} = \sum_\alpha n_\alpha \mathbf{e}_\alpha + \frac{1}{2} \rho \mathbf{g}$

LBE - dimensionless form

In lattice units (dimensionless form, bars omitted):

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau} \left(n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t) \right)$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t) \left[1 + 3 \left(\tau - \frac{1}{2} \right) (\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k \right]$
- $n_\alpha^{eq}(\mathbf{r}_k, t) = \omega_\alpha \rho_k \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}_k) + \frac{9}{2} (\mathbf{e}_\alpha \cdot \mathbf{u}_k)^2 - \frac{3}{2} u_k^2 \right]$
- $\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right), \quad p = \frac{1}{3} \rho \text{ (ideal gas),} \quad c_s = 1/\sqrt{3}$
- $\rho = \sum_\alpha n_\alpha, \quad \rho \mathbf{u} = \sum_\alpha n_\alpha \mathbf{e}_\alpha + \frac{1}{2} \rho \mathbf{g}$

LBE - fluid modeling

Fluid properties $(\nu, c_s, \rho_0)|_T$ provide natural scales:

$$\text{time: } \nu/c_s^2, \quad \text{length: } \nu/c_s, \quad \text{mass: } \rho_0 (\nu/c_s)^3$$

The dimensionless parameter τ then sets the model's physical time and length scales:

$$\tau = \frac{3\nu}{c_s^2 \delta t} + \frac{1}{2} \Rightarrow \delta t = \frac{(\nu/c_s^2)}{\tau - \frac{1}{2}}, \quad \delta x = (\sqrt{3}c_s)\delta t$$

Conflict:

- For most fluids: $10^{-13}s < (\nu/c_s^2) < 10^{-9}s$
- In simulations we would like: $0.50 < \tau < 1.00$

LBE - fluid modeling

$[T \sim 20^\circ C]$	ν ($10^{-6} m^2/s$)	c_s (m/s)	ν/c_s^2 (s)
Air	15	343	1.275×10^{-10}
Glycerine	648	1920	1.758×10^{-10}
Castor Oil	292	1474	1.344×10^{-10}
Water	1	1482	4.550×10^{-13}

(<https://www.engineeringtoolbox.com>)

Example: $\tau = 0.51 \Rightarrow \delta t = 100 \times (\nu/c_s^2)$, $\delta x = \sqrt{3}c_s\delta t$

	δt	δx
Air	12.8 ns	7.6 μm
Glycerine	17.6 ns	58.5 μm
Castor Oil	13.4 ns	34.3 μm
Water	0.05 ns	0.1 μm

- In this introductory course we will simply choose τ so as to ensure the stability of our simulations.

LBE - fluid modeling

$[T \sim 20^\circ C]$	ν ($10^{-6} m^2/s$)	c_s (m/s)	ν/c_s^2 (s)
Air	15	343	1.275×10^{-10}
Glycerine	648	1920	1.758×10^{-10}
Castor Oil	292	1474	1.344×10^{-10}
Water	1	1482	4.550×10^{-13}

(<https://www.engineeringtoolbox.com>)

Example: $\tau = 0.51 \Rightarrow \delta t = 100 \times (\nu/c_s^2)$, $\delta x = \sqrt{3}c_s\delta t$

	δt	δx
Air	12.8 ns	7.6 μm
Glycerine	17.6 ns	58.5 μm
Castor Oil	13.4 ns	34.3 μm
Water	0.05 ns	0.1 μm

- In this introductory course we will simply choose τ so as to ensure the stability of our simulations.

LBE - fluid modeling

$[T \sim 20^\circ C]$	ν ($10^{-6} m^2/s$)	c_s (m/s)	ν/c_s^2 (s)
Air	15	343	1.275×10^{-10}
Glycerine	648	1920	1.758×10^{-10}
Castor Oil	292	1474	1.344×10^{-10}
Water	1	1482	4.550×10^{-13}

(<https://www.engineeringtoolbox.com>)

Example: $\tau = 0.51 \Rightarrow \delta t = 100 \times (\nu/c_s^2)$, $\delta x = \sqrt{3}c_s\delta t$

	δt	δx
Air	12.8 ns	7.6 μm
Glycerine	17.6 ns	58.5 μm
Castor Oil	13.4 ns	34.3 μm
Water	0.05 ns	0.1 μm

- In this introductory course we will simply choose τ so as to ensure the stability of our simulations.

The basic LB algorithm

Given an initial state $\{n_\alpha(\mathbf{r}_k, 0)\}$ time propagation is carried out by iterating two simple operations:

- **Collide:** compute collision term and update local populations (using a buffer array)

$$n_\alpha^*(\mathbf{r}_k, t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

(obs: hydrodynamic moments updated here)

- **Stream:** copy updated populations to neighboring sites

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha^*(\mathbf{r}_k, t)$$

(obs: special rules apply at boundary nodes)

The basic LB algorithm

Given an initial state $\{n_\alpha(\mathbf{r}_k, 0)\}$ time propagation is carried out by iterating two simple operations:

- **Collide:** compute collision term and update local populations (using a buffer array)

$$n_\alpha^*(\mathbf{r}_k, t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

(obs: hydrodynamic moments updated here)

- **Stream:** copy updated populations to neighboring sites

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha^*(\mathbf{r}_k, t)$$

(obs: special rules apply at boundary nodes)

The basic LB algorithm

Given an initial state $\{n_\alpha(\mathbf{r}_k, 0)\}$ time propagation is carried out by iterating two simple operations:

- **Collide:** compute collision term and update local populations (using a buffer array)

$$n_\alpha^*(\mathbf{r}_k, t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

(obs: hydrodynamic moments updated here)

- **Stream:** copy updated populations to neighboring sites

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha, t + 1) = n_\alpha^*(\mathbf{r}_k, t)$$

(obs: special rules apply at boundary nodes)

The basic LB algorithm

**shock waves in a periodic domain*

- **Collide**: compute collision term and update local populations (using a buffer array)

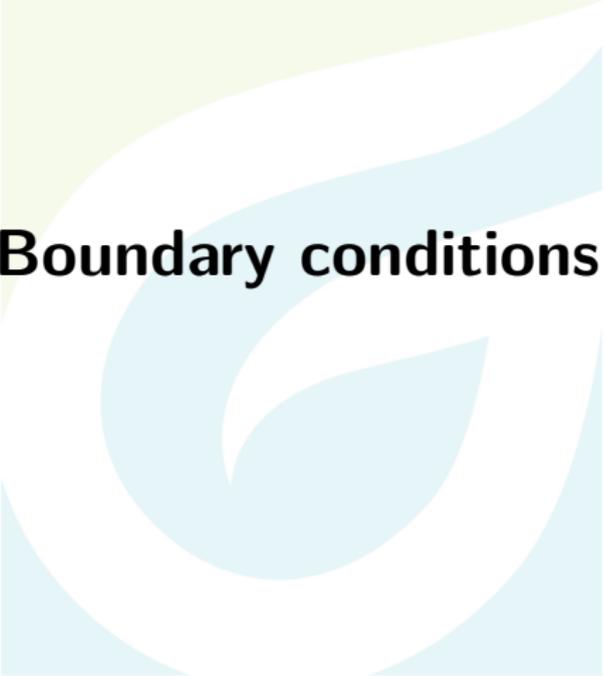
$$n_{\alpha}^*(\mathbf{r}_k, t) = n_{\alpha}(\mathbf{r}_k, t) + \Omega_{\alpha}(\mathbf{r}_k, t)$$

(obs: hydrodynamic moments updated here)

- **Stream**: copy updated populations to neighboring sites

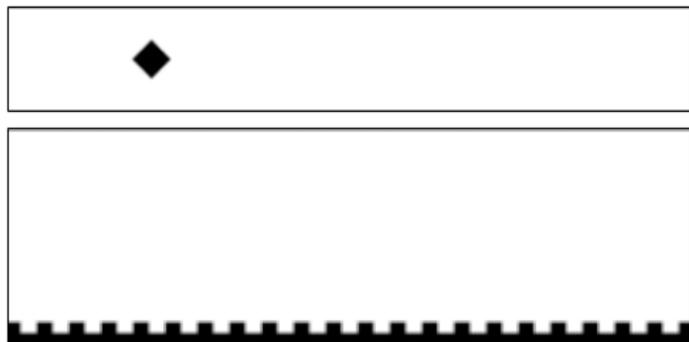
$$n_{\alpha}(\mathbf{r}_k + \mathbf{e}_{\alpha}, t + 1) = n_{\alpha}^*(\mathbf{r}_k, t)$$

(obs: special rules apply at boundary nodes)

A stylized logo consisting of a light green square in the top-left corner, a white central shape resembling a leaf or a flame, and light blue shapes in the bottom-left and bottom-right corners. The text "Boundary conditions" is centered over the white shape.

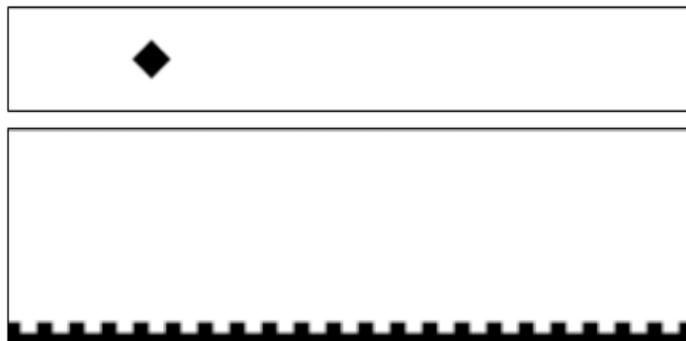
Boundary conditions

Boundary conditions in the LB method



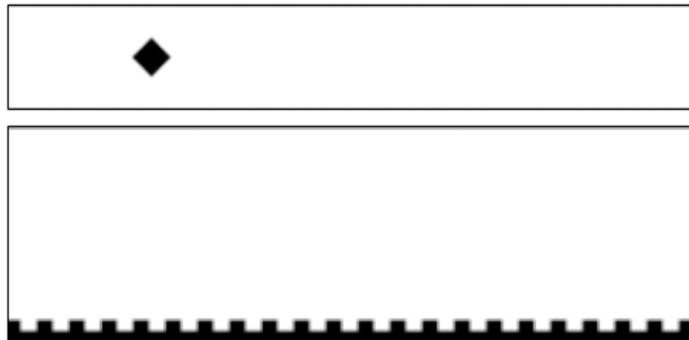
- Some populations on *boundary nodes* are left unspecified after a streaming step
- Bottom-up: a more fundamental theory could tell us how to assign the missing values
- Top-down: unknown populations are adjusted so that standard fluid-dynamics boundary conditions are obtained

Boundary conditions in the LB method



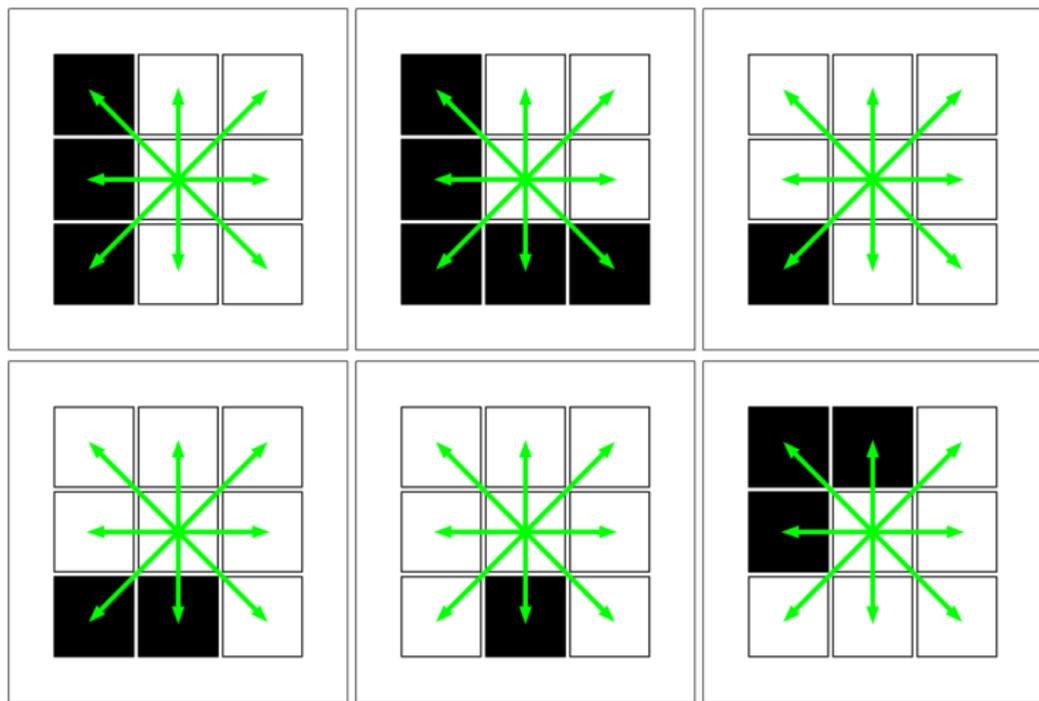
- Some populations on *boundary nodes* are left unspecified after a streaming step
- Bottom-up: a more fundamental theory could tell us how to assign the missing values
- Top-down: unknown populations are adjusted so that standard fluid-dynamics boundary conditions are obtained

Boundary conditions in the LB method



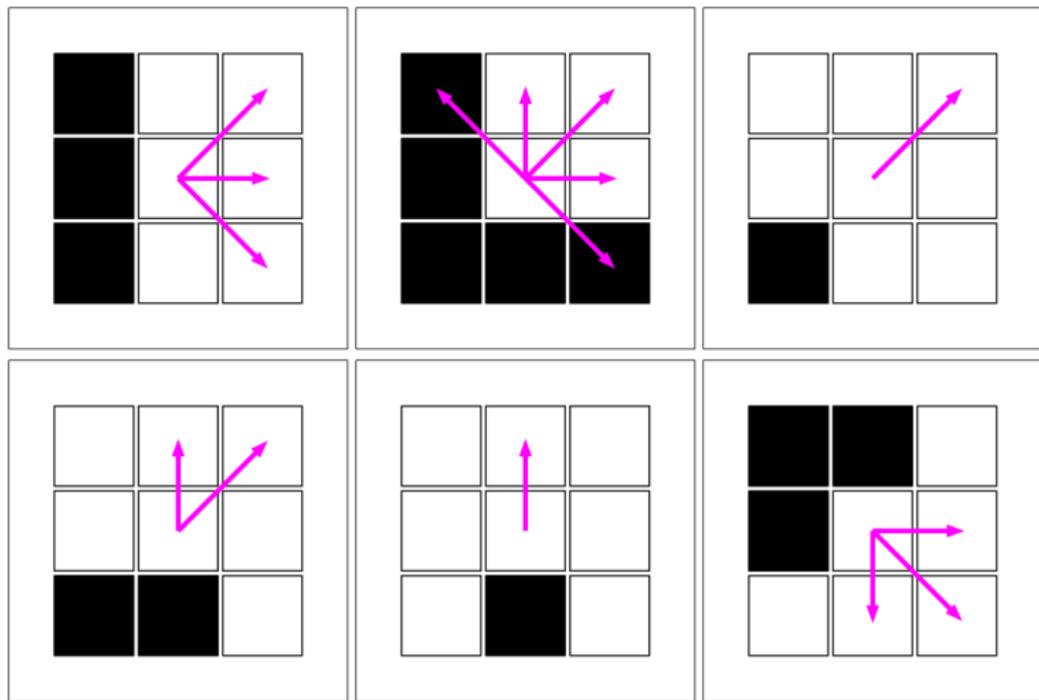
- Some populations on *boundary nodes* are left unspecified after a streaming step
- Bottom-up: a more fundamental theory could tell us how to assign the missing values
- Top-down: unknown populations are adjusted so that standard fluid-dynamics boundary conditions are obtained

Boundaries: undetermined populations



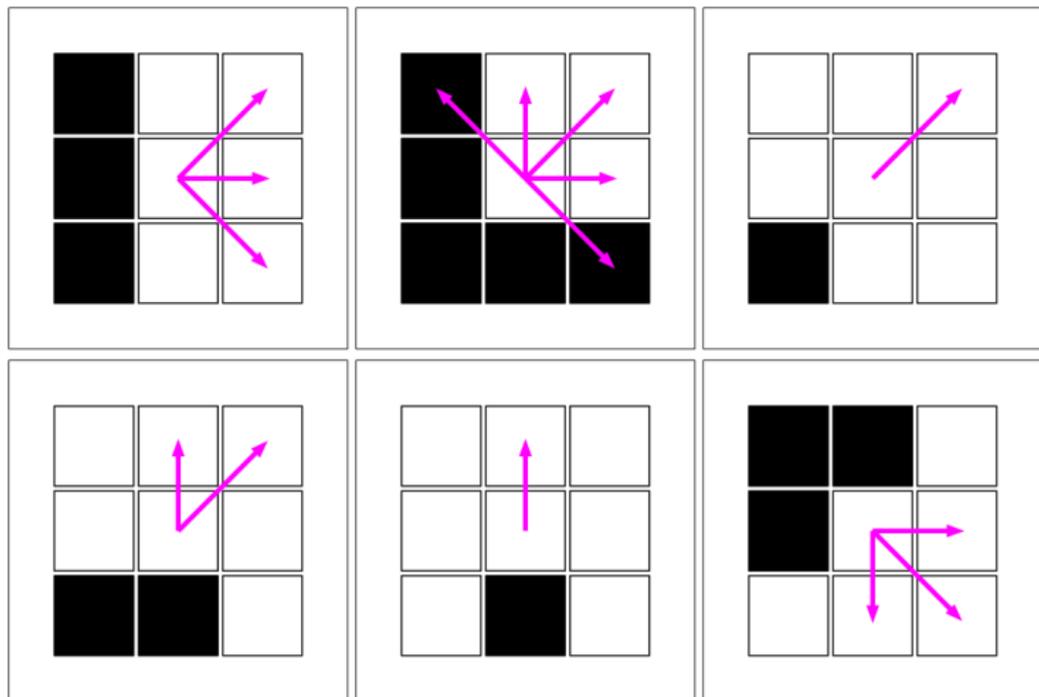
- the simplest way to specify the unknown populations is through the *bounce-back scheme*

Boundaries: undetermined populations



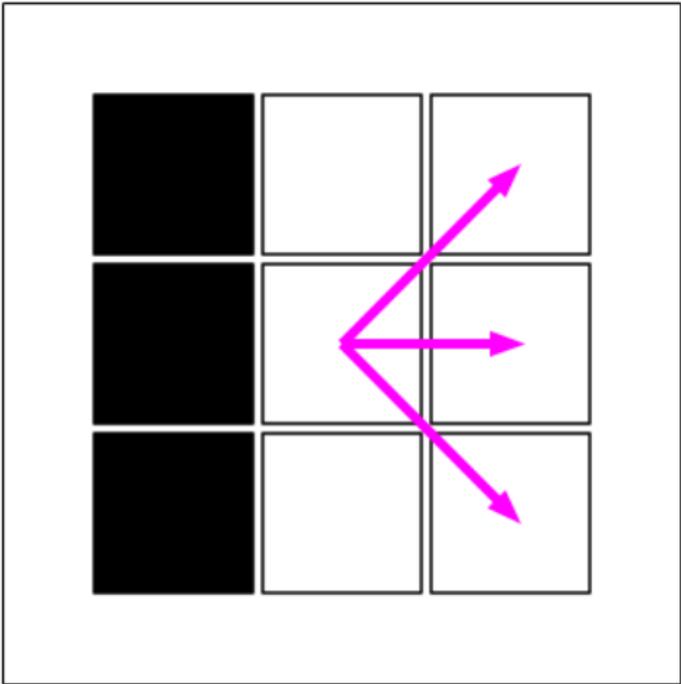
- the simplest way to specify the unknown populations is through the *bounce-back scheme*

Boundaries: undetermined populations



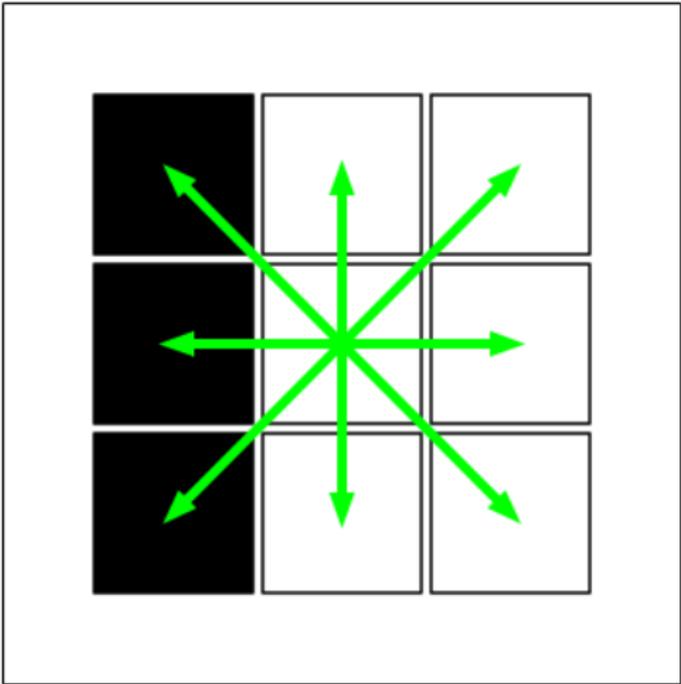
- the simplest way to specify the unknown populations is through the *bounce-back scheme*

Bounce back scheme



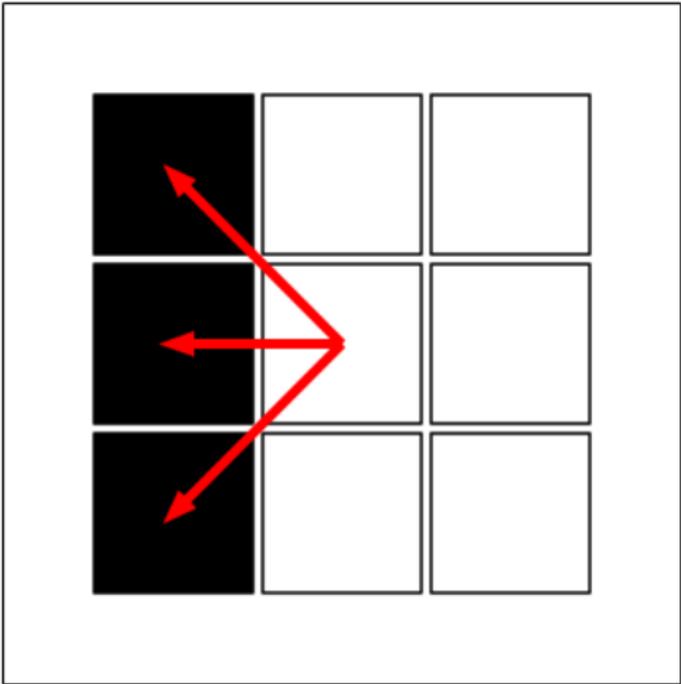
west wall/inlet: undetermined populations

Bounce back scheme



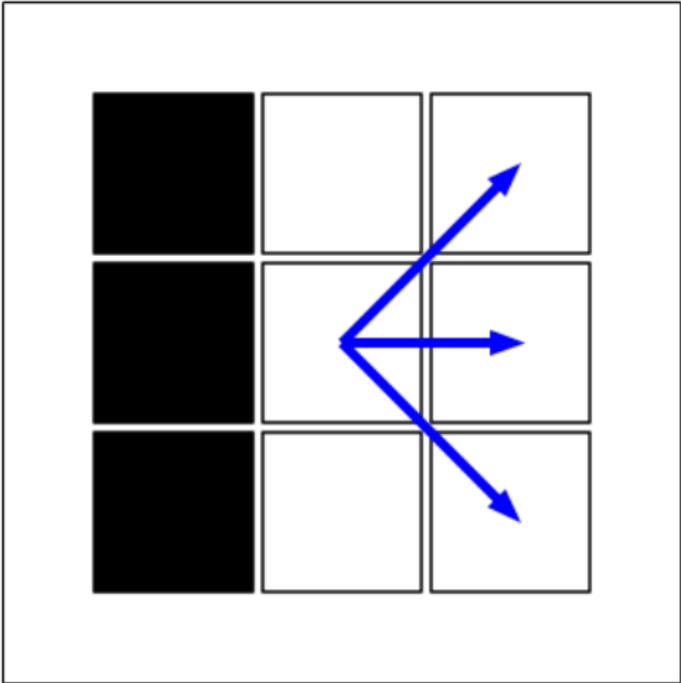
after colliding; before streaming

Bounce back scheme



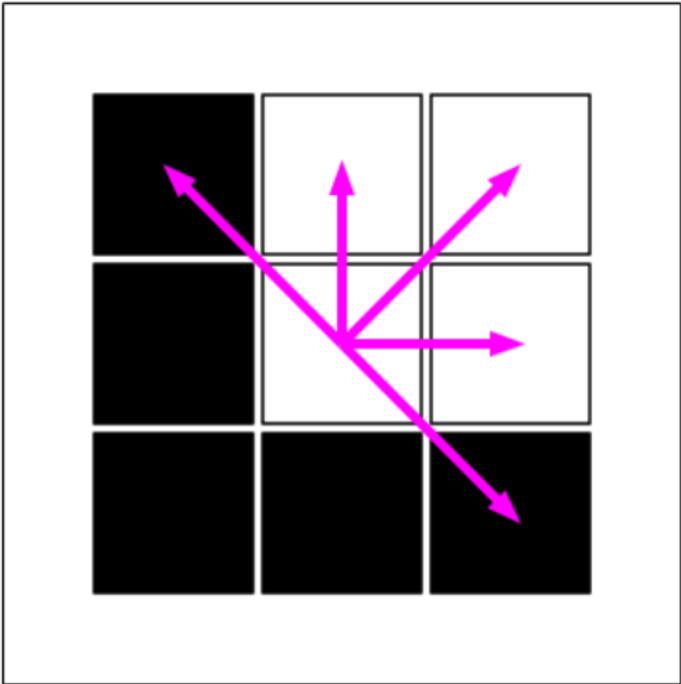
populations going into the wall...

Bounce back scheme



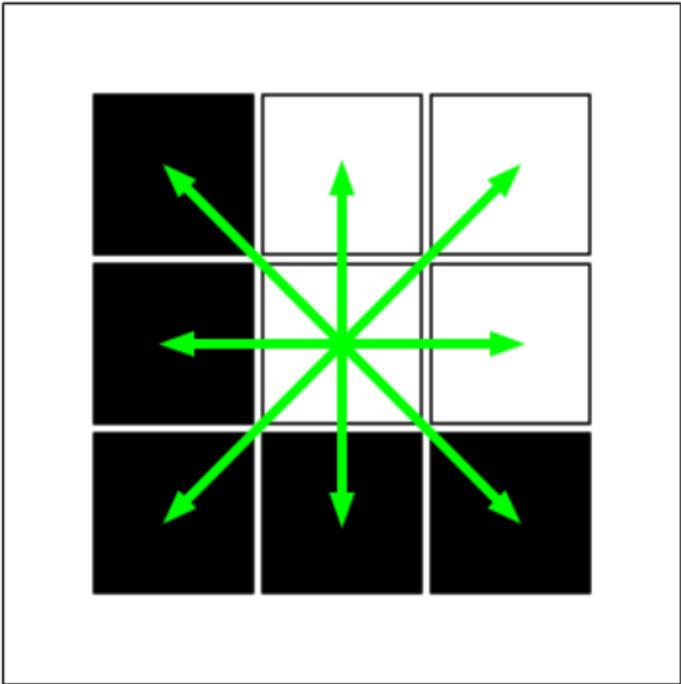
... are bounced to their opposite direction

Bounce back scheme



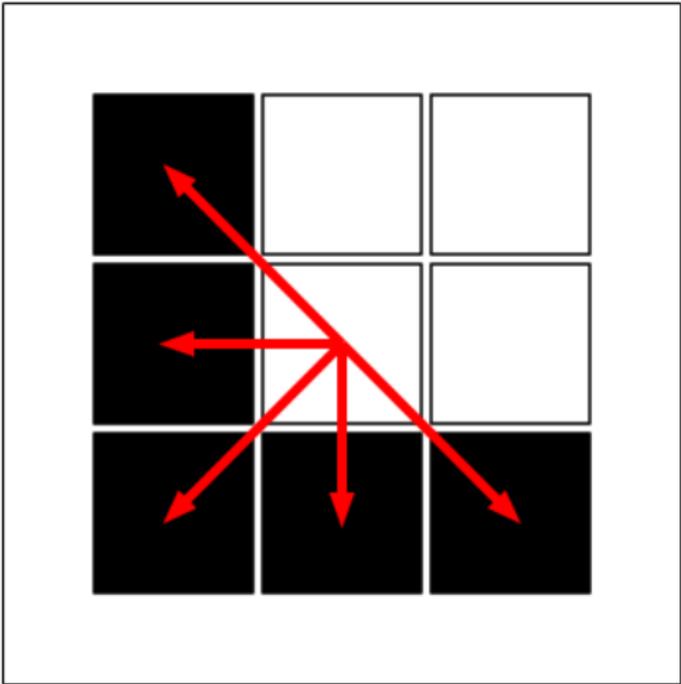
Southwest edge: undetermined populations

Bounce back scheme



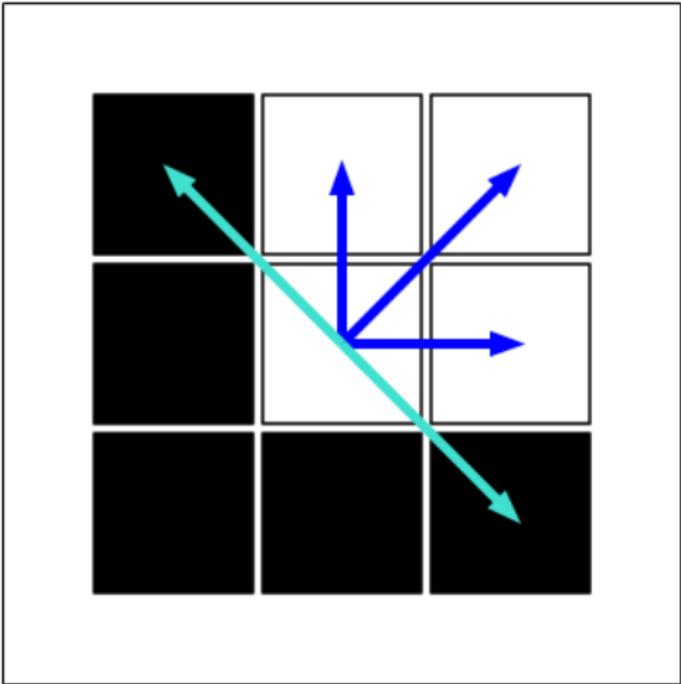
after colliding; before streaming

Bounce back scheme



populations going into the wall...

Bounce back scheme



... are bounced to their opposite direction

Bounce back scheme

Single time-step bounce back:

- Completely general
- Extremely simple to implement
- No-slip velocity condition holds on average
- No-slip boundary lies midway between solid and fluid nodes

Zou-He boundary conditions

On pressure and velocity boundary conditions for the lattice Boltzmann BGK model

Qisu Zou

*Theoretical Division, Los Alamos National Lab, Los Alamos, New Mexico 87545
and Department of Mathematics, Kansas State University, Manhattan, Kansas 66506*

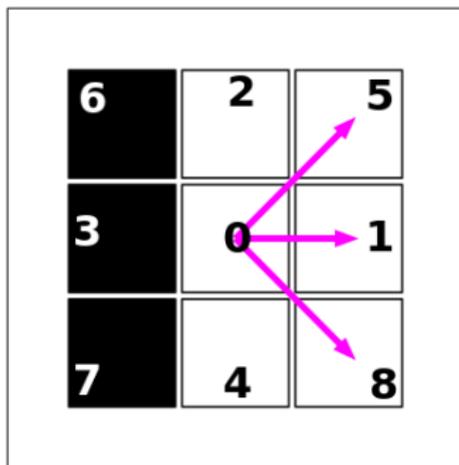
Xiaoyi He

Center for Nonlinear Studies and Theoretical Biology and Biophysics Group, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 10 August 1995; accepted 24 February 1997)

- Fix inlet/outlet pressure (density)
- Fix inlet/outlet velocity
- Fix wall velocity

Zou-He: fix inlet density (bulk)



4 unknowns:

$$(u_x, n_1, n_5, n_8)$$

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3$$

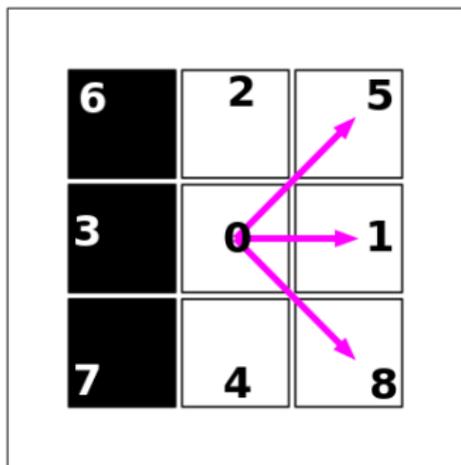
$$n_1 + n_5 + n_8 = n_0 + n_2 + n_3 + n_4 + n_6 + n_7 - \rho$$

$$n_1 + n_5 + n_8 - \rho u_x = n_3 + n_6 + n_7$$

$$n_5 - n_8 = n_4 - n_2 + n_7 - n_6$$

$$n_1 - n_1^{eq} = n_3 - n_3^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix inlet density (bulk)



4 unknowns:

$$(u_x, n_1, n_5, n_8)$$

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3$$

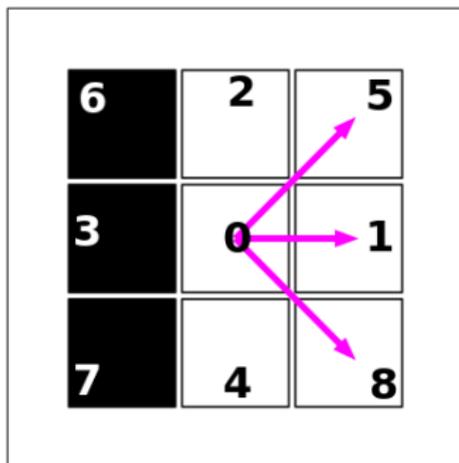
$$n_1 + n_5 + n_8 = n_0 + n_2 + n_3 + n_4 + n_6 + n_7 - \rho$$

$$n_1 + n_5 + n_8 - \rho u_x = n_3 + n_6 + n_7$$

$$n_5 - n_8 = n_4 - n_2 + n_7 - n_6$$

$$n_1 - n_1^{eq} = n_3 - n_3^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix inlet density (bulk)



4 unknowns:

$$(u_x, n_1, n_5, n_8) \checkmark$$

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3$$

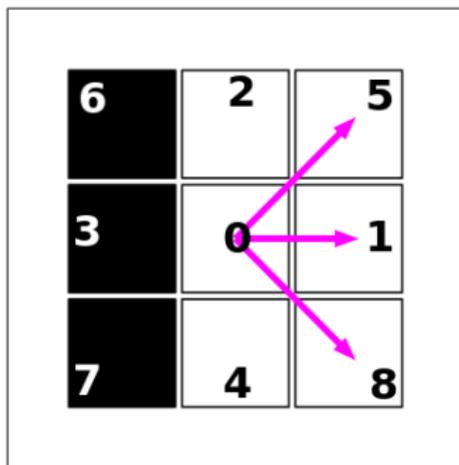
$$n_1 + n_5 + n_8 = n_0 + n_2 + n_3 + n_4 + n_6 + n_7 - \rho$$

$$n_1 + n_5 + n_8 - \rho u_x = n_3 + n_6 + n_7$$

$$n_5 - n_8 = n_4 - n_2 + n_7 - n_6$$

$$n_1 - n_1^{eq} = n_3 - n_3^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix inlet density (bulk)



4 unknowns:

(u_x, n_1, n_5, n_8) ✓

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3$$

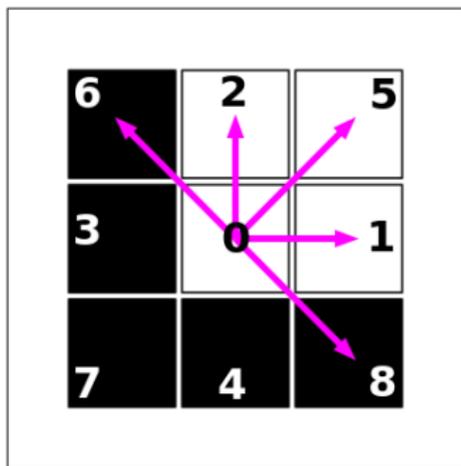
$$u_x = 1 - [n_0 + n_2 + n_4 + 2(n_3 + n_6 + n_7)]/\rho$$

$$n_1 = n_3 + \frac{2}{3}\rho u_x$$

$$n_5 = n_7 - \frac{1}{2}(n_2 - n_4) + \frac{1}{6}\rho u_x$$

$$n_6 = n_8 + \frac{1}{2}(n_2 - n_4) + \frac{1}{6}\rho u_x$$

Zou-He: fix inlet density (edge)



5 unknowns:

$(n_1, n_2, n_5, n_6, n_8)$

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3, \quad \delta n_2 = \delta n_4$$

$$n_1 + n_2 + n_5 + n_6 + n_8 = n_3 + n_4 + n_7 + n_8 - \rho$$

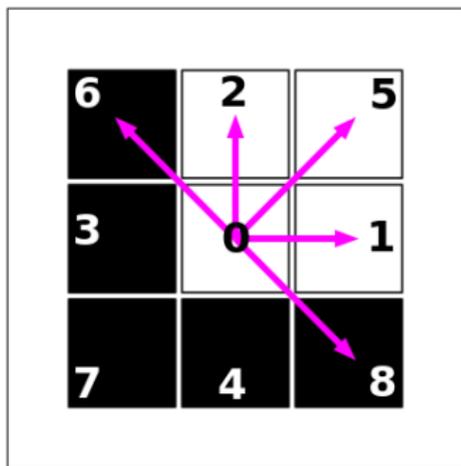
$$n_1 + n_5 - n_6 + n_8 = n_3 + n_7$$

$$n_2 + n_5 + n_6 - n_8 = n_4 + n_7$$

$$n_1 - n_1^{eq} = n_3 - n_3^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

$$n_2 - n_2^{eq} = n_4 - n_4^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix inlet density (edge)



5 unknowns:

$$(n_1, n_2, n_5, n_6, n_8)$$

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3, \quad \delta n_2 = \delta n_4$$

$$n_1 + n_2 + n_5 + n_6 + n_8 = n_3 + n_4 + n_7 + n_8 - \rho$$

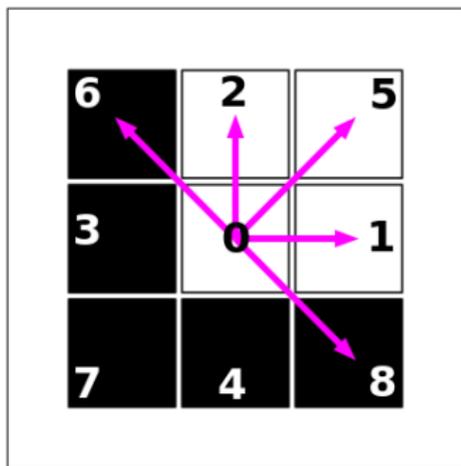
$$n_1 + n_5 - n_6 + n_8 = n_3 + n_7$$

$$n_2 + n_5 + n_6 - n_8 = n_4 + n_7$$

$$n_1 - n_1^{eq} = n_3 - n_3^{eq} \quad \leftarrow \text{non-equilibrium bounce-back}$$

$$n_2 - n_2^{eq} = n_4 - n_4^{eq} \quad \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix inlet density (edge)



5 unknowns:

$(n_1, n_2, n_5, n_6, n_8)$ ✓

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3, \quad \delta n_2 = \delta n_4$$

$$n_1 + n_2 + n_5 + n_6 + n_8 = n_3 + n_4 + n_7 + n_8 - \rho$$

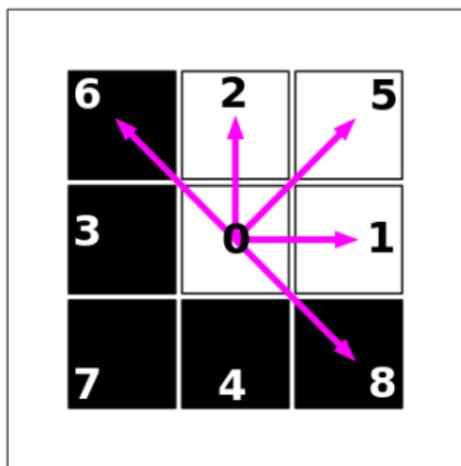
$$n_1 + n_5 - n_6 + n_8 = n_3 + n_7$$

$$n_2 + n_5 + n_6 - n_8 = n_4 + n_7$$

$$n_1 - n_1^{eq} = n_3 - n_3^{eq} \quad \leftarrow \text{non-equilibrium bounce-back}$$

$$n_2 - n_2^{eq} = n_4 - n_4^{eq} \quad \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix inlet density (edge)



5 unknowns:

$(n_1, n_2, n_5, n_6, n_8)$ ✓

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$0 = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_1 = \delta n_3, \quad \delta n_2 = \delta n_4$$

$$n_1 = n_3$$

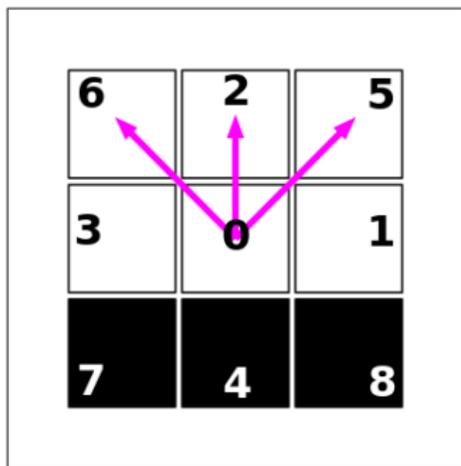
$$n_2 = n_4$$

$$n_5 = n_7$$

$$n_6 = \frac{1}{2}[\rho - n_0 - 2(n_3 + n_4 + n_7)]$$

$$n_8 = \frac{1}{2}[\rho - n_0 - 2(n_3 + n_4 + n_7)]$$

Zou-He: fix velocity (wall)



4 unknowns: (ρ, n_2, n_5, n_6)
3 equations

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$\rho u_y = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_2 = \delta n_4$$

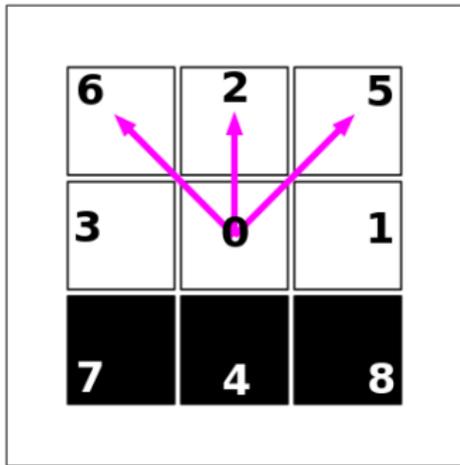
$$\rho + n_2 + n_5 + n_6 = n_0 + n_1 + n_3 + n_4 + n_7 + n_8$$

$$n_2 + n_5 + n_6 - \rho u_y = n_4 + n_7 + n_8$$

$$n_5 - n_6 - \rho u_x = n_3 - n_1 + n_7 - n_8$$

$$n_2 - n_2^{eq} = n_4 - n_4^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix velocity (wall)



4 unknowns: (ρ, n_2, n_5, n_6)
3 equations

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$\rho u_y = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_2 = \delta n_4$$

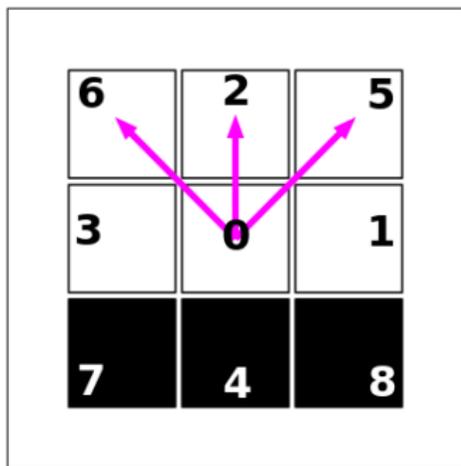
$$\rho + n_2 + n_5 + n_6 = n_0 + n_1 + n_3 + n_4 + n_7 + n_8$$

$$n_2 + n_5 + n_6 - \rho u_y = n_4 + n_7 + n_8$$

$$n_5 - n_6 - \rho u_x = n_3 - n_1 + n_7 - n_8$$

$$n_2 - n_2^{eq} = n_4 - n_4^{eq} \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix velocity (wall)



4 unknowns: (ρ, n_2, n_5, n_6)

4 equations ✓

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$\rho u_y = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_2 = \delta n_4$$

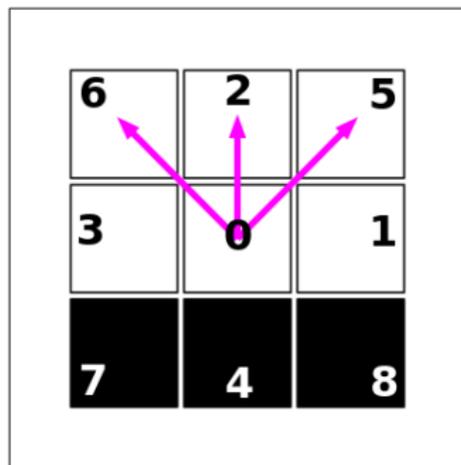
$$\rho + n_2 + n_5 + n_6 = n_0 + n_1 + n_3 + n_4 + n_7 + n_8$$

$$n_2 + n_5 + n_6 - \rho u_y = n_4 + n_7 + n_8$$

$$n_5 - n_6 - \rho u_x = n_3 - n_1 + n_7 - n_8$$

$$n_2 - n_2^{eq} = n_4 - n_4^{eq} \quad \leftarrow \text{non-equilibrium bounce-back}$$

Zou-He: fix velocity (wall)



4 unknowns: (ρ, n_2, n_5, n_6)

4 equations ✓

$$\rho = \sum_{\alpha} n_{\alpha}$$

$$\rho u_x = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_x$$

$$\rho u_y = \sum_{\alpha} n_{\alpha} (\mathbf{e}_{\alpha})_y$$

$$\delta n_2 = \delta n_4$$

$$n_2 = n_4 + \frac{2}{3} \rho u_y$$

$$n_5 = n_7 - \frac{1}{2} (n_1 - n_3) + \frac{1}{2} \rho u_x + \frac{1}{6} \rho u_y$$

$$n_6 = n_8 + \frac{1}{2} (n_1 - n_3) - \frac{1}{2} \rho u_x + \frac{1}{6} \rho u_y$$

$$\rho = [n_0 + n_1 + n_3 + 2(n_4 + n_7 + n_8)] / (1 - u_y)$$

The complete LB algorithm (1 timestep)

- Fix boundary conditions: stream-unspecified populations are set to their target values
- Collide:

$$n_{\alpha}^*(\mathbf{r}_k, t) = n_{\alpha}(\mathbf{r}_k, t) + \Omega_{\alpha}(\mathbf{r}_k, t)$$

(hydrodynamic moments updated, *forces computed*)

- Stream and bounce-back:

$$\begin{aligned} n_{\alpha}(\mathbf{r}_k + \mathbf{e}_{\alpha}, t + 1) &= n_{\alpha}^*(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is fluid} \\ n_{\alpha''}(\mathbf{r}_k + \mathbf{e}_{\alpha}'', t + 1) &= n_{\alpha}^*(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is solid} \end{aligned}$$

(no conflict with boundary conditions)

The complete LB algorithm (1 timestep)

- **Fix boundary conditions:** stream-unspecified populations are set to their target values
- **Collide:**

$$n_{\alpha}^*(\mathbf{r}_k, t) = n_{\alpha}(\mathbf{r}_k, t) + \Omega_{\alpha}(\mathbf{r}_k, t)$$

(hydrodynamic moments updated, *forces computed*)

- **Stream and bounce-back:**

$$\begin{aligned} n_{\alpha}(\mathbf{r}_k + \mathbf{e}_{\alpha}, t + 1) &= n_{\alpha}^*(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is fluid} \\ n_{\alpha''}(\mathbf{r}_k + \mathbf{e}_{\alpha}'', t + 1) &= n_{\alpha}^*(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is solid} \end{aligned}$$

(no conflict with boundary conditions)

The complete LB algorithm (1 timestep)

- **Fix boundary conditions:** stream-unspecified populations are set to their target values
- **Collide:**

$$n_{\alpha}^*(\mathbf{r}_k, t) = n_{\alpha}(\mathbf{r}_k, t) + \Omega_{\alpha}(\mathbf{r}_k, t)$$

(hydrodynamic moments updated, *forces computed*)

- **Stream and bounce-back:**

$$\begin{aligned} n_{\alpha}(\mathbf{r}_k + \mathbf{e}_{\alpha}, t + 1) &= n_{\alpha}^*(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is fluid} \\ n_{\alpha''}(\mathbf{r}_k + \mathbf{e}_{\alpha}'', t + 1) &= n_{\alpha}^*(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is solid} \end{aligned}$$

(no conflict with boundary conditions)

The complete LB algorithm (1 timestep)

- **Fix boundary conditions:** stream-unspecified populations are set to their target values
- **Collide:**

$$n_{\alpha}^{*}(\mathbf{r}_k, t) = n_{\alpha}(\mathbf{r}_k, t) + \Omega_{\alpha}(\mathbf{r}_k, t)$$

(hydrodynamic moments updated, *forces computed*)

- **Stream and bounce-back:**

$$\begin{aligned} n_{\alpha}(\mathbf{r}_k + \mathbf{e}_{\alpha}, t + 1) &= n_{\alpha}^{*}(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is fluid} \\ n_{\alpha''}(\mathbf{r}_k + \mathbf{e}_{\alpha}'', t + 1) &= n_{\alpha}^{*}(\mathbf{r}_k, t) && \text{if } \mathbf{r}_k + \mathbf{e}_{\alpha} \text{ is solid} \end{aligned}$$

(no conflict with boundary conditions)

A stylized logo consisting of overlapping shapes in light green, white, and light blue. The green shape is at the top left, the white shape is in the center, and the blue shape is at the bottom right. The text "Hands-on tutorial" is centered over the white shape.

Hands-on tutorial

Hands on

LB-lab-0:

program usage

LB-lab-1:

profiling a channel flow

LB-lab-2:

visualizing flow past obstacles

References – Part 2



X. He; L-S. Lou

Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation. *Phys. Rev. E*, 56(6), 6811-6817 (1997)



Q. Zou; X. He

On pressure and velocity boundary conditions for the lattice Boltzmann BGK model. *Phys. Fluids*. 9 (6), 1591-1598 (1998)



X. Shan; X. He

Discretization of the Velocity Space in the Solution of the Boltzmann Equation. *Phys. Rev. Lett.*, 80(1), 6811-6817 (1998)



L-S. Lou

Unified Theory of Lattice Boltzmann Models for Nonideal Gases. *Phys. Rev. Lett.*, 81(8), 1618-1621 (1998)



P. J. Dellar

Bulk and shear viscosities in lattice Boltzmann equations. *Phys. Rev. E.*, 64, 031203 (2001)

References – Part 2



X. Shan; H. Chen

Simulation of nonideal gases and liquid-gas phase transitions by the lattice Boltzmann equation. *Phys. Rev. E.*, 49(4), 2941-2948 (1994)



S. Nekoeian; A. S. Goharrizi; M. Jamialahmadi; S. Jafari; F. Sotoudeh

A novel Shan and Chen type Lattice Boltzmann two phase method to study the capillary pressure curves of an oil water pair in a porous media. *Petroleum*, 4, 347-357 (2018)



S. Chen; G. D. Doolen

Lattice Boltzmann Method for Fluid Flow. *Annu. Rev. Fluid Mech.*, 30 (1998)



X. He; G. D. Doolen

Thermodynamic Foundations of Kinetic Theory and Lattice Boltzmann Models for Multiphase Flows. *Journal of Statistical Physics*, 107(1-2), 309-328 (2002)



J. Zhang

Lattice Boltzmann method for microfluidics: models and applications. *Microfluid Nanofluid* 10:1–28 (2011)

References – Part 2



S. Succi

The Lattice Boltzmann Equation for Fluid Dynamics and Beyond



Q. Chang; J. Iwan; D. Alexander

Application of Lattice Boltzmann Method: Thermal Multiphase Fluid Dynamics



J. G. Zhou

Lattice Boltzmann Methods for Shallow Water Flows