LATTICE BOLTZMANN METHOD for CFD

More @ LBE

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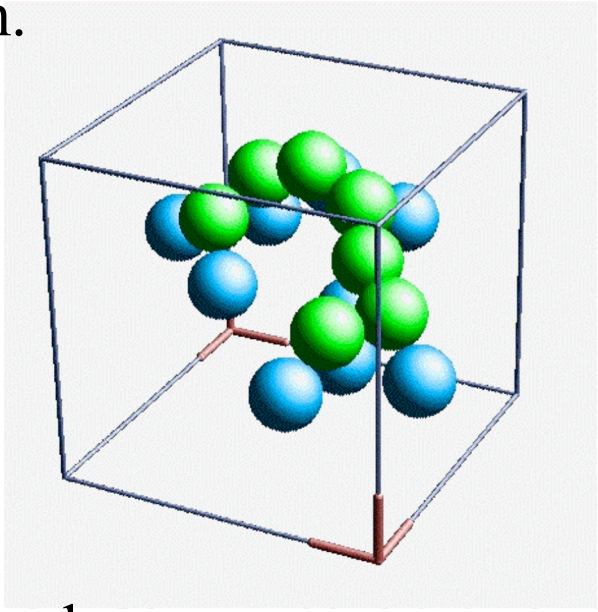
What makes up fluids

- Fluid made of small, individual molecules.
- Molecules are in a state of constant motion.
- Molecules are at continuous collision with each other.
- Molecule has internal structure.
- There are intermolecular forces.
- Macroscopic variables, such as pressure, temperature, and internal energy, are determined by the mass, velocity, and internal structure of molecules.



Modeling Fluids

Knudsen number $Kn \equiv \dfrac{\text{Mean free path}}{\text{Characteristic hydrodynamic length}}$

- Microscopic Method : Molecular dynamics

  $Kn<\infty$

- Mesoscopic Method : Boltzmann Equation

  $Kn<\infty$

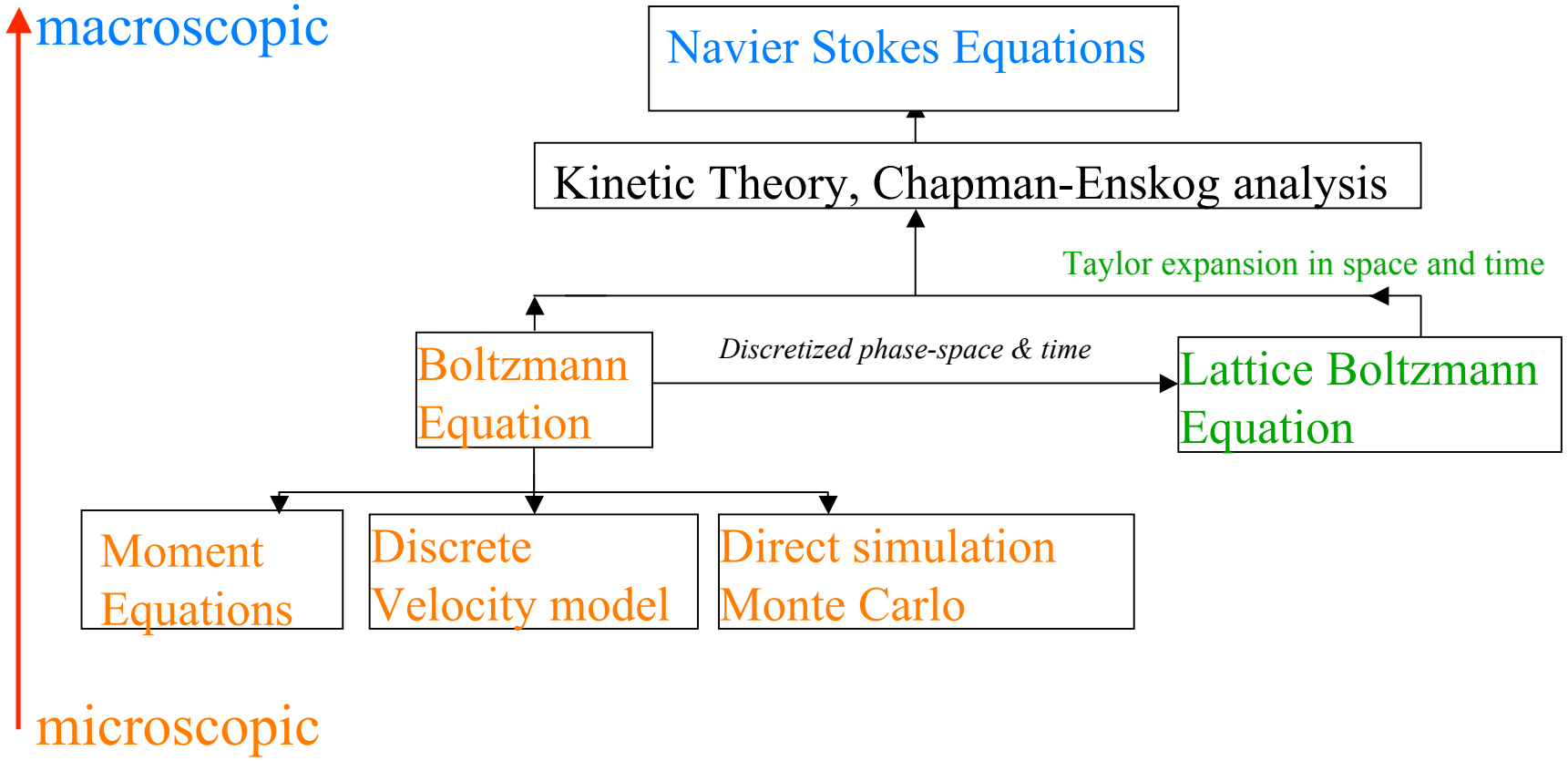
- Macroscopic Method: Navier-Stokes Equations

  $Kn<0.1$

- A Novel Method : Lattice Boltzmann Method

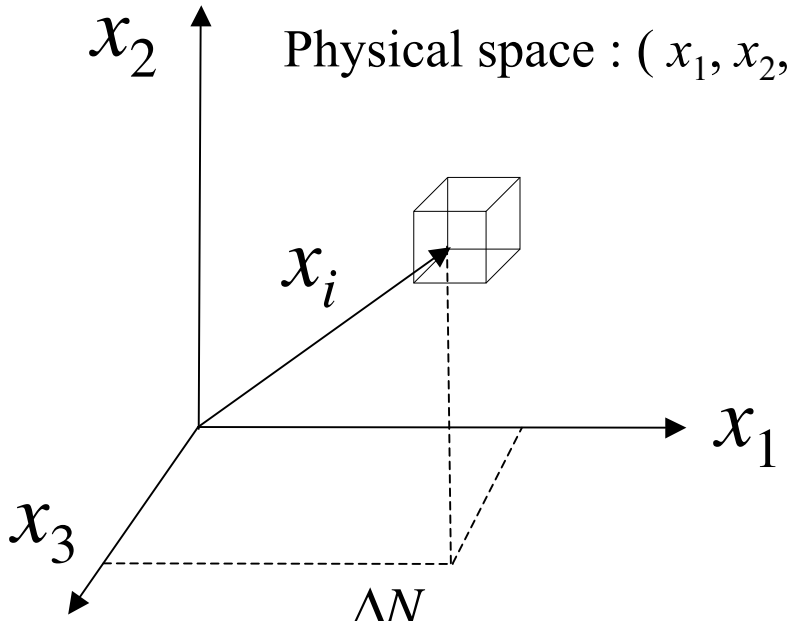
  $Kn<0.1$

Modeling of Fluids

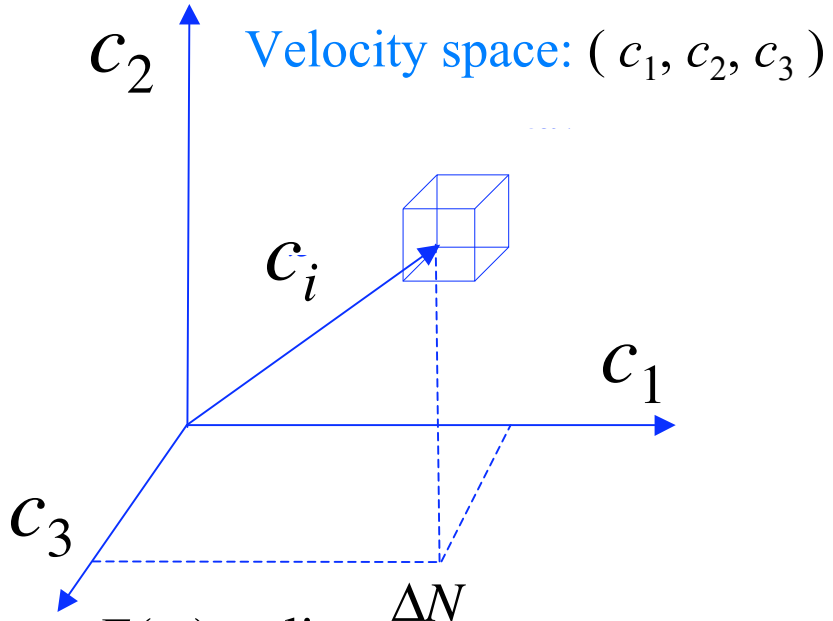


Velocity distribution function

- Velocity distribution function: $F(c_i)$



$$\rho = \lim_{\Delta V_x \to 0} m \frac{\Delta N}{\Delta V_x} = mn(x_i)$$



$$F(c_i) = \lim_{\Delta V_c \to 0} \frac{\Delta N}{\Delta V_c}$$

m : *mass of molecule*

ΔN : *number of molecules in* ΔV_x

$n(x_i)$: *local number density*

Velocity Distribution Function

- Normalized Velocity distribution Function

  $f(c_i) = F(c_i) / N$

  N: Number of molecules in system

- Characteristics of Distribution Function f

  1. $\int_{-\infty}^{\infty} Nf(c_i)dV_c = N \Rightarrow \int_{-\infty}^{\infty} f(c_i)dV_c = 1$

  2. $\overline{Q} = \dfrac{\int_N QdN}{N} = \dfrac{\int_{-\infty}^{\infty} Q(c_i)Nf(c_i)dV_c}{N} = \int_{-\infty}^{\infty} QfdV_c$

  $\overline{Q}$ is the average value of Q for all molecules

  Macrosopic velocity: $\vec{u} = \mathbf{u} = \bar{\mathbf{c}} = \int_{-\infty}^{\infty} c_i f dV_c$

Velocity Distribution Function under Equilibrium State

- Equilibrium State

  In equilibrium state, the number of molecules in c_i is constant.

- Distribution function under equilibrium state is the Maxwellian distribution:

$$f^{eq}(c_i) = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{m}{2kT}\left[(c_1-u_1)^2+(c_2-u_2)^2+(c_3-u_3)^2\right]}$$

  T: temperature;

  k : Boltzmann constant (1.38054×10^{-16} erg-K)

  m: mass of molecule

  u : macroscopic velocity

Boltzmann Equation

- Under non-equilibrium state distribution function

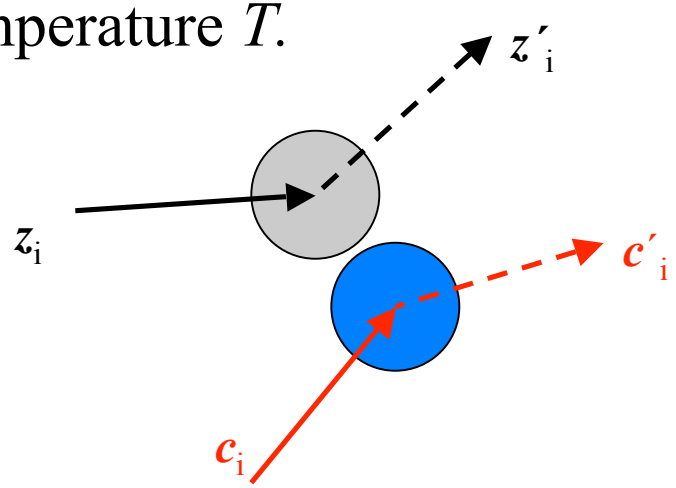
  $f = f(x_i, c_i, t) = f(\mathbf{x}, \mathbf{c}, t)$

- The molecular velocity distribution function has a rate of change, with respect to position and time, that is described by

$$\frac{\partial}{\partial t}[nf(c_i)] + c_j \frac{\partial}{\partial x_j}[nf(c_i)] = \left\{\frac{\partial}{\partial t}[nf(c_i)]\right\}_{collision}$$

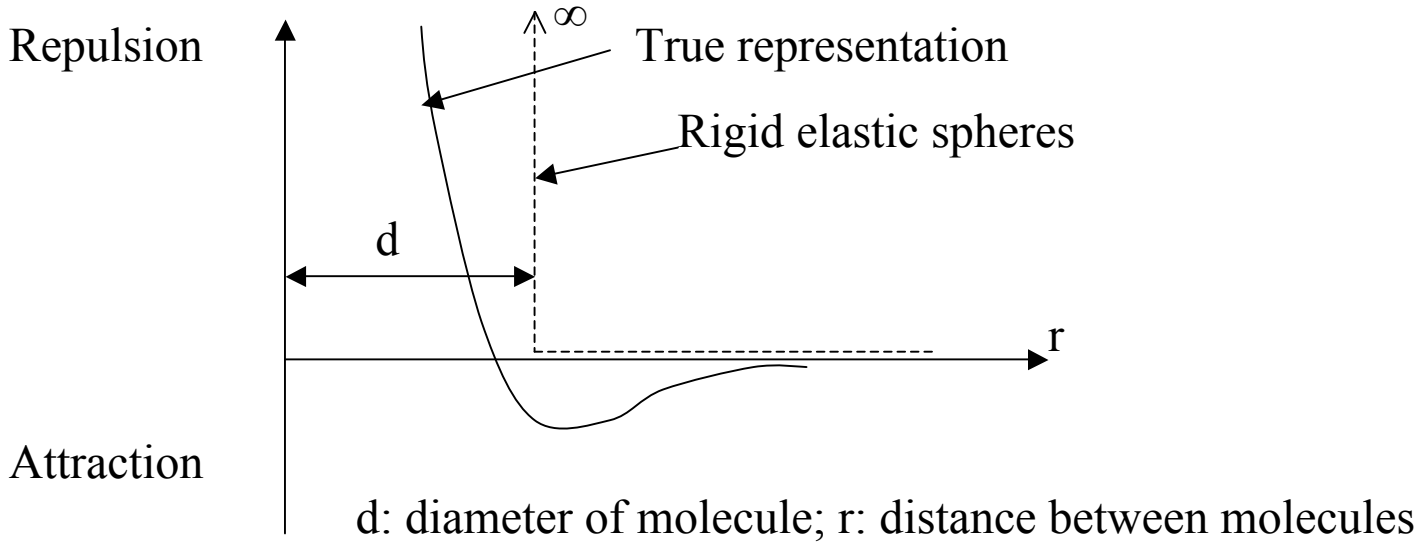
Collisions in fluids

- Molecules constantly collide with each other.
- Collision will change the velocity of molecules.
- In collision, the translational energy of molecule may transfer to internal energy, if molecule has internal structure.
- In general, the rate of collision depends on the molecule velocity, number density $n(\boldsymbol{x})$, and temperature T.



Collision Operator in Boltzmann Equation

- Elastic-sphere molecule model
  1. no internal structure of molecule,
  2. the molecule is treated as a rigid ball,
  3. so no rotation and vibration,
  4. only translation.
- no attraction force between molecules.



Collision operator

- Rigid ball model gives:

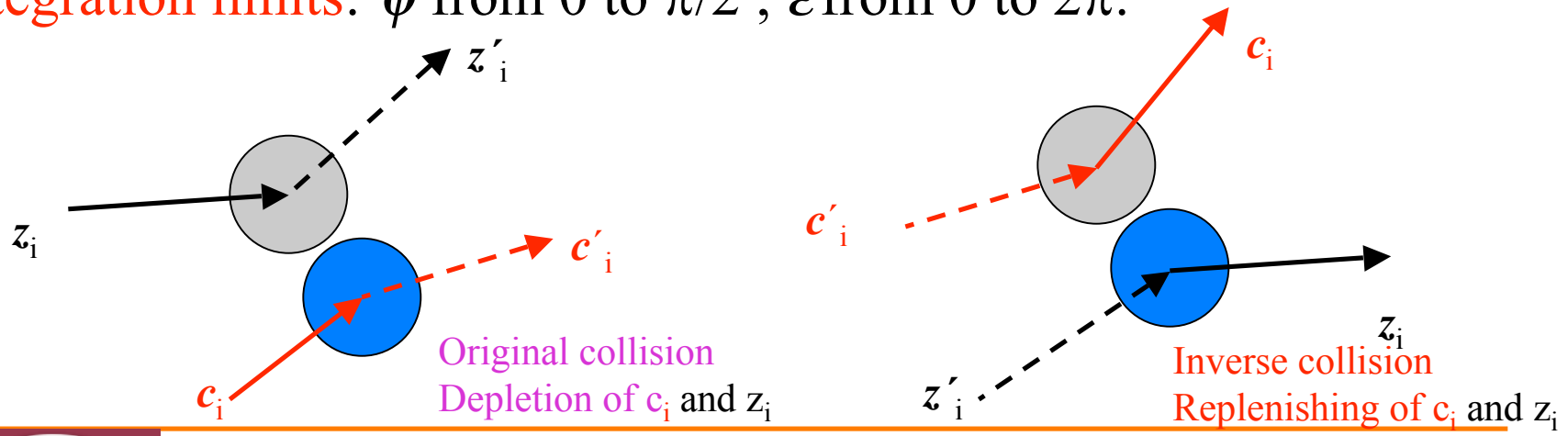
$$\left\{\frac{\partial}{\partial t}[nf(c_i)]\right\}_{collision} = \int_{-\infty}^{\infty}\int_{0}^{2\pi}\int_{0}^{\pi/2} n^2 \mathrm{d}^2\left[f(c'_i)f(z'_i) - f(c_i)f(z_i)\right] g \sin\psi\cos\psi d\psi d\varepsilon dV_x$$

g: relative velocity between two collided molecules

$f(\mathbf{c}'_i)f(\mathbf{z}'_i)$: replenishing of the molecules of class c_i

$f(\mathbf{c}_i)f(\mathbf{z}_i)$: depleting of the molecules of class c_i

Integration limits: ψ from 0 to $\pi/2$; ε from 0 to 2π.



Macroscopic variables

Quantities of interest

- Density $$\rho = \int_{-\infty}^{\infty} mf dV_c$$
- Momentum $$\rho \mathbf{u} = \int_{-\infty}^{\infty} m\mathbf{c} f dV_c$$
- Translational energy $$e_{tr} = \int_{-\infty}^{\infty} \frac{1}{2}(\mathbf{c} - \bar{\mathbf{c}})^2 f dV_c$$

Moments of the Boltzmann Equation

- Let $Q(c_i)$ be a function of c_i but not of position and time, the equation of transfer of $Q(c_i)$ is

$$\int_{-\infty}^{\infty} Q(c_i)\left\{\frac{\partial}{\partial t}[nf(c_i)] + c_j\frac{\partial}{\partial x_j}[nf(c_i)]\right\}dV_c = \int_{-\infty}^{\infty} Q(c_i)\left\{\frac{\partial}{\partial t}[nf(c_i)]\right\}_{collision} dV_c$$

$$\Downarrow$$

- $$\frac{\partial}{\partial t}[n\overline{Q}] + \frac{\partial}{\partial x_j}[n\overline{Qc_i}] = \Delta[Q]$$

if $Q=m$, mc_i, $mc^2/2$, the change in Q for both molecules must be zero in collision. We have

$$\frac{\partial}{\partial t}[n\overline{Q}] + \frac{\partial}{\partial x_j}[n\overline{Qc_i}] = 0$$

Let Q = m, we have the continuity equation in NS. We recover the momentum and energy equations in NS when $Q=mc_i$, $mc^2/2$

The Conservation Equations from the Boltzmann Equation

$Q = m$ $$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \bar{c}_j\right) = 0$$

$Q = mc_i$ $$\frac{\partial}{\partial t}\left(\rho \bar{c}_j\right) + \frac{\partial}{\partial x_i}\left(\rho \bar{c}_j \bar{c}_i\right) = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i}$$

$Q = mc^2/2$ $$\frac{\partial}{\partial t}\left[\rho\left(e + \bar{c}^2\right)\right] + \frac{\partial}{\partial x_i}\left[\rho \bar{c}_i\left(h + \frac{1}{2}\bar{c}^2\right)\right] = \frac{\partial}{\partial x_i}\left(\tau_{ij}\bar{c}_k - q_i\right)$$

Kinetic theory: $e = e_{tr} = \overline{C^2}/2$ $\qquad h = h_{tr} = e_{tr} + p/\rho = 5RT/2$

$\rho = nm$ $\qquad p = \rho[\overline{C_1^2} + \overline{C_2^2} + \overline{C_3^2}]/3$

New definition: $\tau_{ij} = -[\rho \overline{C_i C_j} - p\,\delta_{ij}]$ $\qquad q_j = \rho\,\overline{C_j\,C^2}$

$\mathbf{C} = \mathbf{c} - \bar{\mathbf{c}}$ $\qquad$ tr: translational

The Chapmen-Enskog Solution of Boltzmann Equation

- Non-dimensional form

$$\xi\left\{\frac{\partial}{\partial \hat{t}}\left[\hat{n}\hat{f}\right]+\hat{c}_j\frac{\partial}{\partial \hat{x}_j}\left[\hat{n}\hat{f}\right]\right\}=\left\{\frac{\partial}{\partial \hat{t}}\left[\hat{n}\hat{f}\right]\right\}_{collision}$$

c_r: reference molecule speed ; L: characteristic length

ν_r: reference collision frequency

$\xi = c_r / L\,\nu_r$ is proportional to the Knudsen #, the ratio of the mean free path to a characteristic length, thus it is a very small value.

- Chapman-Enskog expansion (simplifying definitions ($f = \hat{n}\hat{f}$):

$$f(\mathbf{x}, \mathbf{c}, t) = f^{(eq)}(\mathbf{x}, \mathbf{c}, t) + \xi f^{(1)}(\mathbf{x}, \mathbf{c}, t) + \ldots$$

Solve the $f^{(1)}$, then we get the solution for f

Chapman-Enskog Procedure

- Taking the 1st order departure of *f* from the Maxwellian distribution as:

$$f(\mathbf{x}, \mathbf{c}, t) = f^{(eq)}(\mathbf{x}, \mathbf{c}, t) + \xi f^{(1)}(\mathbf{x}, \mathbf{c}, t) + \ldots$$

- Substituting into the Boltzmann equation:

$$\left(\frac{\partial f}{\partial t}\right)_c = \int\int\left[f^{(1)'}(\mathbf{x},\mathbf{c}',t) f^{(eq)'}(\mathbf{x},\mathbf{z}',t) + f^{(1)'}(\mathbf{x},\mathbf{z}',t) f^{(eq)'}(\mathbf{x},\mathbf{c}',t)\right]|\mathbf{z}-\mathbf{c}| n\sigma(\Omega) d\mathrm{V}_z d\Omega$$

$$-\int\int\left[f^{(1)}(\mathbf{x},\mathbf{c},t) f^{(eq)}(\mathbf{x},\mathbf{z},t) + f^{(1)}(\mathbf{x},\mathbf{z},t) f^{(eq)}(\mathbf{x},\mathbf{c},t)\right]|\mathbf{z}-\mathbf{c}| n\sigma(\Omega) d\mathrm{V}_z d\Omega$$

Chapman-Enskog Procedure

- Keeping only 1st order terms in the expansion:

$$\left(\frac{\partial f}{\partial t}\right)_c = \int\int\left[f^{(1)}(\mathbf{x},\mathbf{c},t)f^{(eq)'}(\mathbf{x},\mathbf{z},t)\right]|\mathbf{z}-\mathbf{c}|n\sigma(\Omega)d\mathrm{V}_z d\Omega \approx -f^{(1)}(\mathbf{x},\mathbf{c},t)n\sigma_{tot}\bar{c}_{rel}$$

- Where
  - The average relative velocity btwn particles is $\bar{\mathbf{c}}_{rel}$
  - The total collision cross-section is σ_{tot}
- The collision frequency is $\nu_r = \nu_c = n\sigma_{tot}\bar{c}_{rel}$

The "1st Order" Boltzmann Equation

- So the Boltzmann equation becomes, to 1st order:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = -\frac{1}{\lambda}\left(f - f^{(eq)}\right)$$

- Or

$$\frac{df}{dt} + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(eq)}$$

- On the characteristic line $\mathbf{c} = d\mathbf{x}/dt$
- Where $\lambda = 1 / \nu_r$

Integrating the "1st Order" BE

- Integrating the "1st Order" BE over a time step δ_t:

$$f(\mathbf{x}+\mathbf{c}\delta_t,\mathbf{c},t+\delta_t)=\frac{1}{\lambda}e^{-\delta_t/\lambda}\int_0^{\delta_t}e^{t'/\lambda}f^{(eq)}(\mathbf{x}+\mathbf{c}t',\mathbf{c},t+t')dt'+e^{-\delta_t/\lambda}f(\mathbf{x},\mathbf{c},t)$$

- Assuming δ_t is small enough & $f^{(eq)}$ is smooth enough locally, then for $0 \le t' \le \delta_t$:

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

Integrating the "1st Order" BE

- Putting these last 2 eqs. together:

$$f(\mathbf{x}+\mathbf{c}\delta_t,\mathbf{c},t+\delta_t)-f(\mathbf{x},\mathbf{c},t)=\left(e^{-\delta_t/\lambda}-1\right)\left[f(\mathbf{x},\mathbf{c},t)-f^{(eq)}(\mathbf{x},\mathbf{c},t)\right]$$
$$+\left[1+\frac{\lambda}{\delta_t}\left(e^{-\delta_t/\lambda}-1\right)\right]\left[f^{(eq)}(\mathbf{x}+\mathbf{c}\delta_t,\mathbf{c},t+\delta_t)-f^{(eq)}(\mathbf{x},\mathbf{c},t)\right]$$

- Expanding $e^{-\delta_t/\lambda}$ in a Taylor series while neglecting terms of $O(\delta_t^2)$ and also defining $\tau=\lambda/\delta_t$:

$$f(\mathbf{x}+\mathbf{c}\delta_t,\mathbf{c},t+\delta_t)-f(\mathbf{x},\mathbf{c},t)=-\frac{1}{\tau}\left[f(\mathbf{x},\mathbf{c},t)-f^{(eq)}(\mathbf{x},\mathbf{c},t)\right]$$

Low Mach Number Approximation

- In LBE, the equilibrium distribution

$$f^{(eq)} = \left(\frac{m}{2\pi kT}\right)^{D/2} e^{-\frac{m}{2kT}(\mathbf{c}-\mathbf{u})^2} = \left(\frac{m}{2\pi kT}\right)^{D/2} e^{-\frac{m}{2kT}\mathbf{c}^2} e^{-\frac{m}{2kT}(2\mathbf{c}\bullet\mathbf{u}-\mathbf{u}\bullet\mathbf{u})}$$

- is obtained from a truncated small velocity expansion or low-Mach-number approximation

$$f^{(eq)} = \left(\frac{m}{2\pi kT}\right)^{D/2} e^{-\frac{m}{2kT}\mathbf{c}^2}\left[1+\frac{\mathbf{c}\bullet\mathbf{u}}{kT}+\frac{1}{2}\left(\frac{\mathbf{c}\bullet\mathbf{u}}{kT}\right)^2-\frac{\mathbf{u}\bullet\mathbf{u}}{2kT}\right]+O\left(u^3\right)$$

- D = number of dimensions (e.g., D = 3 for 3D)

Discretization of Phase Space

- Discretization of momentum space is coupled to that of configuration space such that a lattice structure is obtained
- This is a special characteristic of LBE
- Quadrature must be accurate enough to
  - Preserve conservation constraints exactly
  - Retain necessary symmetries of Navier-Stokes

Discretization of Phase Space

- The first 2 order approximations of the distribution function ($f^{(eq)}$, $f^{(1)}$) are used to derive Navier-Stokes
- So quadrature used must evaluate hydrodynamic moments w.r.t $f^{(eq)}$ exactly:

  ρ: $1, c_i, c_i c_j,$

  $\mathbf{u}$: $c_i, c_i c_j, c_i c_j c_k,$

  T: $c_i c_j, c_i c_j c_k, c_i c_j c_k c_l,$

- Assuming particle has linear d.o.f. only, d.o.f=D

Discretization of Phase Space

- To obtain Navier-Stokes, must evaluate moments of 1, $\mathbf{c}$, …, $\mathbf{c}^6$, w.r.t. wt. fnctn $e^{-m\mathbf{c}\bullet\mathbf{c}/2kT}$ exactly
- Hydro-dynamic moments of $f^{(eq)}$: $I = \int \psi(\mathbf{c})\, f^{(eq)}\, d\mathbf{c}$

$$I = \left(\frac{m}{2\pi kT}\right)^{D/2} \int \psi(\mathbf{c}) e^{-\frac{m}{2kT}\mathbf{c}^2} \left[1 + \frac{\mathbf{c}\bullet\mathbf{u}}{kT} + \frac{1}{2}\left(\frac{\mathbf{c}\bullet\mathbf{u}}{kT}\right)^2 - \frac{\mathbf{u}\bullet\mathbf{u}}{2kT}\right] d\mathbf{c}$$

- Use Gaussian-type quadrature to evaluate

$$\int \psi(x) e^{-x^2}\, dx$$

Square Lattice-Boltzmann Model 9-bit 2D

- In Cartesian coordinates: $\psi_{mn}(\mathbf{c}) = c_x^m c_y^n$
- Then

$$I = \int_{-\infty}^{\infty} \psi_{mn}(\mathbf{c}) f^{(eq)} d\mathbf{c} = \frac{m}{\pi}\left(\sqrt{2kT}\right)^{m+n} \times$$

$$\left\{\left(1 - \frac{\mathbf{u}^2}{2kT}\right) I_m I_n + \frac{2\left(u_x I_{m+1} I_n + u_y I_m I_{n+1}\right)}{\sqrt{2kT}} + \frac{u_x^2 I_{m+2} I_n + 2u_x u_y I_{m+1} I_{n+1} + u_x^2 I_m I_{n+2}}{RT}\right\}$$

- Where

$$I_m = \int_{-\infty}^{\infty} e^{-\zeta^2} \zeta^m d\zeta, \zeta = c/\sqrt{2kT}$$

Square Lattice-Boltzmann Model 9-bit 2D

- Use 3rd order Hermite formula to evaluate

$$I_m = \int_{-\infty}^{\infty} e^{-\zeta^2} \zeta^m d\zeta = \sum_{j=1}^{3} \omega_j \zeta_j^m$$

- Where the 3 abscissas of the quadrature are:

$$\zeta_1 = -\sqrt{3/2},\ \zeta_2 = 0,\ \zeta_3 = \sqrt{3/2}$$

- And the corresponding weight coefficients are:

$$\omega_1 = \sqrt{\pi}/6,\ \omega_2 = 2\sqrt{\pi}/3,\ \omega_3 = \sqrt{\pi}/6$$

2D Square Lattice-Boltzmann Model 9-bit

- Moment integral becomes

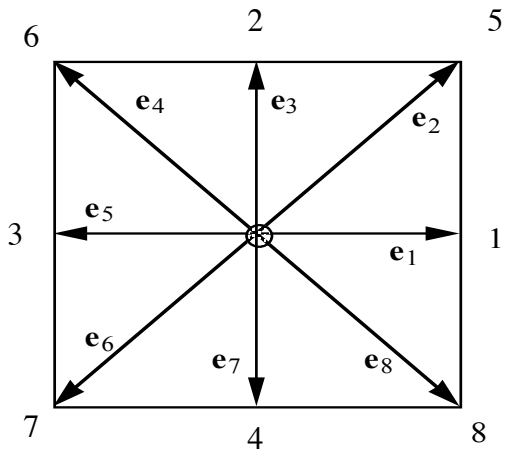
$$I_m = \frac{m}{\pi}\sum_{i,j=1}^{3}\omega_i\omega_j\psi\left(c_{i,j}\right)\left\{1+\frac{c_{i,j}\bullet\mathbf{u}}{kT}+\frac{\left(c_{i,j}\bullet\mathbf{u}\right)^2}{2\left(kT\right)^2}-\frac{\mathbf{u}^2}{2kT}\right\}$$

- From which, parts of the equilibrium distribution function are identified as

$$f_{i,j}^{(eq)} = \frac{m}{\pi}\omega_i\omega_j\left\{1+\frac{c_{i,j}\bullet\mathbf{u}}{kT}+\frac{\left(c_{i,j}\bullet\mathbf{u}\right)^2}{2\left(kT\right)^2}-\frac{\mathbf{u}^2}{2kT}\right\}$$

2D Square Lattice-Boltzmann Model 9-bit

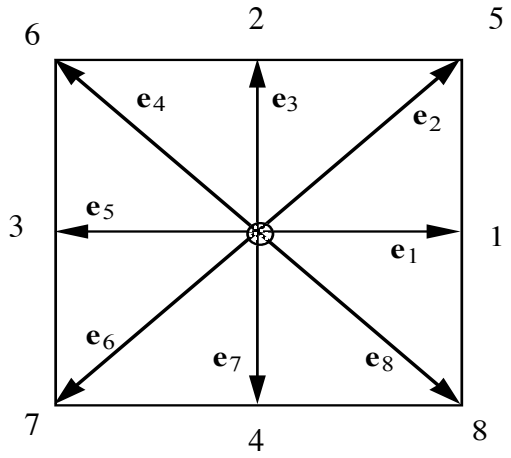
- Select possible molecular velocities on 2D square lattice to go in as many directions of such square
- The chosen velocities have a certain symmetry to account for molecules moving in any and all directions independent of directions (isotropy)
- For square this means sides & corners
- This means 9 possible velocities
- To go w/at least 9 terms in $\psi_{mn}(\mathbf{c})$



2D Square Lattice-Boltzmann Model 9-bit

- The 9 possible velocities are:

$$e_\alpha = \begin{cases} (0,0), & & \alpha = 0, \\ (\cos\theta_\alpha, \sin\theta_\alpha)c, & \theta_\alpha = (\alpha-1)\pi/2, & \alpha = 1,2,3,4, \\ \sqrt{2}(\cos\theta_\alpha, \sin\theta_\alpha)c, & \theta_\alpha = (\alpha-5)\pi/2 + \pi/4, & \alpha = 5,6,7,8 \end{cases}$$



2D Square Lattice-Boltzmann Model 9-bit

- Then parts of the equilibrium distribution function are identified as

$$f_\alpha^{(eq)} = m w_\alpha \left\{ 1 + \frac{\mathbf{e}_\alpha \bullet \mathbf{u}}{c^2} + \frac{(\mathbf{e}_\alpha \bullet \mathbf{u})^2}{2c^4} - \frac{\mathbf{u}^2}{2c^2} \right\}$$

- Where the corresponding weight coefficients are now

$$w_\alpha = \frac{\omega_i \omega_j}{\pi} = \begin{cases} 4/9, & i = j = 2, \quad \alpha = 0, \\ 1/9, & i = 1, j = 2, \ldots, \quad \alpha = 1,2,3,4, \\ 1/36, & i = j = 1, \quad \alpha = 5,6,7,8 \end{cases}$$

- And $RT = c_s^2 = c^2/3$ or

$$\left\| \sqrt{RT}\vec{\zeta} \right\| = \sqrt{3RT} = c$$

3D Cube Lattice-Boltzmann Model 27-bit

- This is a straight-forward extension of 2D:

$$I_m = \frac{m}{\pi^{3/2}} \sum_{i,j,k=1}^{3} \omega_i \omega_j \omega_k \psi\left(c_{i,j,k}\right)\left\{1 + \frac{c_{i,j,k} \bullet \mathbf{u}}{kT} + \frac{\left(c_{i,j,k} \bullet \mathbf{u}\right)^2}{2(kT)^2} - \frac{\mathbf{u}^2}{2kT}\right\}$$

- where

$$e_\alpha = \begin{cases} (0,0,0) & \alpha = 0, \\ (\pm 1,0,0)c, (0,\pm 1,0)c, (0,0,\pm 1)c, & \alpha = 1,2,\ldots,6, \\ (\pm 1,\pm 1,0)c, (\pm 1,0,\pm 1)c, (0,\pm 1,\pm 1)c, & \alpha = 7,8,\ldots,18, \\ (\pm 1,\pm 1,\pm 1)c, & \alpha = 19,20,\ldots,26 \end{cases}$$

3D Cube Lattice-Boltzmann Model 27-bit

- Then parts of the equilibrium distribution function are identified as

$$f_\alpha^{(eq)} = m w_\alpha \left\{ 1 + \frac{3\mathbf{e}_\alpha \bullet \mathbf{u}}{c^2} + \frac{9(\mathbf{e}_\alpha \bullet \mathbf{u})^2}{2c^4} - \frac{3\mathbf{u}^2}{2c^2} \right\}$$

- where

$$w_\alpha = \begin{cases} 8/27 & i=j=k=2 & \alpha = 0, \\ 2/27, & i=j=2, k=1,\ldots, & \alpha = 1,2,\ldots,6, \\ 1/54, & i=j=1, k=2,\ldots, & \alpha = 7,8,\ldots,18, \\ 1/216, & i=j=k=1,\ldots., & \alpha = 19,20,\ldots,26 \end{cases}$$

Lattice Boltzmann Equation

- Equilibrium distribution function for f_α

$$f_\alpha^{(eq)} = \rho w_\alpha [1 + \frac{3}{c^2} \boldsymbol{e}_\alpha \cdot \boldsymbol{u} + \frac{9}{2c^4} (\boldsymbol{e}_\alpha \cdot \boldsymbol{u})^2 - \frac{3}{2c^2} \boldsymbol{u} \cdot \boldsymbol{u}]$$

Δ 9-velocity model(2D):

$$w_\alpha = \begin{cases} 4/9, & \alpha = 0 \\ 1/9, & \alpha = 1,3,5,7 \\ 1/36, & \alpha = 2,4,6,8 \end{cases}$$

Δ 15-velocity model:

$$w_\alpha = \begin{cases} 2/9, & \alpha = 0 \\ 1/9, & \alpha = 1,2,...6 \\ 1/72, & \alpha = 7,8,...14. \end{cases}$$

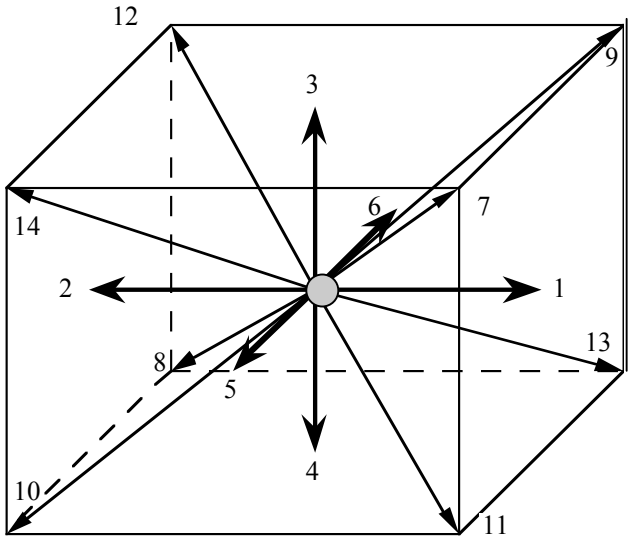
Δ 19-velocity model:

$$w_\alpha = \begin{cases} 1/3, & \alpha = 0 \\ 1/18, & \alpha = 1,2,...6 \\ 1/36, & \alpha = 7,8,...18. \end{cases}$$

Qian YH, d'Humieres D, Lallemand P. Lattice BGK Models for Navier Stokes Equation. Europhys Lett 1992;17:479-484.

Examples of 3-D lattice models

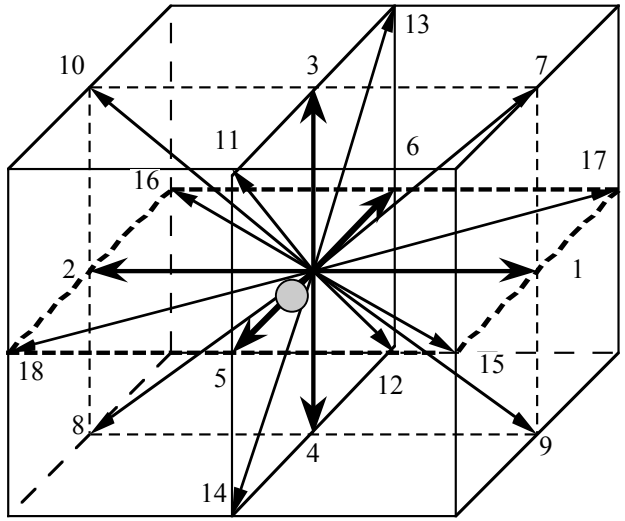
15-velocity **3-D** lattice model



Q15D3 lattice

$2\delta x$

19-velocity **3-D** lattice model



Q19D3 lattice

$2\delta x$

Lattice Boltzmann Equation

- Macroscopic variables is obtained from:

$$\rho = \sum_{\alpha=0}^{N} f_\alpha = \sum_{\alpha=0}^{N} f_\alpha^{(eq)}, \qquad \rho \boldsymbol{u} = \sum_{\alpha=1}^{N} \boldsymbol{e}_\alpha f_\alpha = \sum_{\alpha=1}^{N} \boldsymbol{e}_\alpha f_\alpha^{(eq)}$$

- Chapman-Enskog analysis (multi-scale expansion) $\Rightarrow$

  NS Eqs. recovered in near incompressible flow limit.

- Equation of state: $p = \rho c_s^2 = \rho / 3$

- What are the advantages?
- What are potential benefits comparing with the standard CFD methods for the Navier-Stokes equations?
- Let's look at the actual implementation:

  LBGK scheme.

Lattice Boltzmann Equation

LBGK Scheme: discretization in time & space $\Rightarrow$

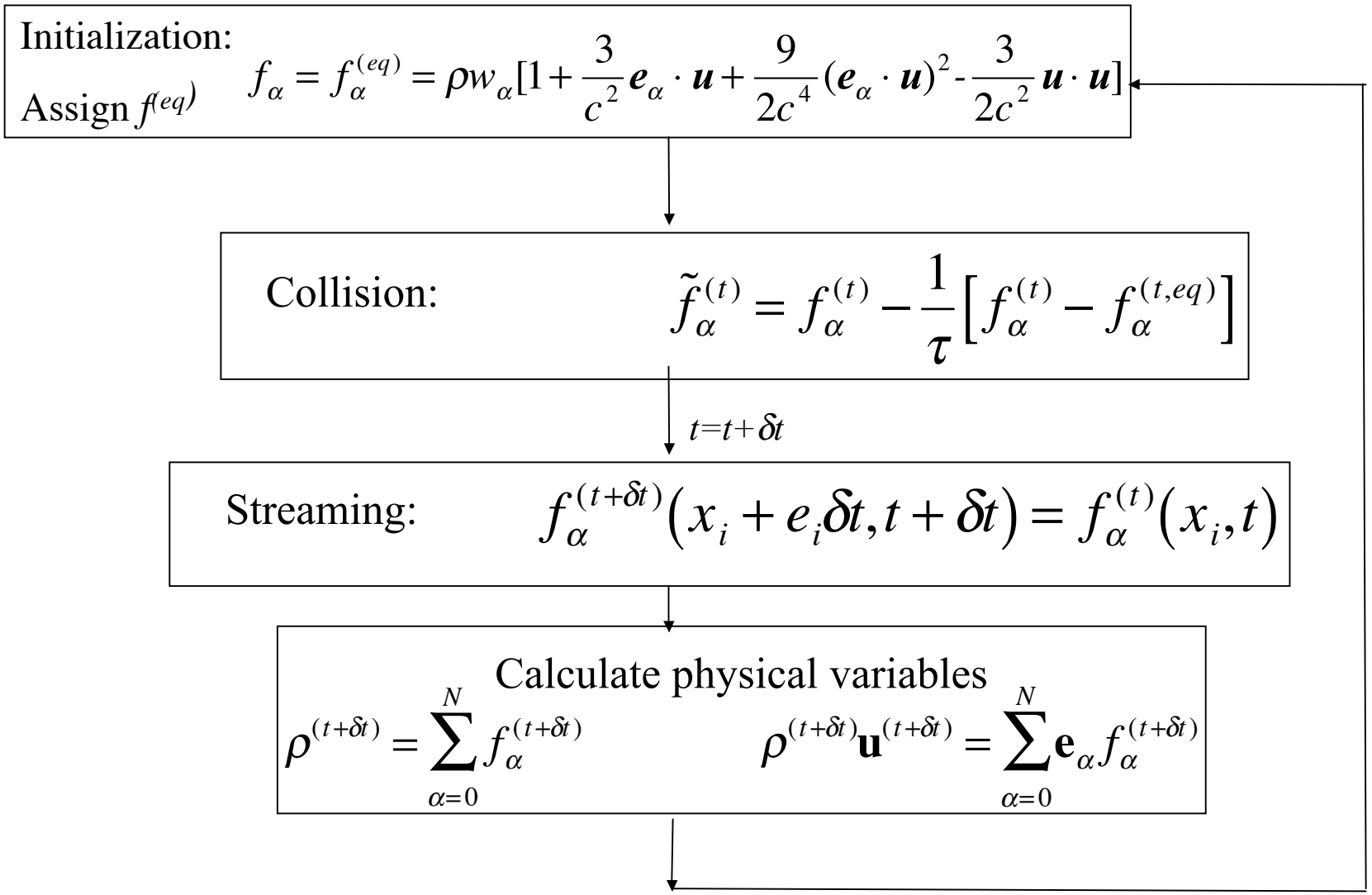
$$f_a(\boldsymbol{x}_i + \boldsymbol{e}_a dt,\ t + dt) - f_a(\boldsymbol{x}_i,\ t) = -\frac{1}{\tau}[f_\alpha(\boldsymbol{x}_i,t) - f_\alpha^{(eq)}(\boldsymbol{x}_i,t)]$$

- Viscosity: $\nu = (\tau\text{-}1/2)\, c_s^2 \delta t$
- Order of accuracy: 2nd in $\boldsymbol{x}$ & 1st in t.
- Computation:

  collision step: $\tilde{f}_\alpha(\boldsymbol{x}_i,\ \mathrm{t}) - f_\alpha(\boldsymbol{x}_i,\ \mathrm{t}) = -\frac{1}{\tau}[f_\alpha(\boldsymbol{x}_i,t) - f_\alpha^{(eq)}(\boldsymbol{x}_i,t)]$

  streaming step: $f_a(\boldsymbol{x}_i + \boldsymbol{e}_a dt,\ t + dt) = \tilde{f}_\alpha(\boldsymbol{x}_i,\ t)$
- **Advantages**:
  - collision step is local; streaming step takes no computation.
  - explicit in form, easy to implement, and natural to parallelize.
  - Pressure is obtained simply as: $p = \rho c_s^2 = \rho/3$

Computational Procedure



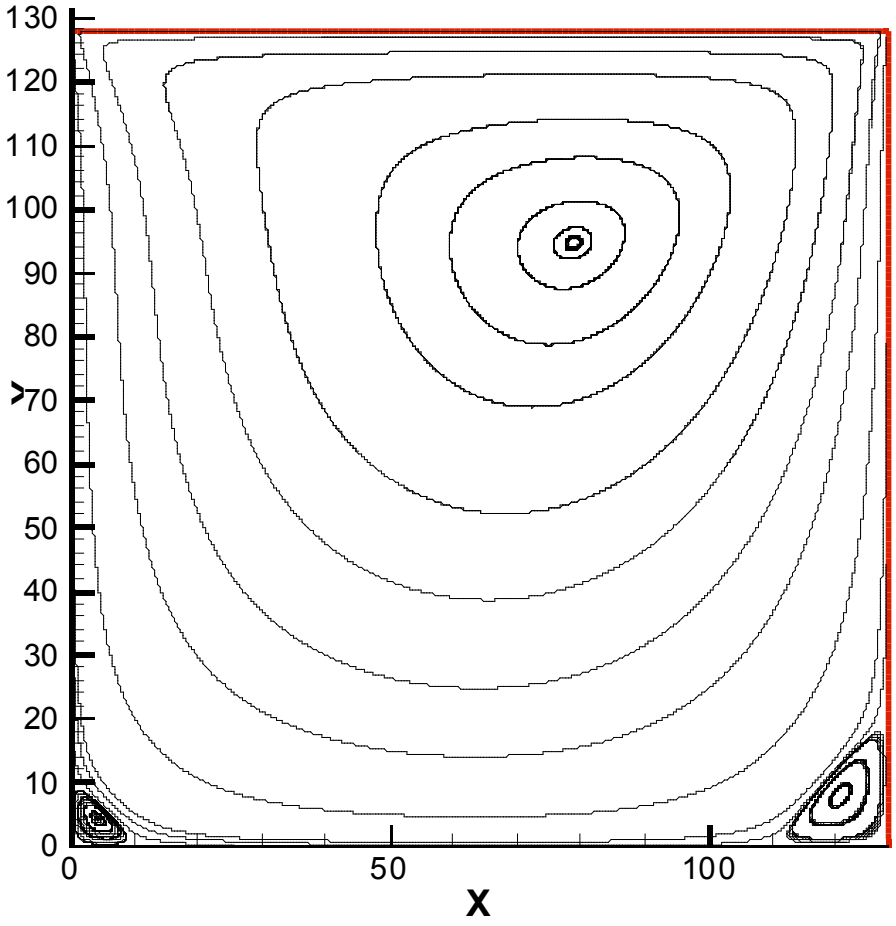
Boltzmann's *H*-theorem

- Generally, macroscopic processes are irreversible.
- The relaxation to a Maxwellian distribution as a result of collisions, is an irreversible process.
- *H*-theorem states that if the distribution function evolves according to the Boltzmann equation, then for a uniform gas in the absence of external forces H can never increase: $\frac{dH}{dt} < 0$ $\qquad H = \int_{-\infty}^{\infty} f \log f dV_c$
- if we begin with a uniform gas having a non-equilibrium distribution function, H decreases until the gas relaxes to the equilibrium distribution when H attains a minimum value

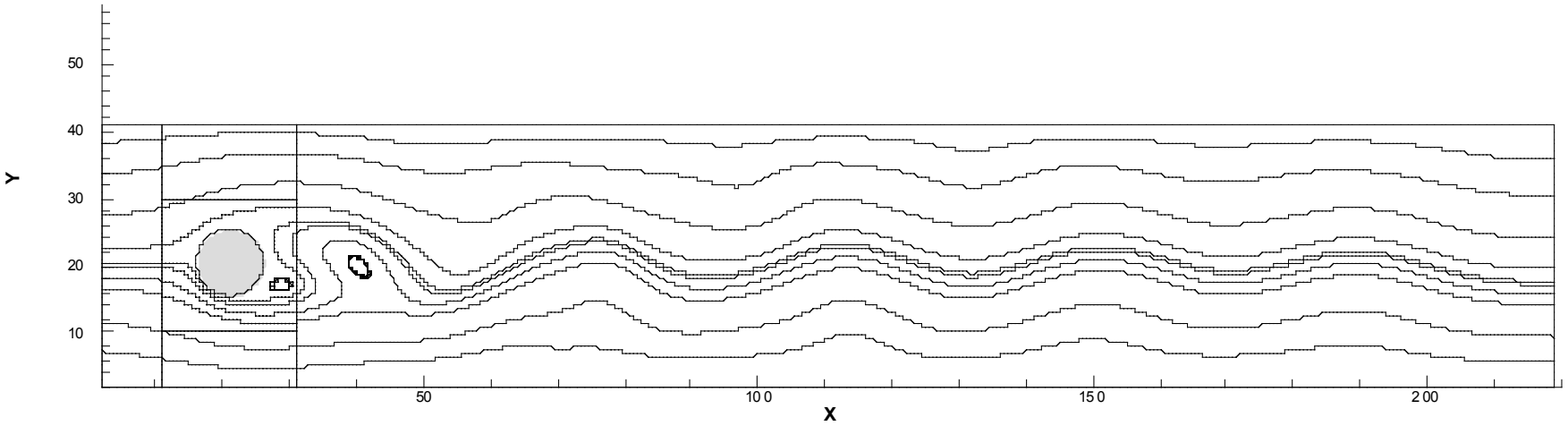
Applications of LBE

- Simulation of incompressible flows
- Fully compressible and thermal flows
- Multi-phase and multi-component flows
- Particulate Suspensions
- Turbulent Flows
- Micro Flows

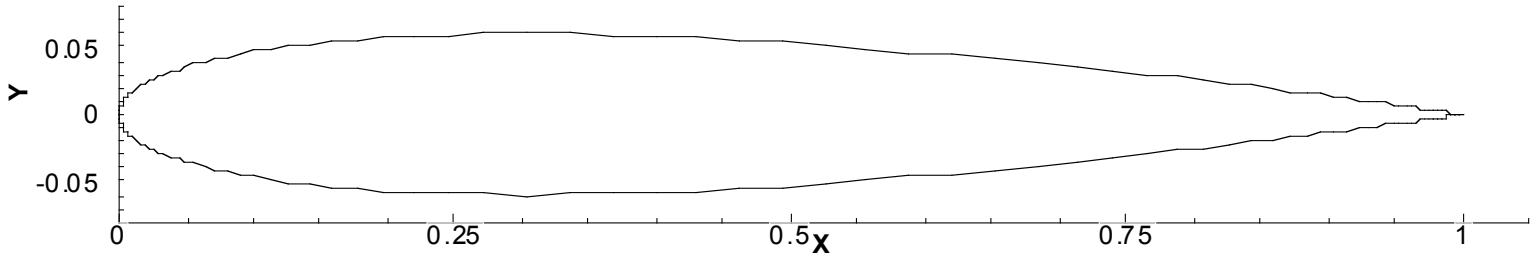
Streamlines in the cavity flow at Re=100



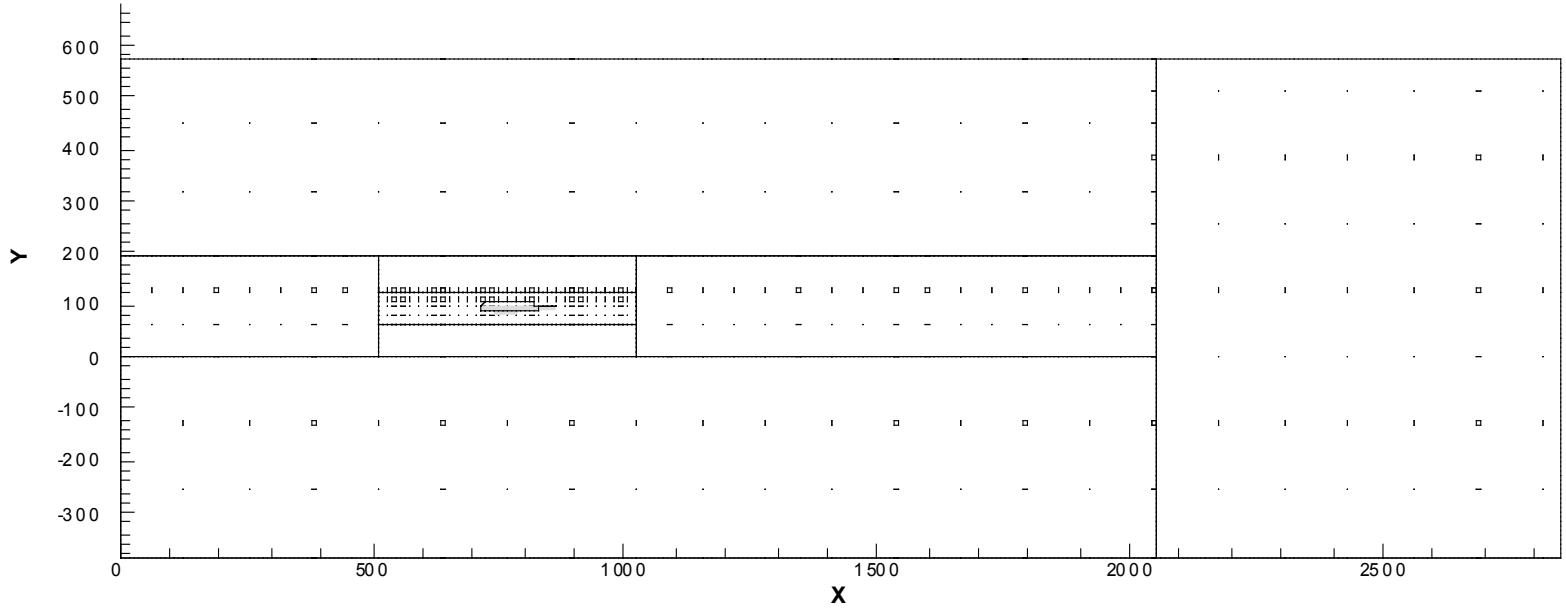
Instantaneous streamlines for channel flow over an asymetrically placed cylinder at Re=100



NACA 0012 airfoil

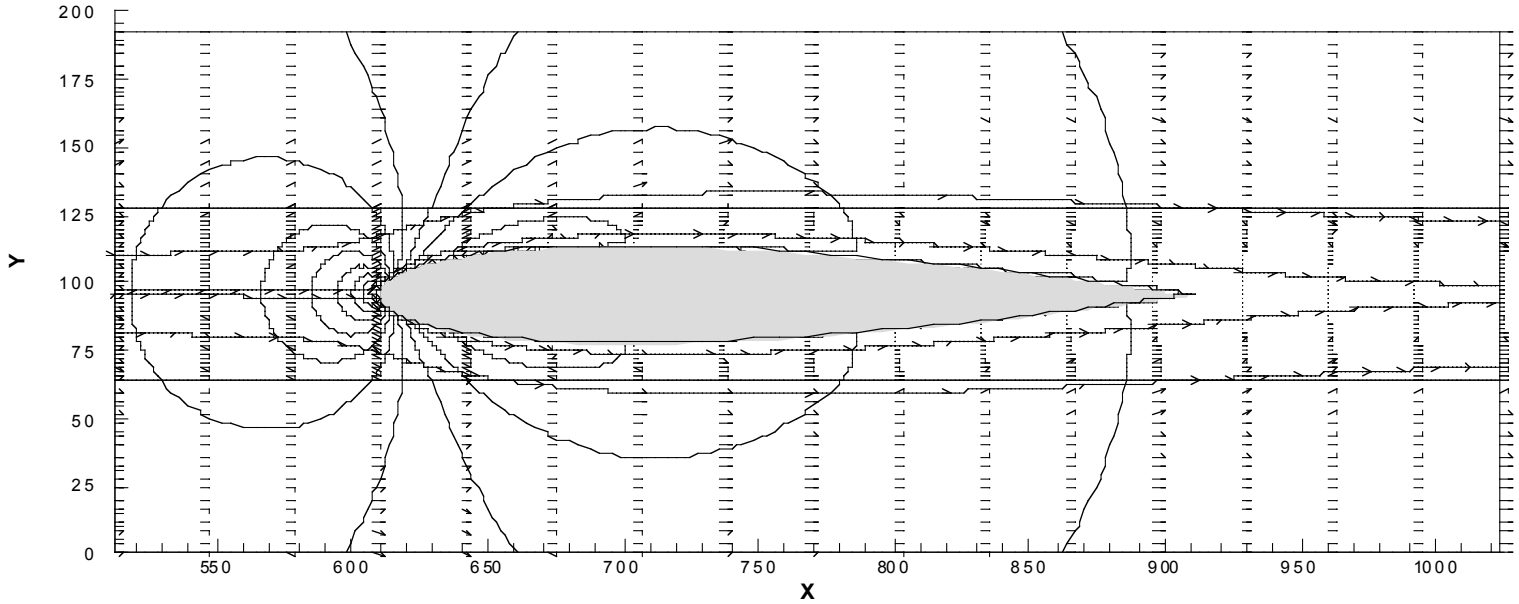


Block and lattice layout for flow over NACA 0012

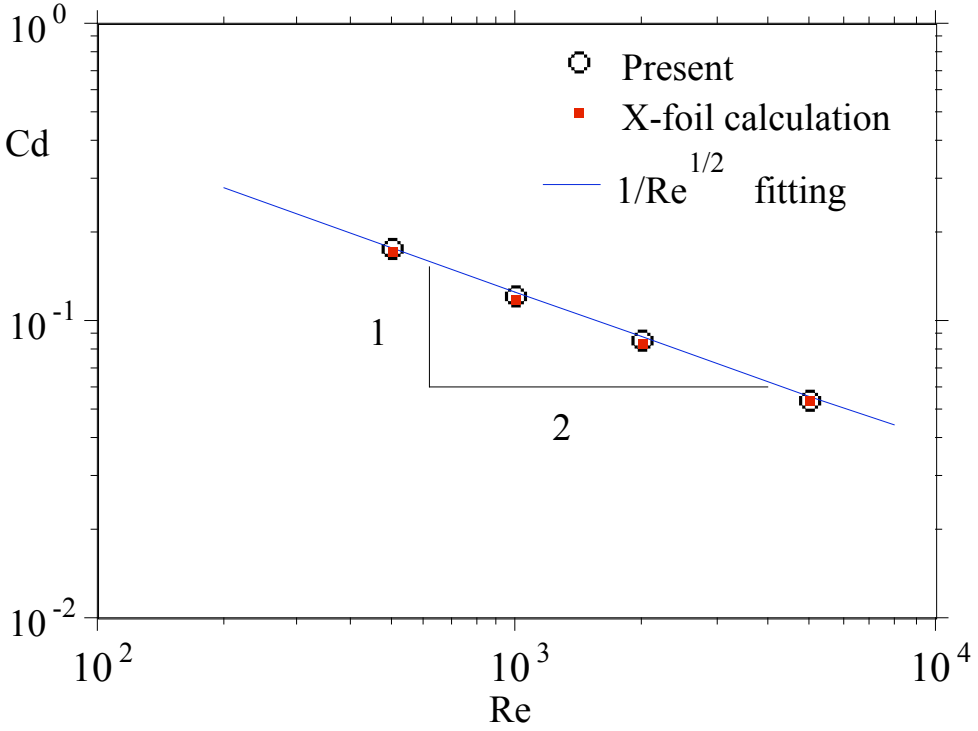


- The lattice spacing is reduced by a factor 32 for graphical clarity

Streamlines, pressure contour, velocity vector for uniform flow over NACA 0012 airfoil at Re=2000.



Comparing *Cd* between present simulation and Xfoil calculation vs. *Re* for NACA0012 flow.



- The straight line is the slope according to the laminar boundary layer theory

Rayleigh-Taylor Instabil

Single mode perturbation

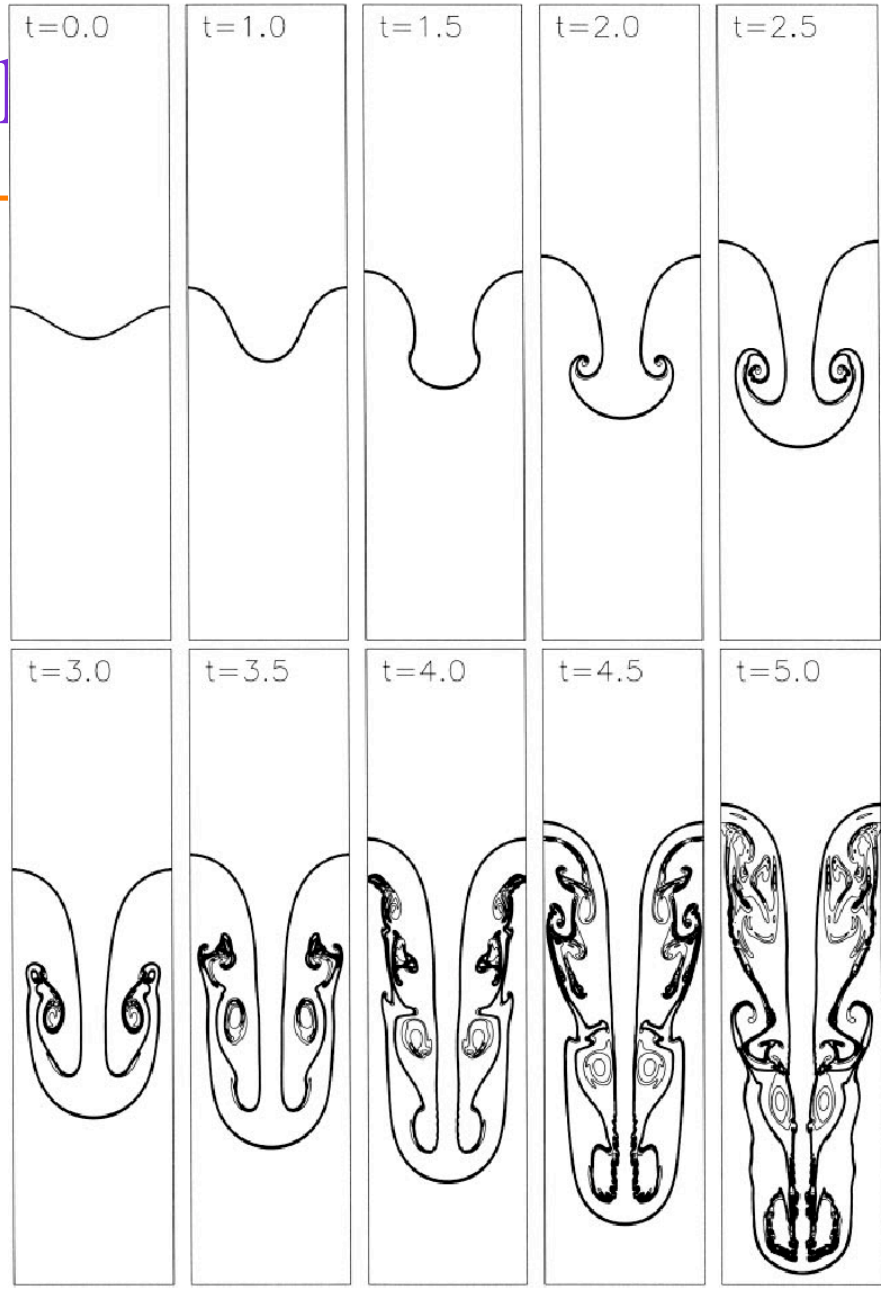
W = channel width

ρ_h= heavy fluid

ρ_l= lighter fluid

$$\mathrm{Re} = \frac{W\sqrt{Wg}}{\nu} = 2048$$

$$A = \frac{\rho_h - \rho_l}{\rho_h + \rho_l} = 0.5$$



Implementation of complex LBE model.

- For complicated problems, new LBE models may need to be designed.
- The number of particle velocities in new models can vary.
- Hybrid modes which incorporate finite different method in LBE need to be considered.

References for LBE

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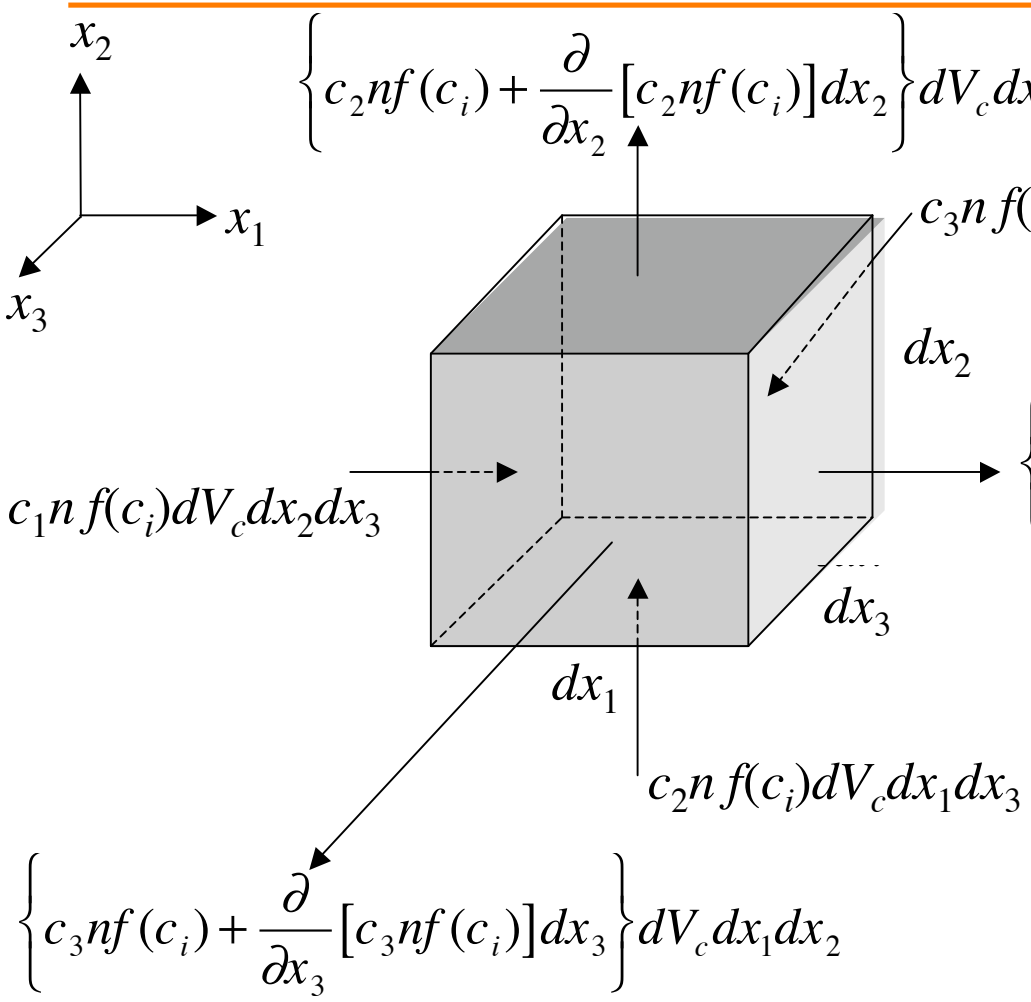
Boltzmann Equation

- Studying molecules (class c_i) inside dV_x, we see total number of molecules whose velocity is between c_i and $c_i + dV_c$ is

  $nf(c_i)\, dV_x\, dV_c$

- Change of number of molecules in class c_i must result from convection of molecules across the surface of dV_c and dV_x or from intermolecular collision within

Number increased by convection thru dV_x



The total number increase by convection through surface of dV_x in unit time is:

$$-c_j \frac{\partial}{\partial x_j}[nf(c_i)]dV_c dV_x$$

c_i is taken out of the differentiation because of it is independent of x_i

Boltzmann Equation

- If there is no external force, the convection of molecules through the surface of dV_c is zero.
- The rate of increase of number of molecules in class c_i results from collision is:

$$\left\{\frac{\partial}{\partial t}[nf(c_i)]\right\}_{collision} dV_c dV_x$$

- The total rate of increase of number of molecules of class c_i is:

$$\frac{\partial}{\partial t}[nf(c_i)]dV_c dV_x$$

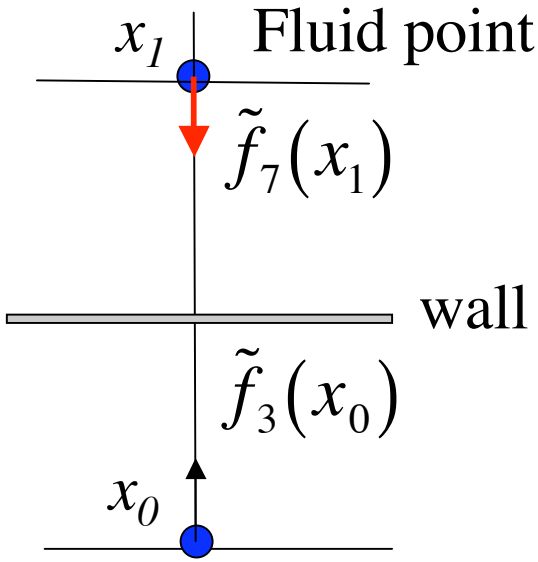
Boltzmann Equation

- The rate of increase of the number of molecules of class c_i in the volume element is equal to the rate of increase by convection through surface of dV_x plus the rate of increase by collision.
- This gives the Boltzmann Equation:

$$\frac{\partial}{\partial t}[nf(c_i)] + c_j \frac{\partial}{\partial x_j}[nf(c_i)] = \left\{\frac{\partial}{\partial t}[nf(c_i)]\right\}_{collision}$$

- How to determine the collision operator?

Solid wall boundary



After collision, set:

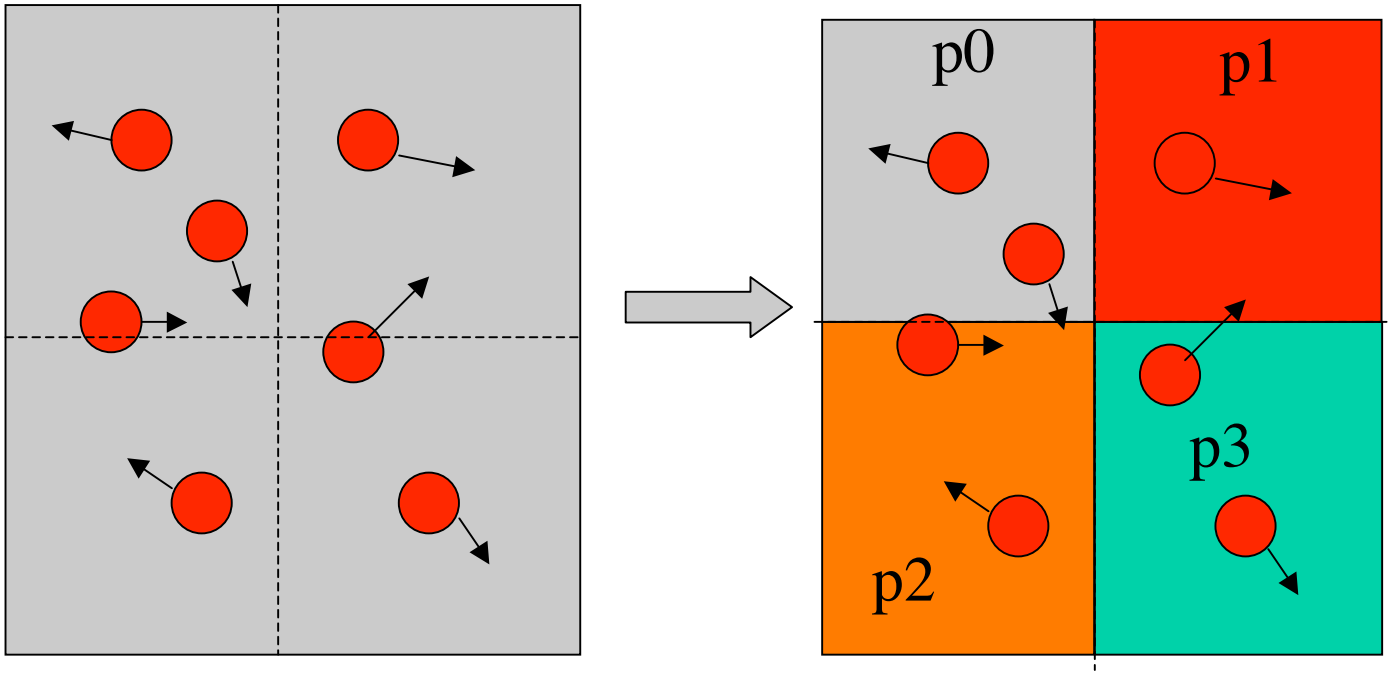
$$\tilde{f}_3(x_0) = \tilde{f}_7(x_1)$$

bounce back idea

If the wall has a velocity ***u***, momentum flux can be added:

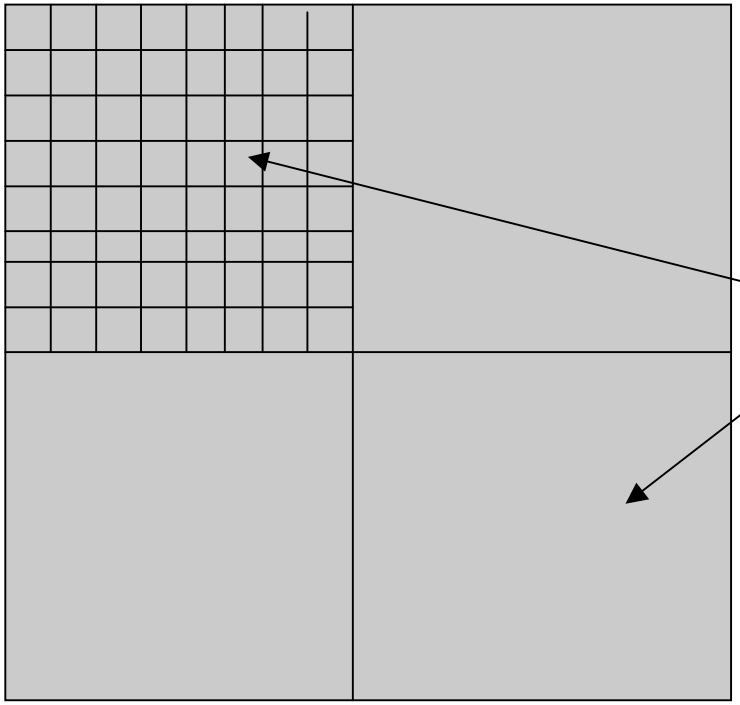
$$\tilde{f}_3(x_0) = \tilde{f}_7(x_1) + 6\rho w_3(\mathbf{e}_3 \cdot \mathbf{u})$$

Implementation in moving boundary problems



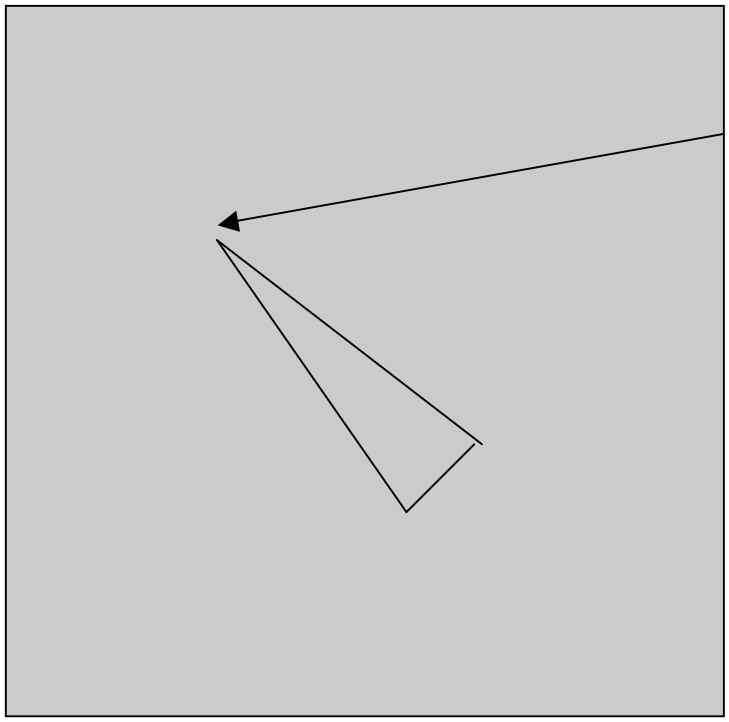
Particles are moving; they may belong to different processors at different time.

Multi-block method in LBE



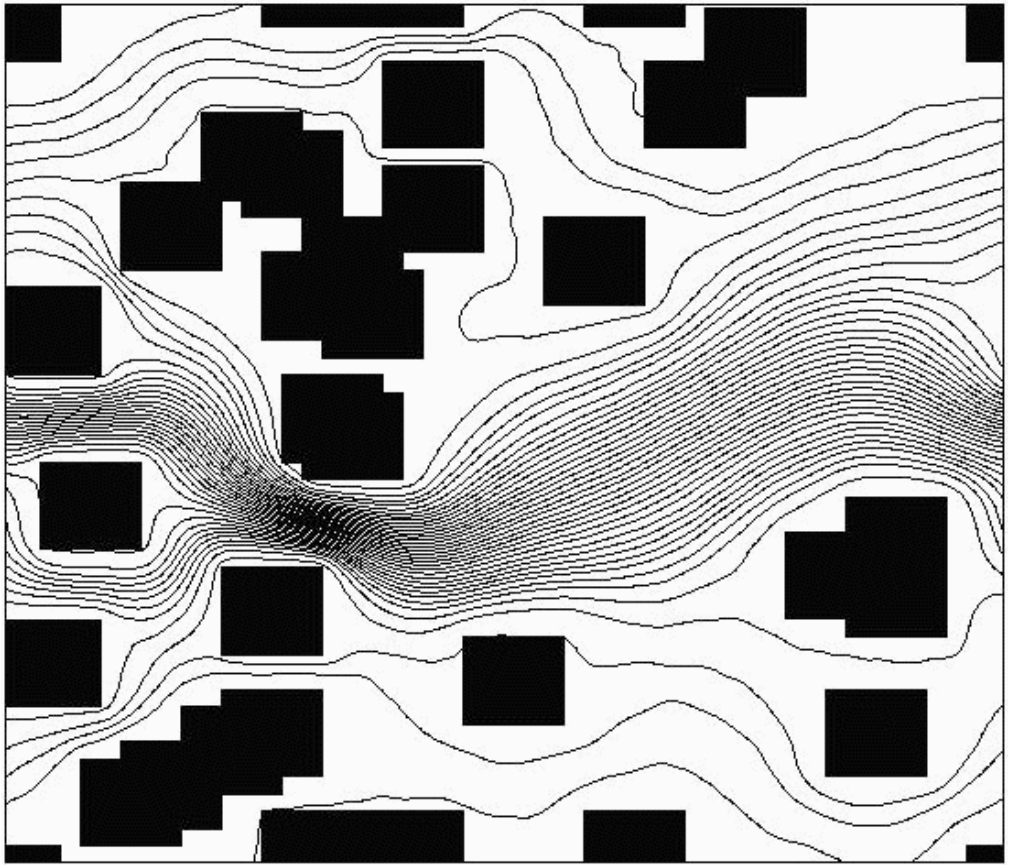
Different grid resolution
in different block.

Implementation of adaptive grid method in LBE



Around the corner, we put fine grids. We may also need to increase grid resolution during computation.

Flows in porous media



In solid region, computation and memory are not required.

Boltzmann's *H* Theorem

- Generally, entropy, S, is defined to be related to the # of possible arrangements of molecules
- In other words, entropy is a function of # of possible micro-states, Ω
- The probability distribution function provides a way of determining the # of possible macro-states,
- Because Ω for combined systems of certain micro-states is a product of each, $\Omega_{AB} = \Omega_A \ \Omega_B$
- And because total entropy is $S_{AB} = S_A + S_B$

$$S = - k \log \Omega = - k \int f \log f \, dV_c,$$

Boltzmann's *H* Theorem

- Differentiating *H*, using Boltzmann's eq., & combining terms:

$$\frac{dH}{dt} = -\frac{1}{4}\iint \left[f(\mathbf{c}')f(\mathbf{z}') - f(\mathbf{c})f(\mathbf{z})\right]\log\frac{f(\mathbf{c})f(\mathbf{z})}{f(\mathbf{c}')f(\mathbf{z}')}|\mathbf{c}-\mathbf{z}|\sigma d\Omega dV_z \le 0$$

- *H* theorem shows why entropy is automatically satisfied if Boltzmann's eq. is satisfied
- Many CFD schemes do not easily guarantee that they will not violate entropy
- Through solving BE,
  - entropy is inherently & automatically satisfied and
  - fluid field is found from *f* rather than using *f* to find properties to use in Navier-Stokes eqs. derived from BE