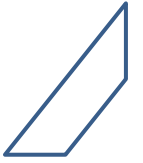


# 参考: Lattice Boltzmann Method

IPCST  
Seoul National University



# Modeling Scales



- Microscopic
  - Small particles or individuals.
- Macroscopic
  - Averaged quantities of groups (ex.: particle group). Approximation to continuum.
- **Mesosopic**
  - Large particles or small clusters. Ensembles. Kinetic type. Often stochastic.
- Multi-scale: Combination of different scales



# Kinetic Theory



- Object of interest
  - Particle distribution function (PDF)
    - Phase space probability density
- BBGKY hierarchy
  - Bogoliubov, Born, Green, Kirkwood, and Yvon
  - A set of equations for many particles
    - Each equation describes  $k$ -particle probability density function ( $k = 1, 2, \dots, N$ )
  - Boltzmann equation
    - Truncation at the first or the second equation



# Boltzmann Equation



- Boltzmann equation
  - Considering 1-particle probability density function  $f(\mathbf{x}, \mathbf{v}, t)$

$$\partial_t f = (\partial_t f)_{\text{ext. force}} + (\partial_t f)_{\text{diffusion}} + (\partial_t f)_{\text{collision}}$$

$$\partial_t f + (\mathbf{v} \cdot \nabla) f + \mathbf{F} \cdot \partial f / \partial \mathbf{p} = \Omega(f, f)$$

- $\mathbf{F}$ : external force field
- $\Omega(f, f)$ : collision effect term

$$\Omega(f, f) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \sigma(\omega) |\mathbf{w} - \mathbf{v}| (f(\mathbf{v}') f(\mathbf{w}') - f(\mathbf{v}) f(\mathbf{w})) d\omega d\mathbf{w}$$



# Boltzmann Equation



- Boltzmann equation
  - $\Omega(f, f)$ : collision effect term (also called collision operator)

$$\Omega(f, f) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \sigma(\omega) |\mathbf{w} - \mathbf{v}| (f(\mathbf{v}')f(\mathbf{w}') - f(\mathbf{v})f(\mathbf{w})) d\omega d\mathbf{w}$$

- Collision of particles with velocity  $\mathbf{v}$  and particles with velocity  $\mathbf{w}$
- $\sigma(\omega)$ : scattering cross section
- $\omega$  : scattering angle



# Boltzmann Equation



- Detailed balance
  - At equilibrium, (net gain) = (net loss)
    - $\Omega(f, f) = 0$
  - ◆  $f_0(\mathbf{v}') f_0(\mathbf{w}') = f_0(\mathbf{v}) f_0(\mathbf{w})$  for gas model (no  $\mathbf{F}$  case)
    - $f_0(\mathbf{v})$ : a one-particle probability density function at equilibrium
- Maxwell-Boltzmann distribution
$$f_0(\mathbf{v}) = n (m\beta/2\pi)^{3/2} \exp(-m\beta|\mathbf{v}-\mathbf{v}^0|^2/2) \text{ where } \beta = 1/(k_B T)$$
  - $n = 1$  after normalization  $k_B$ : Boltzmann constant
  - The equilibrium state for Boltzmann equation without external forces
    - Accurate for rarefied gases

# Boltzmann Equation

- Conservation laws

- Average value of  $A$ :  $\langle A \rangle = \int A f d\mathbf{v} / \int f d\mathbf{v}$

- Mass conservation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (\rho = mn, n = \int f d\mathbf{v}, \mathbf{u} = \langle \mathbf{v} \rangle)$$

- Momentum conservation

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \cdot \boldsymbol{\tau} = n \mathbf{F} \quad \left( \boldsymbol{\tau} = \frac{1}{m} \int \mathbf{v}' \otimes \mathbf{v}' f d\mathbf{v}' \right)$$

- $\boldsymbol{\tau}$ : stress by fluctuation

$$\mathbf{v} \otimes \mathbf{w} = \begin{bmatrix} v_1 w_1 & v_1 w_2 & \cdots & v_1 w_m \\ v_2 w_1 & v_2 w_2 & \cdots & v_2 w_m \\ \vdots & \vdots & \ddots & \vdots \\ v_n w_1 & v_n w_2 & \cdots & v_n w_m \end{bmatrix}$$

# Boltzmann Equation

- Conservation laws

- Average value of  $A$ :  $\langle A \rangle = \int A f d\mathbf{v} / \int f d\mathbf{v}$

- Mass conservation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (\rho = mn, n = \int f d\mathbf{v}, \mathbf{u} = \langle \mathbf{v} \rangle)$$

- Momentum conservation

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \cdot \boldsymbol{\tau} = n \mathbf{F} \quad (\boldsymbol{\tau} = \frac{1}{m} \int \mathbf{v}' \otimes \mathbf{v}' f d\mathbf{v}')$$

- $\boldsymbol{\tau}$ : stress by fluctuation

- Energy conservation

$$\partial_t E + \nabla \cdot (E \mathbf{u} + \boldsymbol{\tau} \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} = n \mathbf{F} \cdot \mathbf{u} \quad (\mathbf{q} = \frac{1}{m} \int \frac{|\mathbf{v}'|^2}{2} \mathbf{v}' f d\mathbf{v}')$$

- $E = \rho |\mathbf{u}|^2 / 2 + (\text{thermal } E)$ ,  $\mathbf{q}$ : heat flux





# Boltzmann Equation



- Knudsen number (Kn)

$$\text{Kn} = \lambda/L$$

- $\lambda$  : mean free path (typical order:  $\mu\text{m}$  or  $\text{nm}$ )
  - $L$  : system size (typical order: meter)
- Dimensionless Boltzmann equation

$$\partial_t f + (\mathbf{v} \cdot \nabla) f + \mathbf{F} \cdot \partial f / \partial \mathbf{p} = \Omega(f, f) / \text{Kn}$$

- Local equilibrium approximation

- Assuming  $\mathbf{F} = 0$ ,

*If*  $\text{Kn} \ll 1 \rightarrow \Omega(f, f) = 0 \rightarrow \text{M.-B. Distribution}$



# BGK Approximation



– Bhatnagar, Gross, and Krook

- In most cases, the collision effect results a distribution not far from the equilibrium distribution.

$$\partial_t f + (\mathbf{v} \cdot \nabla) f + \mathbf{F} \cdot \partial f / \partial \mathbf{p} = (f_0 - f) / \tau$$

–  $\tau$ : relaxation time

- Elementary time of collisions
- Related to transport coefficient or diffusion coefficient



# Lattice Boltzmann Method



- Computational fluid dynamics method
- Discrete-velocity version of approximated Boltzmann equation
  - When we ignore the external force term,

$$\partial_t f_i + (\mathbf{v}_i \cdot \nabla) f_i = \Omega(f_i, f_i) \quad (i: \text{velocity index})$$

$$\rightarrow f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Delta t \cdot \Omega[f_i(\mathbf{x}, t), f_i(\mathbf{x}, t)]$$

- Propagation and collision of fictitious particles (quasiparticles)
  - Mesoscopic viewpoint



# Advantages of LBM



- Easy to include a particular molecular interaction
- Easy to be parallelized.
  - Massive-parallelism such as GPUs and supercomputers
- Suitable to mass-conserving flows in porous media
- Moving boundaries can be implemented.
- Multiphase and multicomponent methods are available.
- Various couplings between different flows are available.
  - Wave with sound, heat-transfer or chemical reactions
- Thermal fluctuations can be applied.
- Appropriate for simulating mesoscopic physics



# Disadvantages of LBM



- Memory-intensive
- Time-dependent, even for steady flows
- Spurious currents near fluid-fluid interfaces, as in other lattice-based methods
- The range of viscosities and densities are limited in multiphase and multicomponent simulations
- Energy-conserving thermal simulations are not straightforward
- Inappropriate for long-range propagation of sound at real viscosity
- Inappropriate for strongly compressible flows



# Lattice Boltzmann Models



- Lattice Boltzmann equation

$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Delta t \cdot \Omega[f_i(\mathbf{x}, t), f_i(\mathbf{x}, t)]$$

- Discretization: time & velocity

- The BGK approximation is usually used in LBM.

$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + [f_{0,i}(\mathbf{x}, t) - f_i(\mathbf{x}, t)] \cdot \Delta t / \tau$$

- ❖ Naturally,  $(\mathbf{v} \text{ lattice unit}) = (\mathbf{x} \text{ lattice unit}) / \Delta t$
- ❖ Velocity lattice notation:  $DdQq$ 
  - $d$ : dimension,  $q$ : number of linkages

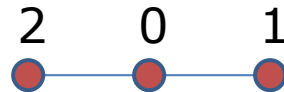
# 1-D Lattice Arrangements

- D1Q2



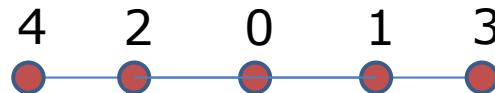
- Weighting factors:  $w_1=1/2$ ,  $w_2=1/2$ .

- D1Q3



- Weighting factors:  $w_0=2/3$ ,  $w_1=1/6$ ,  $w_2=1/6$ .

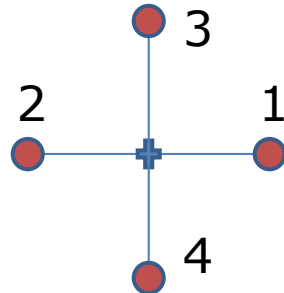
- D1Q5



- Weighting factors:  $w_0=1/2$ ,  $w_1=1/6$ ,  $w_2=1/6$ ,  $w_3=1/12$ ,  $w_4=1/12$ .

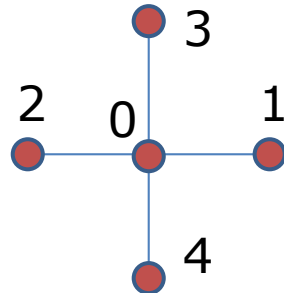
# 2-D Lattice Arrangements

- D2Q4



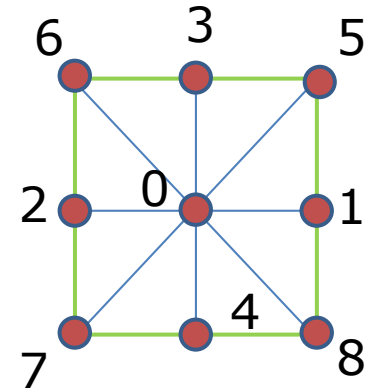
- Weighting factors:  
 $w_i = 1/4$

- D2Q5



- Weighting factors:  
 $w_0 = 1/3$ ,  $w_1 = 1/6$ ,  
 $w_2 = 1/6$ ,  $w_3 = 1/6$ ,  
 $w_4 = 1/6$ .

- D2Q9



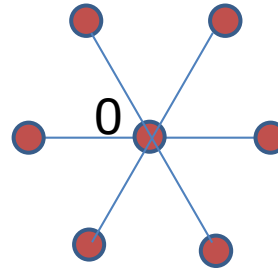
- Weighting factors:  
 $w_0 = 4/9$ ,  $w_1 = 1/9$ ,  
 $w_2 = 1/9$ ,  $w_3 = 1/9$ ,  
 $w_4 = 1/9$ ,  $w_5 = 1/36$ ,  
 $w_6 = 1/36$ ,  $w_7 = 1/36$ ,  
 $w_8 = 1/36$



# 2-D Lattice Arrangements

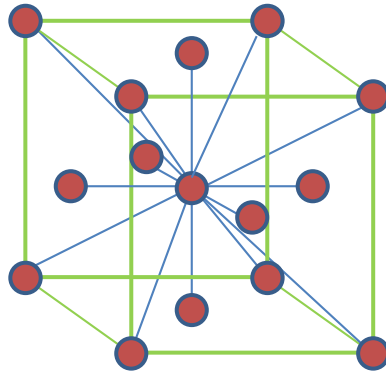
- D2Q7
  - Hexagonal grid
  - Weighting factors:  $w_0 = 1/2$ ,  $w_1 = 1/12$ , ..... ,  $w_6 = 1/12$ ,

$$c_s = \Delta x / (2\Delta t)$$



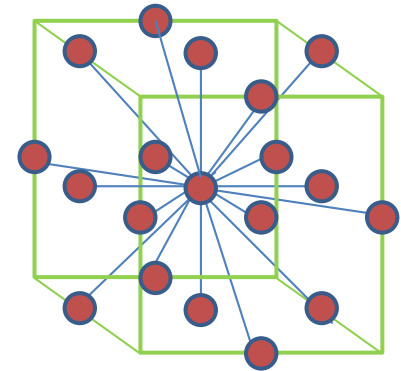
# 3-D Lattice Arrangements

- D3Q15



- Weighting factors:  
 $w_0 = 2/9$ ,  $w_1 = 1/9$ ,  
.....,  $w_6 = 1/9$ ,  
 $w_7 = 1/72$ , ..... ,  
 $w_{14} = 1/72$ .

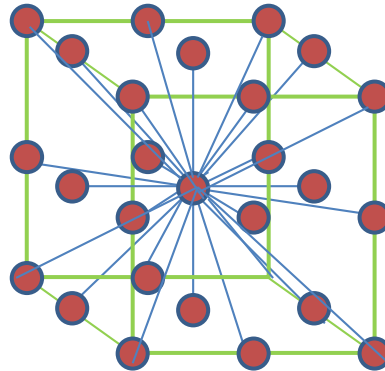
- D3Q19



- Weighting factors:  
 $w_0 = 1/3$ ,  $w_1 = 1/18$ ,  
.....,  $w_6 = 1/18$ ,  
 $w_7 = 1/36$ , ..... ,  
 $w_{18} = 1/36$ .

# 3-D Lattice Arrangements

- D3Q27
  - Weighting factors:  $w_0 = 8/27$ ,  $w_1 = 2/27$ , ..... ,  
 $w_6 = 2/27$ ,  $w_7 = 1/216$ , ..... ,  $w_{14} = 1/216$ ,  
 $w_{15} = 1/54$ , ..... ,  $w_{26} = 1/54$ .





# Macroscopic Variables



$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + [f_{0,i}(\mathbf{x}, t) - f_i(\mathbf{x}, t)] \cdot \Delta t / \tau$$

- Density  $\rho(\mathbf{x}, t) = \Sigma f_i(\mathbf{x}, t)$
- Velocity  $\mathbf{u}(\mathbf{x}, t) = \Sigma f_i(\mathbf{x}, t) \mathbf{v}_i / \rho(\mathbf{x}, t)$
- Kinematic shear viscosity (or diffusivity)

$$\nu = c_s^2 (\tau - \Delta t / 2)$$

–  $c_s$ : speed of sound (or an equivalent speed)

- Kinematic bulk viscosity  $\nu_B = 2\nu/3$
- Viscous stress tensor

$$\sigma_{\alpha\beta} \approx - [1 - \Delta t / (2\tau)] \Sigma_i v_{i\alpha} v_{i\beta} (f_i - f_{0,i})$$



# Equilibrium Distribution Function



- Maxwell-Boltzmann distribution

$$f_0(\mathbf{v}) = (m\beta/2\pi)^{3/2} \exp(-m\beta|\mathbf{v}-\mathbf{v}^0|^2/2) \text{ where } \beta = k_B T$$

$$\rightarrow f_0(\mathbf{v}) = (m\beta/2\pi)^{3/2} \exp(-m\beta|\mathbf{v}-\mathbf{u}|^2/2) \text{ where } \beta = k_B T$$

This can be approximated by Hermite expansion.

- So  $f_{0,i}$  can have a form of

$$f_{0,i} = \rho w_i [A + B \mathbf{v}_i \cdot \mathbf{u} + C(\mathbf{v}_i \cdot \mathbf{u})^2 + D|\mathbf{u}|^2], \rho = \sum f_i(\mathbf{x}, t)$$

- For general fluids with constant density,

$$f_{0,i} = \rho_0 w_i \left[ 1 + \frac{\mathbf{v}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{v}_i \cdot \mathbf{u})^2}{2 c_s^4} + \frac{|\mathbf{u}|^2}{2 c_s^2} \right]$$



# General LBM Algorithm



## 1. Initialization

❖ Ex.)  $f_{0,i}$  at prev. page &  $\rho = 1$  &  $\mathbf{u} = 0$

## 2. Calculation: $\rho$ & $\mathbf{u}$

## 3. Calculation: $f_{0,i}$ (and optionally, $\sigma_{\alpha\beta}$ )

✓ You can save  $\rho$  &  $\mathbf{u}$  at this point.

## 4. Collision: $f_i(\mathbf{x}, t) + [f_{0,i}(\mathbf{x}, t) - f_i(\mathbf{x}, t)] \cdot \Delta t / \tau$

## 5. Streaming: $f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t)$

& Applying boundary conditions

## 6. Time stepping: $t \rightarrow t + \Delta t$

## 7. Back to 2 or Stop



# Memory and Loops in LBM



- Memory usage
  - $\rho$ :  $N_x \times N_y \times N_z$
  - $u_x, u_y, u_z$ :  $N_x \times N_y \times N_z$
  - $f_i$ :  $N_x \times N_y \times N_z \times q$  (q: number of  $v_i$ )
    - You need  $f_{i,old}$  &  $f_{i,new}$ , or you should arrange updating carefully with or without some buffer memory (some functions such as `circshift` in Matlab, `numpy.roll` in Python, and `CSHIFT` in Fortran may be helpful).
- Loops
  - $\rho$ : for each position, summation over  $i$
  - $u_x, u_y, u_z$ : for each position, summation over  $i$
  - $f_i$ : for each position



# Dimensionless Variables



$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + [f_{0,i}(\mathbf{x}, t) - f_i(\mathbf{x}, t)] \cdot \Delta t / \tau$$

- Let's assume your system has the characteristic length  $l$ , velocity  $V$ , and density  $\rho_0$ ,
- $t \rightarrow tV/l$ ,  $\mathbf{x} \rightarrow \mathbf{x}/l$ ,  $\mathbf{v} \rightarrow \mathbf{v}/V$ ,  $\rho \rightarrow \rho/\rho_0$
- $f \rightarrow fV^d/\rho_0$  ( $d$ : space dimension)





# BGK Stability



- Sufficient condition

$$f_{0,i} \geq 0 \text{ for all } i \text{ and } \tau/\Delta t > 1/2$$

- Optimal condition for  $\tau/\Delta t \geq 1$

$$f_{0,0} > 0 \text{ and } \tau/\Delta t \geq 1$$



$$|\mathbf{u}| < \sqrt{\frac{2}{3}} \frac{\Delta x}{\Delta t}$$

- If unstable,
  - Adjust  $\Delta t$  and  $\Delta x$ , or
  - Try MRT(Multi-Relaxation-Time) or TRT(Two-Relaxation-Time) instead of BGK approx.



# Initial Conditions



- For a steady-state solution,  
 $f_i = f_{0,i}$  &  $\rho = 1$  &  $\mathbf{u} = 0$
- For a time-dependent solution,  
 $f_i = f_{0,i} + f_{n,i}$  (non-equilibrium part)
  - Consistent initialization
    - Ref.) R. Mei *et al.*, Comput. Fluids **35**, 855 (2006).
    - Through iteration by the LB algorithm,
    - Initial velocity  $\rightarrow f_i \rightarrow \rho \rightarrow f_i \rightarrow \rho \rightarrow \dots \rightarrow$  converged
    - The end step has to be propagation rather than collision.



# LBM for Diffusion Equation



- 1-D diffusion equation  $\phi_t = \mu \phi_{xx} [+ S]$ 
  - Diffusivity  $\mu = c_s^2(\tau - \Delta t/2)$  or  $\rho_0 c_s^2(\tau - \Delta t/2)$
  - In LBM,  $c_s = \Delta x/(\Delta t \cdot \sqrt{c})$ 
    - $c$ : 3 for most  $\mathbf{v}_i$  lattices except D1Q2, D2Q4, & D2Q7
- Equilibrium distribution function
  - At equilibrium,  $\mathbf{u} = 0$ .
  - Thus,  $f_{0,i} = \rho w_i$   
(Note: usually  $\phi = \rho$  in diffusion equation)
- With source term
$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + [f_{0,i}(\mathbf{x}, t) - f_i(\mathbf{x}, t)] \cdot \Delta t / \tau + \Delta t w_i S$$



# LBM for Diffusion Equation



- Boundary conditions (for  $T_t = \mu T_{xx}$ )
  - Constant temperature (Dirichlet B. C.)
    - $\Sigma f_i(\mathbf{x} = \mathbf{x}_0, t) = T_0 \rightarrow f_i(\mathbf{x} = \mathbf{x}_0) + f_j(\mathbf{x} = \mathbf{x}_0) = w_i T_0 + w_j T_0$
  - Adiabatic boundary (insulator, Neumann B. C.)
    - Using forward or backward finite differences
    - $[T(\mathbf{x} = \mathbf{x}_0 + \Delta x) - T(\mathbf{x} = \mathbf{x}_0)] / \Delta x = 0 \rightarrow f_i(\mathbf{x} = \mathbf{x}_0) = f_i(\mathbf{x} = \mathbf{x}_0 + \Delta x)$
  - Constant flux boundary
    - $T_t = S$  at the boundary
    - $T(\mathbf{x} = \mathbf{x}_0 + \Delta x) - T(\mathbf{x} = \mathbf{x}_0) = \Delta x S$
    - $\rightarrow f_i(\mathbf{x} = \mathbf{x}_0) = f_i(\mathbf{x} = \mathbf{x}_0 + \Delta x) - \Delta x w_i S$



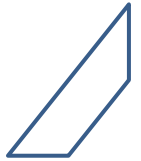
# Do It Yourself



- Consider LBM for 1-D diffusion equation  $T_t = \mu T_{xx}$  with D1Q2 lattice.
  - Set  $\Delta t = \Delta x = 1$  and prepare  $f_i$  and  $T$  for your own space grid (set initial  $f_i(x, t = 0) = 0$  &  $T(x, t = 0) = 0$ )
  - Set  $\tau (> 0.5)$  and b. c. value  $T_0$
  - Loop:  $T(x, t) = \sum f_i(x, t)$ ,  $f_{0,i} = T w_i$ , &  
 $f_i(x + v_i \Delta t, t + \Delta t) = f_i(x, t) + [f_{0,i}(x, t) - f_i(x, t)] \cdot \Delta t / \tau$ 
    - Applying B. C.:  $f_1(x = 0, t) = T_0 - f_2(x = 0, t)$  &  
 $f_2(x = L, t) = -f_1(x = L, t)$
  - Make and run your code. Check out  $T(x, t)$



# Boundary Conditions for Fluids



- Link-wise
  - Bounce-back method
    - Inverting  $f_i$  across the boundary wall. No-slip condition. Simple and stable. Moderate accuracy.
- Wet-node
  - Equilibrium scheme
    - $\rho$  &  $\mathbf{u}$  at the boundary by  $f_{0,i}$ . Simple and stable.
  - Non-equilibrium extrapolation method
    - Non-eq. contribution by nearby fluid. Moderate.
  - Non-equilibrium bounce-back method
    - Complex. Very accurate but less stable.



# Boundary Conditions for Fluids



- Pressure B. C.
  - Periodic B. C.
    - For constant pressure, but periodic pressure gradient is also available if you follow the scheme of Zhang & Kwok (Phys. Rev. E, 2006)
    - You should check dependence and change of velocities
  - Pressure at inlet or outlet
    - Ghost boundary +  $f_{0,i}$  by the desired pressure, or
    - Density at inlet or outlet from the desired pressure, and finding  $f_i$  and normal velocity from the non-equilibrium distribution functions
      - Zou & He (Phys. Fluids, 1997), Guo *et al.* (Phys. Rev. E, 2002)



# LBM for Advection-Diffusion



- 1-D advection-diffusion eq.  $\phi_t + u_0 \phi_x = \mu \phi_{xx}$ 
  - Like LBM for diffusion,  $\mu = c_s^2(\tau - \Delta t/2)$  or  $\rho_0 c_s^2(\tau - \Delta t/2)$
- Equilibrium distribution function
$$f_{0,i} = \rho w_i (1 + \mathbf{v}_i \cdot \mathbf{u}_0 / c_s^2)$$
- Source term: Same as for the diffusion eq.
- Boundary conditions
  - Periodic B. C.
  - Bounce-back wall
  - Neumann B. C.: setting  $u_x = 0$  at the wall if  $x$  is the wall direction. (Remember  $\rho \mathbf{u} = \sum f_i(\mathbf{x}, t) \mathbf{v}_i$ )



# LBM for Navier-Stokes Equation

- 2-D incompressible Navier-Stokes equation

$$\rho u_t + \rho(\mathbf{u} \cdot \nabla)u = -p_x + \mu(u_{xx} + u_{yy})$$

$$\rho v_t + \rho(\mathbf{u} \cdot \nabla)v = -p_y + \mu(v_{xx} + v_{yy})$$

– With the continuity equation:  $\rho(u_x + v_y) = 0$

– where  $\mathbf{u} := (u, v)$

– Dynamic viscosity  $\mu = \rho_0 c_s^2 (\tau - \Delta t/2)$

– Remember  $c_s = \Delta x / (\Delta t \cdot \sqrt{c})$

- Reynolds number  $Re = \rho_0 UL / \mu$

$U$ : characteristic velocity

$L$ : characteristic length

- Mach number  $Ma = U / c_s$


# LBM for Navier-Stokes Equation

- Equilibrium distribution function

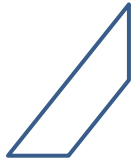
$$f_{0,i} = \rho_0 w_i \left[ 1 + \frac{\mathbf{v}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{v}_i \cdot \mathbf{u})^2}{2 c_s^4} + \frac{|\mathbf{u}|^2}{2 c_s^2} \right]$$

- If  $Ma^2$  is not sufficiently small but  $Ma^3 \ll 1$

$$f_{0,i} = \rho w_i + \rho_0 w_i \left[ \frac{\mathbf{v}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{v}_i \cdot \mathbf{u})^2}{2 c_s^4} + \frac{|\mathbf{u}|^2}{2 c_s^2} \right]$$



# LBM for Navier-Stokes Equation



- Boundary conditions
  - Same as for the advection-diffusion eq., or
  - Dirichlet B. C.: fixing density/pressure at the boundary
    - You need to find  $f_i$  and normal velocity at the wall.
- Gravity: adjust the equilibrium velocity.
- Temperature
  - Compare the result with Maxwell-Boltzmann distribution, or
  - Use an equation of state.



# Accuracy



- Spatial truncation errors
  - Dominated by  $O([\tau - \Delta t/2]^2)$  terms
- Modelling errors
  - Ground concept: LBM can be viewed as an approximation of Navier-Stokes equation.
    - See T. Krüger *et al.* section 4 or M. Junk, Numer. Methods Partial Differential Eq. 17: 383-402 (2001).
  - Space and time accuracy: second order
  - Stress tensor errors:  $O(u^3)$ 
    - In case of standard lattice
    - This limits LBM to weakly compressible flows.
    - Insignificant if  $Ma^2 \ll 1$
  - Compressibility errors:  $O(Ma^2)$ 
    - If you reduce these and spatial truncation errors simultaneously, time accuracy reduces to first order.



# MRT Collision Operator



- $f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Delta t \cdot \Omega[f_i(\mathbf{x}, t), f_i(\mathbf{x}, t)]$   
 $\rightarrow f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Delta t \cdot \mathbf{M}^{-1} \mathbf{S}[\mathbf{m}_0(\mathbf{x}, t) - \mathbf{m}(\mathbf{x}, t)]$
- For DdQq velocity lattice,  
$$m_j = \sum_{i=0}^{q-1} M_{ji} f_i \quad \text{for } j = 0, \dots, q-1$$
$$m_{0,j} = \sum_{i=0}^{q-1} M_{ji} f_{0,i} \quad \text{for } j = 0, \dots, q-1$$
  - See Mohamad or Krüger *et al.* for the values of  $M_{ji}$
- **S**: diagonal matrix of parameters.
  - If  $\mathbf{S} = (1/\tau)\mathbf{I} \rightarrow$  BGK approx.



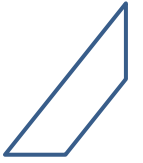
# TRT Collision Operator



- $f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + [f_{0,i}^+(\mathbf{x}, t) - f_i^+(\mathbf{x}, t)] \cdot \Delta t / \tau^+ + [f_{0,i}^-(\mathbf{x}, t) - f_i^-(\mathbf{x}, t)] \cdot \Delta t / \tau^-$
- Two relaxation time parameters
- $f_i^+ = (f_i + f_{-i})/2$ ,  $f_i^- = (f_i - f_{-i})/2$ 
  - where  $f_{-i}$  means that for the opposite velocity (*i.e.*,  $-\mathbf{v}_i$ )
- $f_i = f_i^+ + f_i^-$ ,  $f_{0,i} = f_{0,i}^+ + f_{0,i}^-$
- Dynamic viscosity  $\mu = \rho_0 c_s^2 (\tau^+ - \Delta t/2)$ 
  - while  $\tau^-$  is a free parameter



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