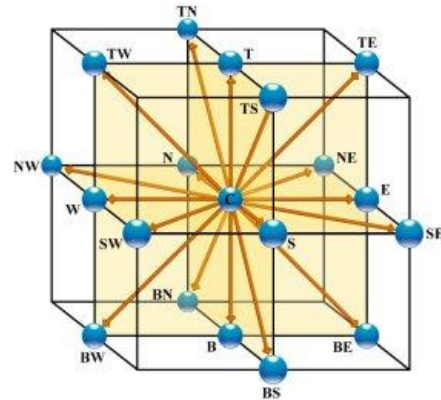
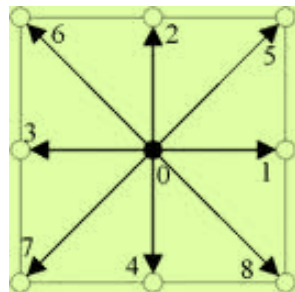
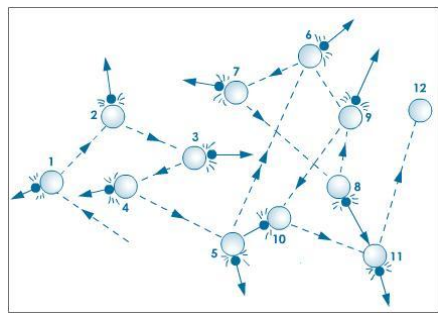


Mesoscopic models and Lattice Boltzmann simulation

Background, ideas, applications

Alexei Heintz

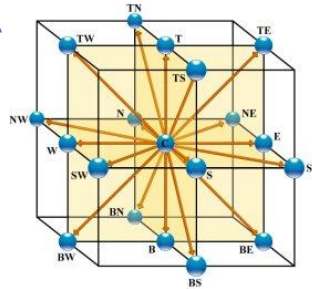




Microscopic picture:

$$(t, \mathbf{x}_k, \mathbf{c}_k)$$

-coordinates and velocities of all particles, cars, cells, rabbits...



Mesoscopic picture:

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

- "number" of particles with velocities \mathbf{c} and positions \mathbf{x}



Macroscopic picture:

average velocity field $\mathbf{v}(t, \mathbf{x})$
or density field
depending on position \mathbf{x}

Systems of ODE - ordinary differential equations
Direct simulation methods
Monte Carlo methods

Boltzmann equation
Lattice – Boltzmann equation
neutron transport

Navier - Stokes equation
diffusion equation
Shallow water equation

Plan

Part 1. Kinetic theory

Macroscopic, microscopic, mesoscopic paradigms.

Distribution function, macroscopic parameters, moments.

Collisionless transport without forces, with forces

Collisions: Boltzmann equation, conservation laws,

Equilibrium, entropy

BGK model.

Transport equations: integrate the kinetic equation.

Non closed macroscopic description.

Euler equation, diffusion equation, Navier Stokes equation.

Transport coefficients: viscosity and diffusion coefficient.

Part 2. Lattice Boltzmann model and simulation

Discrete velocity space. Lattice Boltzmann model.

Various grids. Symmetry requirements. Equilibrium distribution.

Lattice Boltzmann algorithm: advection, relaxation.

Boundary conditions. Neumann, Robin, slip boundary conditions.

Parallel computations.

Discrete viscosity and diffusion coefficients

Multy-phase flows. Shan Chen model. Free energy based models.

Examples

Distribution function

Information is required not only about the spatial distribution of molecules but about their velocities as well.

velocity distribution function, $f(\mathbf{r}, \mathbf{c}, t)$

$f(\mathbf{r}, \mathbf{c}, t)d^3r d^3c$ is the *expected* number of molecules in the volume element d^3r located at \mathbf{r} , whose velocities lie in d^3c about velocity \mathbf{c}

Distribution function and macroscopic parameters

$$n(\mathbf{r}, t) = \int f(\mathbf{r}, \mathbf{c}, t) d^3c. \quad - \text{concentration}$$

$$\rho(\mathbf{r}, t) = mn(\mathbf{r}, t). \quad - \text{density}$$

$$\mathbf{v}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \int m\mathbf{c} f(\mathbf{r}, \mathbf{c}, t) d^3c. \quad - \text{velocity}$$

$$\mathbf{C} = \mathbf{c} - \mathbf{v} \quad - \text{peculiar velocity}$$

$$u(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \int \frac{1}{2}mC^2 f(\mathbf{r}, \mathbf{c}, t) d^3c, \quad - \text{energy}$$

Distribution function and fluxes



Cylinder containing all molecules with peculiar velocity \mathbf{C} which cross the surface element d^2S during the time interval dt .

Distribution function and fluxes

$$P_{\alpha\beta} = m \int C_{\alpha} C_{\beta} f d^3c, \quad \text{- pressure tensor}$$

$$P_{\alpha\alpha} \quad \text{- normal stresses}$$

$$P_{\alpha\beta} \quad \text{- shear stresses – force per unit area in } \alpha\text{- direction exerted on a plane surface with normal in } \beta\text{- direction}$$

$$p = \frac{1}{3} \rho \overline{C^2} = \frac{1}{3} \mathbf{P} : \mathbf{I}. \quad \text{- hydrostatic pressure}$$

$$\mathbf{q} = \frac{1}{2} m \int C^2 f \mathbf{C} d^3c = \frac{1}{2} n m \overline{C^2} \mathbf{C}.$$

- heat flow vector

Transport in absence of collisions

$$f_i(\mathbf{r}, \mathbf{c}_i, t) d^3 r d^3 c_i :$$

$$f_i(\mathbf{r} + \mathbf{c}_i dt, \mathbf{c}_i + \mathbf{F}_i dt, t + dt) d^3 r' d^3 c'_i$$

$$f_i(\mathbf{r} + \mathbf{c}_i dt, \mathbf{c}_i + \mathbf{F}_i dt, t + dt) d^3 r d^3 c_i .$$

$$f_i(\mathbf{r} + \mathbf{c}_i dt, \mathbf{c}_i + \mathbf{F}_i dt, t + dt) = f_i(\mathbf{r}, \mathbf{c}_i, t).$$



The Boltzmann kinetic equation

(1844-1906)

$$f_i(\mathbf{r} + \mathbf{c}_i dt, \mathbf{c}_i + \mathbf{F}_i dt, t + dt) = f_i(\mathbf{r}, \mathbf{c}_i, t) + \left(\frac{\partial f_i}{\partial t} \right)_{\text{coll}} dt$$
$$\left(\frac{\partial f_i}{\partial t} \right)_{\text{coll}} dt = (\Gamma_i^+ - \Gamma_i^-) dt.$$

$$\left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} + \mathbf{F}_i \cdot \nabla_{\mathbf{c}_i} \right) f_i(\mathbf{r}, \mathbf{c}_i, t) = \frac{1}{Kn} (\Gamma_i^+ - \Gamma_i^-)$$

The Knudsen number Kn shows the relation between the collision frequency and the typical macroscopic time scale. In the limit of $Kn \rightarrow 0$ one observes the macroscopic behavior.

The Boltzmann collision operator (terrible formulas!)

$$\Gamma^+(\mathbf{v}) = \int_{\mathbb{R}^3} \int_{S^2} B(|\mathbf{u}|, \theta) f\left(\mathbf{v} - \frac{1}{2}(\mathbf{u} - |\mathbf{u}|\omega)\right) f\left(\mathbf{v} - \frac{1}{2}(\mathbf{u} + |\mathbf{u}|\omega)\right) d\omega d\mathbf{u}$$

$$\Gamma^-(\mathbf{v}) = f(\mathbf{v}) q^-(f)(\mathbf{v})$$

with q^- denoting the *collision frequency* term

$$q^-(f)(\mathbf{v}) = \int_{\mathbb{R}^3} f(\mathbf{v} - \mathbf{u}) \int_{S^2} B(|\mathbf{u}|, \theta) d\omega d\mathbf{u}.$$

The function $B(|\mathbf{u}|, \theta)$ is of the form

$$B(|\mathbf{u}|, \theta) = B_0 \left(|\mathbf{u}|, \frac{|(\mathbf{u}, \omega)|}{|\mathbf{u}|} \right), \mathbf{u} \in \mathbb{R}^3, \omega \in S^2, S^2 = \{\mathbf{q} \in \mathbb{R}^3 : |\mathbf{q}| = 1\}.$$

It contains the information about the binary interactions of particles

For the gas of “hard sphere” molecules $B(|\mathbf{v} - \mathbf{w}|, \theta) = C_\alpha |\mathbf{v} - \mathbf{w}|^\alpha$

Collision invariants

Collision invariants are functions $\psi(\mathbf{c})$ of particles velocities that are preserved during collisions.

Typical examples are:

mass m , momentum $m\mathbf{c}$, and kinetic energy $\frac{1}{2}m\mathbf{c}^2$.

These *conservation laws* are expressed as:

$$\int \psi(\mathbf{c}) \left(\frac{\partial f}{\partial t} \right)_{coll} d\mathbf{c} = 0$$

or
$$\int \psi(\mathbf{c}) (\Gamma^+ - \Gamma^-) d\mathbf{c} = 0$$

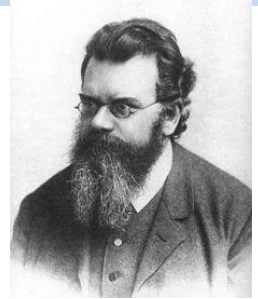
Collision invariants: why these?

$$\begin{aligned} & (\Gamma^+ - \Gamma^-) (\mathbf{c}) = \\ & \int_{\mathbf{R}^3} d\mathbf{c}_1 \int_{S^2} d\omega B(|\mathbf{c} - \mathbf{c}_1|, \theta) [f(\mathbf{c})f(\mathbf{c}_1) - f(\mathbf{c}')f(\mathbf{c}'_1)] \\ & \int \psi(\mathbf{c}) (\Gamma^+ - \Gamma^-) d\mathbf{c} = \\ & \frac{1}{4} \int_{\mathbf{R}^3} d\mathbf{c} \int_{\mathbf{R}^3} d\mathbf{c}_1 \int_{S^2} d\omega B(|\mathbf{c} - \mathbf{c}_1|, \theta) \times \\ & [f(\mathbf{c})f(\mathbf{c}_1) - f(\mathbf{c}')f(\mathbf{c}'_1)] [\psi(\mathbf{c}) + \psi(\mathbf{c}_1) - \psi(\mathbf{c}') + \psi(\mathbf{c}'_1)] \\ & \int \psi(\mathbf{c}) (\Gamma^+ - \Gamma^-) d\mathbf{c} = 0 \end{aligned}$$

Maxwell – Boltzmann equilibrium distribution



$$f^{eq}(t, \mathbf{x}, \mathbf{c}) = \frac{n}{(2\pi T)^{3/2}} \exp \left[\frac{|(\mathbf{c} - \mathbf{v})|^2}{2T} \right]$$



$$n = n(t, \mathbf{x}), \mathbf{v} = \mathbf{v}(t, \mathbf{x}), T = T(t, \mathbf{x})$$

has two important properties: it does not change under collisions

$$\left(\frac{\partial f^{eq}}{\partial t} \right)_{coll} = \Gamma^+(f^{eq}) - \Gamma^-(f^{eq}) = 0$$

It minimizes the H- function $H = \int f \ln f$

for fixed macroscopic velocity, temperature and concentration.

Functional $-\int \int f \ln f d\mathbf{c} d\mathbf{x}$ is called entropy

Macroscopic equations

To see how macro-parameters depend on time and position we use *conservation laws* corresponding to our system.

We multiply the kinetic equation

$$\left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} + \mathbf{F}_i \cdot \nabla_{\mathbf{c}_i} \right) f_i(\mathbf{r}, \mathbf{c}_i, t) = \frac{1}{Kn} (\Gamma_i^+ - \Gamma_i^-)$$

by collision invariants $\psi(\mathbf{c})$ and integrate it over velocities.

Such an operation is called scalar product of functions in analysis.

The integral over collision operator disappears and the rest gives us macroscopic equations.

One says that the collision operator is *orthogonal* to collision invariants.

Macroscopic equations

When $\psi = m$, we obtain the conservation equation for mass,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0.$$

When $\psi = mc$, we obtain the conservation equation for momentum,

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\mathbf{P} + \rho \mathbf{v} \mathbf{v}) = \sum_i \rho_i \mathbf{F}_i \quad (4)$$

Finally, when $\psi = \frac{1}{2}mc^2$ we obtain the conservation equation for kinetic energy,

$$\frac{\partial}{\partial t} \rho(u + \frac{1}{2}v^2) + \nabla \cdot \{ \mathbf{q} + \rho(u + \frac{1}{2}v^2)\mathbf{v} + \mathbf{P} \cdot \mathbf{v} \} = \sum_i \rho_i \mathbf{F}_i \cdot (\mathbf{v} + \mathbf{V}_i) \quad (4.1-26)$$

Macroscopic equations

$$\frac{1}{\rho} \frac{d\rho}{dt} = -\nabla \cdot \mathbf{v},$$

$$\rho \frac{d\mathbf{v}}{dt} = \rho \mathbf{F} - \nabla \cdot \mathbf{P},$$

$$\rho \frac{du}{dt} = -(\nabla \cdot \mathbf{q} + \mathbf{P} : \nabla \mathbf{v}).$$

concept of *substantial derivative*,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla,$$

Closure problem:

Fluxes in the macroscopic equations:
pressure (stress) tensor, mass flux vector,
heat flux etc. depend on the
unknown distribution function.

*How to find macroscopic fluxes
corresponding to kinetic models?
(and vice versa...)*

BGK model

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla_x f = \frac{1}{Kn} [f^{eq} - f]$$

$$f^{eq}(t, \mathbf{x}, \mathbf{c}) = \frac{n}{(2\pi T)^{3/2}} \exp \left[-\frac{|\mathbf{c} - \mathbf{v}|^2}{2T} \right]$$

$$n = n(t, \mathbf{x}), \mathbf{v} = \mathbf{v}(t, \mathbf{x}), T = T(t, \mathbf{x})$$

BGK model keeps most of formal properties of the Boltzmann equation: the same collision invariants, the same equilibrium, H – theorem, but has much simpler structure. Knudsen number Kn shows the relation between collision frequency and the typical macroscopic time scale.

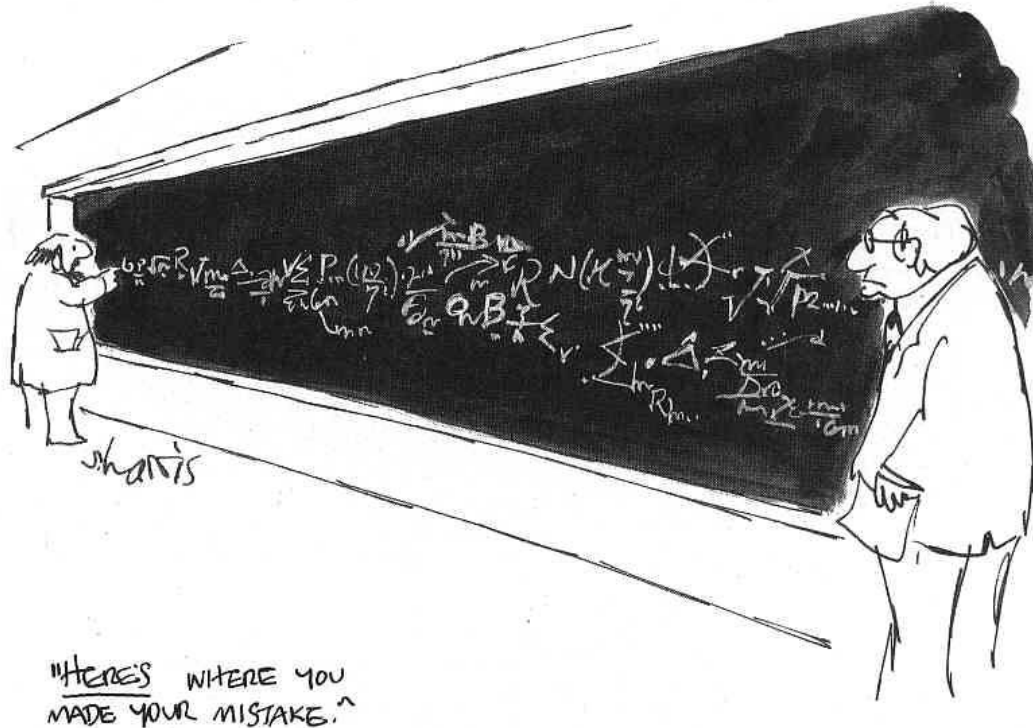
In the limit of $Kn \rightarrow 0$ one observes the macroscopic behavior.

Chapman - Enskog method and method of diffusive scaling (...hard calculations!)



David Enskog
(1917, 1922)

Sydney Chapman
(1916, 1918)



Transport coefficients:

The Chapman-Enskog theory shows that in the limit of $\text{Kn} \rightarrow 0$ density, velocity and temperature:

$$\rho = \rho(x, t), \quad \mathbf{v} = \mathbf{v}(t, \mathbf{x}), \quad T = T(t, \mathbf{x})$$

satisfy up to the second order in Kn number, $\text{Kn} \rightarrow 0$ classical macroscopic equations - Navier Stokes equations for compressible viscous gas.

It is remarkable that this conclusion is valid both for the full Boltzmann equation and for the simplified BGK equation.

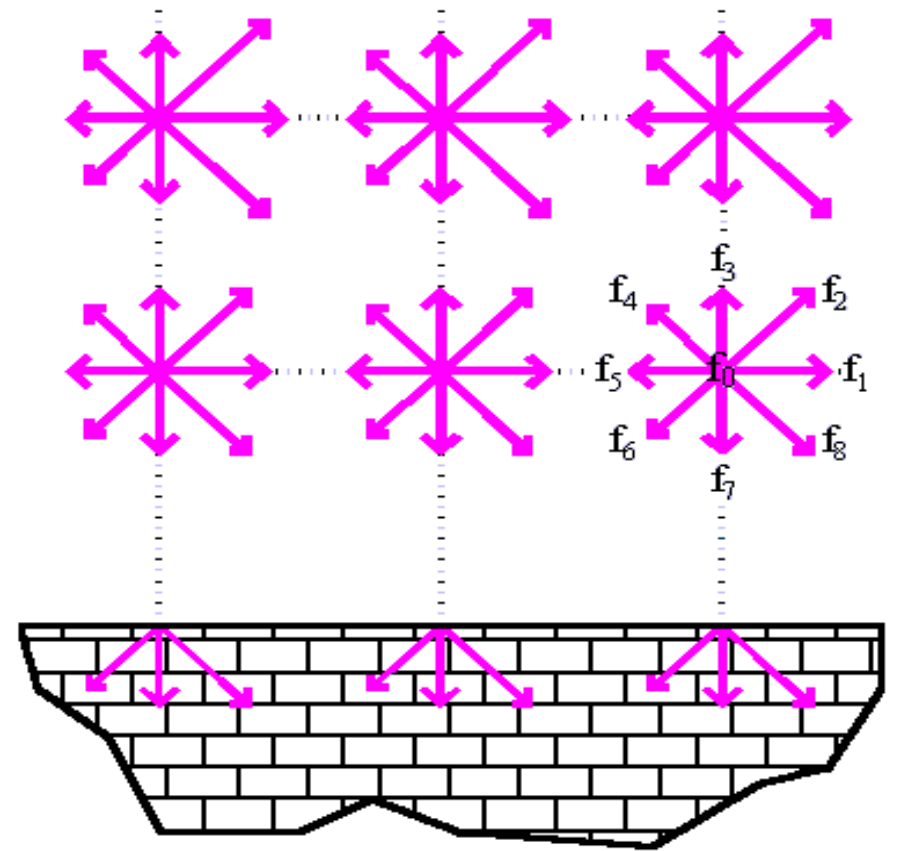
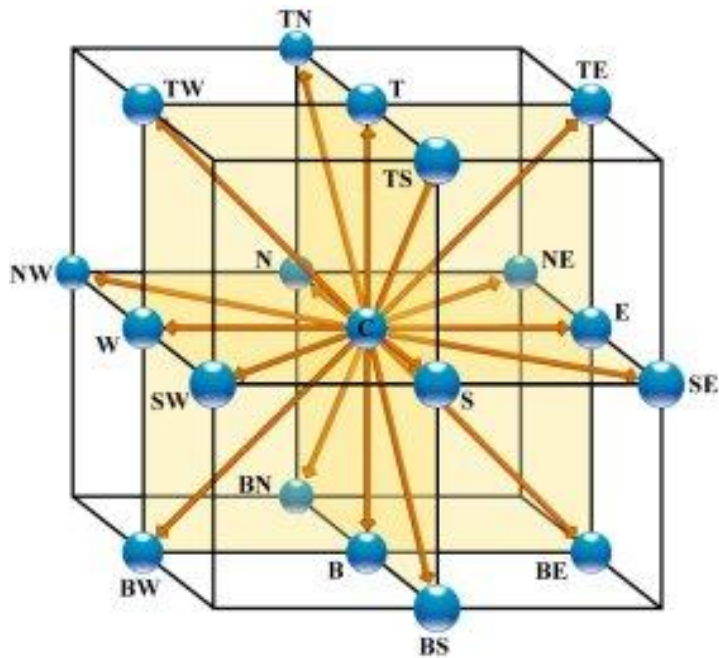
Viscosity, heat conduction and diffusion coefficients of real gases are rather complicated functionals of particular collision models (intermolecular potentials). The theory becomes even more complicated for mixtures of gases.

Lattice Boltzmann equation

A kind of artificial particles with a small number N of possible velocities c_i with $i = 0, 1, 2, \dots, N$ are used to describe the state of the fluid. The state of the fluid in the point x at time t is described by a distribution function as $f_i(x, t)$ that gives the density of "particles" of each type with velocity c_i in point x at time t .

Macroscopic variables for flow - density (pressure) $\rho(x, t)$ and velocity $v(x, t)$ are calculated in a natural way as the averages of $f_i(x, t)$:

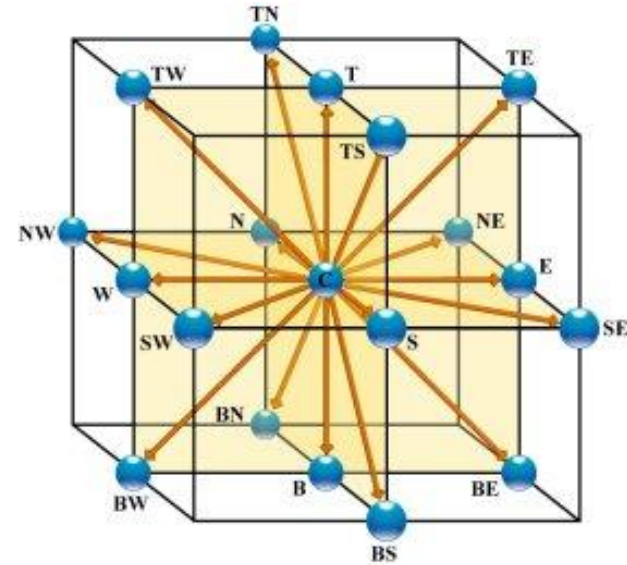
*Distribution function $f_i(x, t)$
for discrete velocity space:*



Macroscopic variables - density $\rho(x, t)$, velocity $v(x, t)$ are calculated in a natural way as the averages of $f_i(x, t)$:

$$\rho(x, t) = \sum_i f_i(x, t)$$

$$v(x, t) = \left(\frac{\mathbf{1}}{\rho(x, t)} \right) \sum_i \mathbf{c}_i f_i(x, t)$$



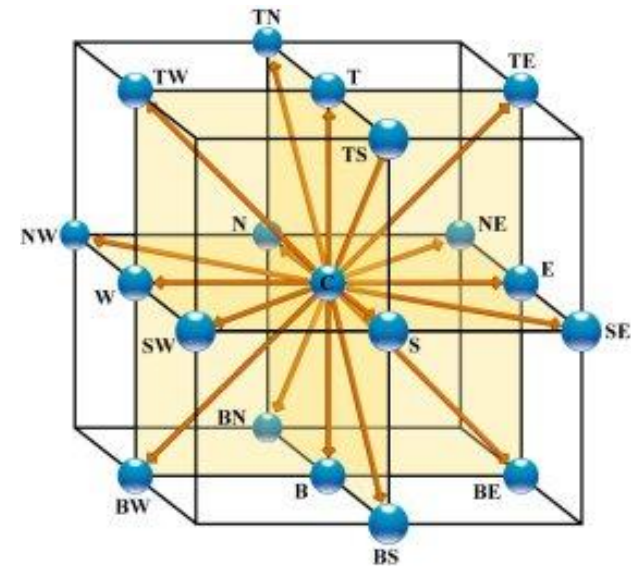
Similarly the stress tensor is calculated:

$$\mathbf{P}_{\alpha\beta}(x, t) = \sum_i (\mathbf{c}_{i,\alpha} - \mathbf{v}_\alpha) (\mathbf{c}_{i,\beta} - \mathbf{v}_\beta) f_i(x, t)$$

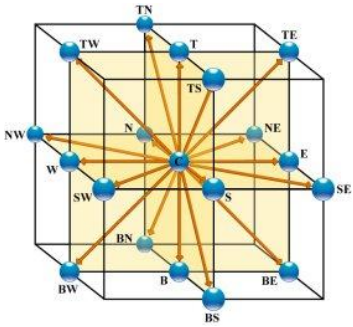
Macroscopic variables for diffusion - density $\rho(x, t)$ and flux $u(x, t)$ are calculated in a natural way as the averages of $f_i(x, t)$:

$$\rho(x, t) = \sum_i f_i(x, t)$$

$$u(x, t) = \sum_i \mathbf{c}_i f_i(x, t)$$



Lattice Boltzmann equation

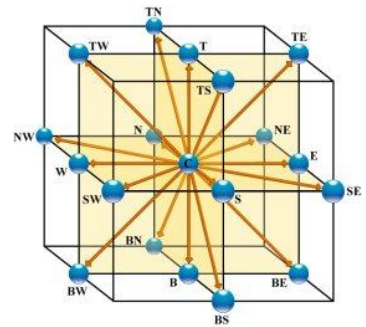


The Lattice-Boltzmann equation describes changes in $f_i(x, t)$ after a time step Δt :

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

The equilibrium distribution $f_i^{eq}(x, t)$ depends only on macroscopic variables density $\rho(x, t)$ and velocity $v(x, t)$ and is a polynomial of \mathbf{c}_i vectors.

Many macroscopic models
can be simulated by
the Lattice Boltzmann equation
by choosing a appropriate
equilibrium distribution

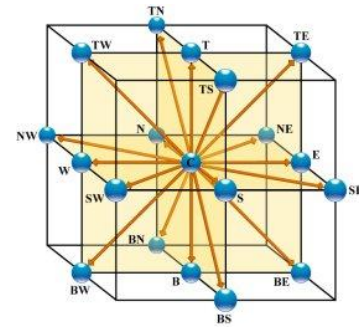


In the case of flow the equilibrium distribution $f_i^{eq}(x, t)$ looks as

$$f_i^{eq}(x, t) = \omega_i \left[\rho + \left(3v \cdot \mathbf{c}_i + \frac{9}{2} (v \cdot \mathbf{c}_i)^2 - \frac{3}{2} |v|^2 \right) \right]$$

Weights ω_i are some fixed numbers such that $\sum_i \omega_i = 1$ and the fluid with distribution f_i^{eq} has

density ρ and velocity v that are used in the expression for f_i^{eq} .



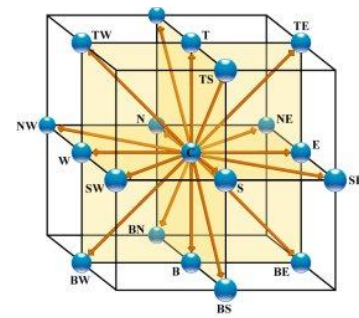
Lattice Boltzmann for advection – diffusion

In the case of diffusion of a solute in a moving solvent the equilibrium distribution $f_i^{eq}(x, t)$ looks as

$$f_i^{eq}(x, t) = \omega_i \rho [1 + (3v \cdot c_i)]$$

and the solute with distribution f_i^{eq} has density ρ .

Velocity v in the expression for f_i^{eq} is the solvent velocity.

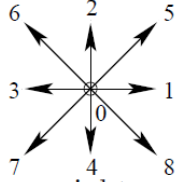


Equilibrium distribution is given by:

$$f_i^0 = nw_i \left[1 + \frac{3}{c^2} \mathbf{u} \cdot \mathbf{v}_i + \frac{9}{2c^4} (\mathbf{u} \cdot \mathbf{v}_i)^2 - \frac{3}{2c^2} \mathbf{u} \cdot \mathbf{u} \right]. \quad ($$

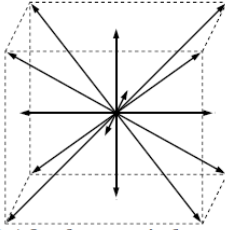
The weights w_i depend on the set of velocities. The values for commonly used models are below.

For D2Q9 we have



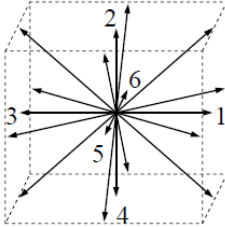
$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1, 2, 3, 4 \\ 1/36 & i = 5, 6, 7, 8 \end{cases}$$

For D3Q15 the weights are:



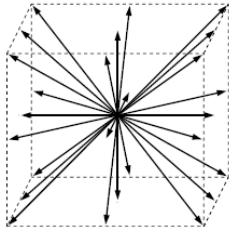
$$w_i = \begin{cases} 2/9 & i = 0 \\ 1/9 & i = 1 - 6 \\ 1/72 & i = 7 - 14 \end{cases}$$

For D3Q19 the weights are:



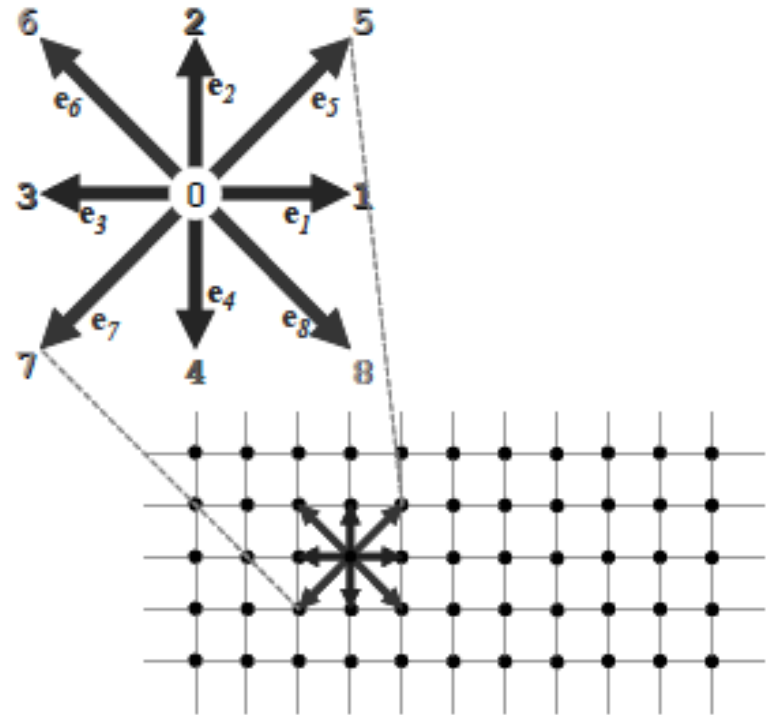
$$w_i = \begin{cases} 1/3 & i = 0 \\ 1/18 & i = 1 - 6 \\ 1/36 & i = 7 - 18 \end{cases}$$

For D3Q27 the weights are:



$$w_i = \begin{cases} 8/27 & i = 0 \\ 2/27 & i = 1 - 6 \\ 1/216 & i = 7 - 14 \\ 1/54 & i = 15 - 26 \end{cases}$$

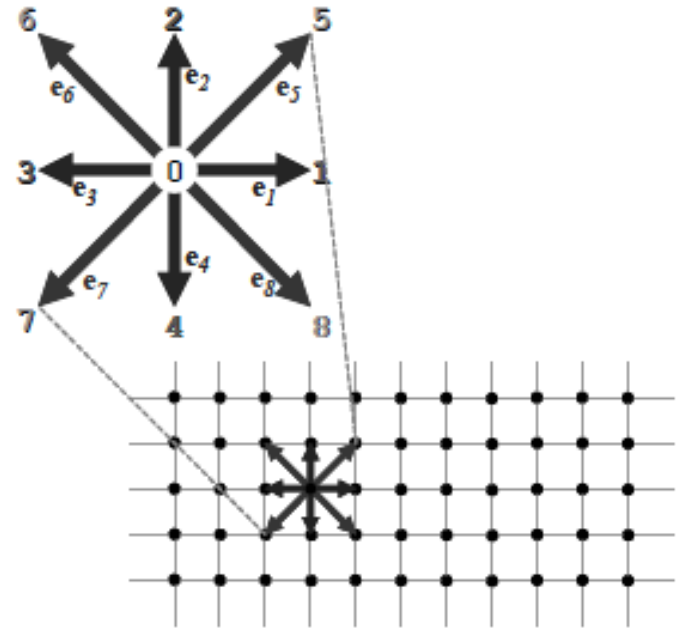
Lattice- Boltzmann algorithm: -transport



1. Transport of "particles" or shift of data along velocities e_i - independently for each "trajectory" $r = x + \mathbf{c}_i l$:

$$\hat{f}_i(x + \mathbf{c}_i \Delta t, t + \Delta t) := f_i(x, t)$$

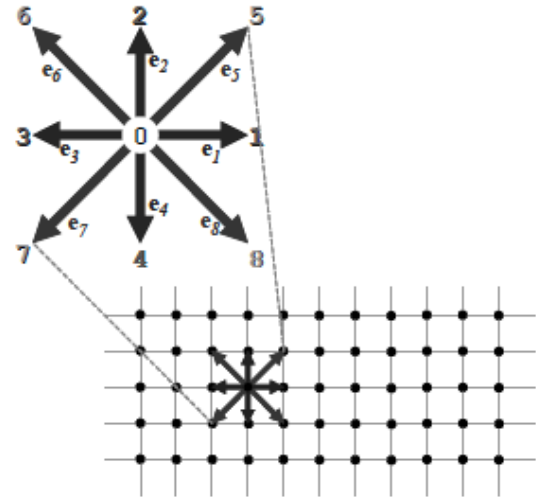
Lattice- Boltzmann algorithm: -macroparameters



2. New density $\rho(x, t + \Delta t) = \sum_i \hat{f}_i(x, t + \Delta t),$

velocity $v(x, t) = \left(\frac{1}{\rho(x, t + \Delta t)} \right) \sum_i \mathbf{c}_i \hat{f}_i(x, t + \Delta t) ,$

Lattice- Boltzmann algorithm: -relaxation



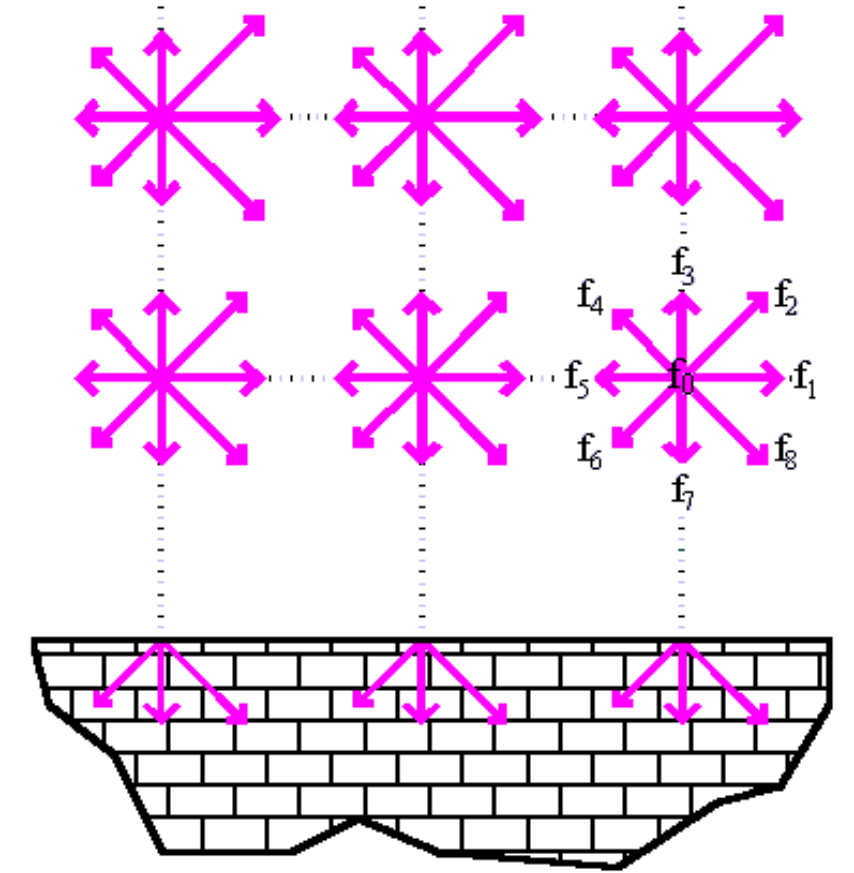
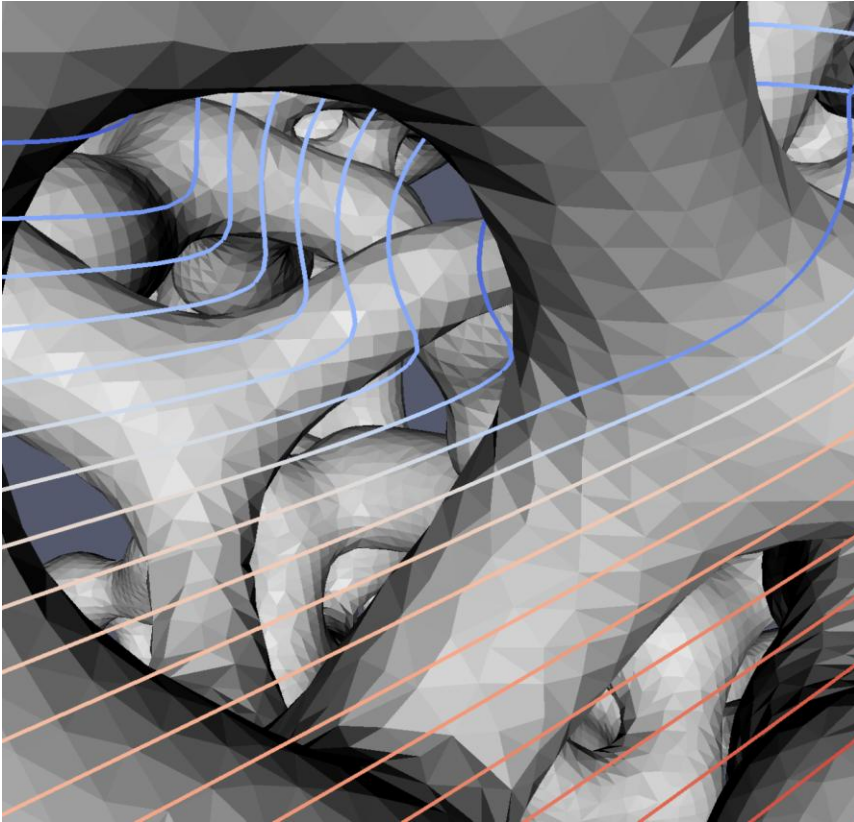
3. Relaxation and possibly applying forcing terms g_i - independently in each node x :

$$f_i(x, t + \Delta t) := \hat{f}_i(x, t + \Delta t) +$$

$$\frac{1}{\tau} \left[f_i^{eq}(x, t + \Delta t) - \hat{f}_i(x, t + \Delta t) \right] + g_i$$

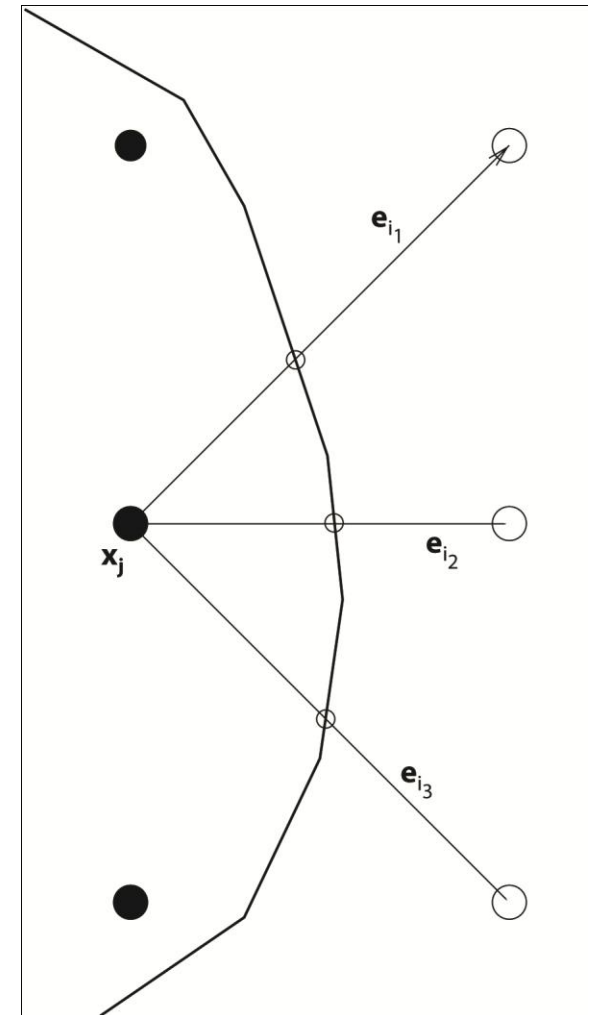
4. Back to step 1.

Boundary conditions



Boundary conditions for flow

- 1) *Bounce back* boundary conditions imply zero (non-slip) velocity for flow and zero **total flux** for diffusion.
- 2) Fixed pressure (for flow) or density (for diffusion)
- 3) Slip boundary conditions for flow: friction depending on tangential velocity
- 4) Zero normal flux of solute particles (no absorption)
- 5) Robin boundary conditions: normal flux is a function of the concentration on the wall (interaction with the structure)
- 6) Mirror and periodic boundary conditions.



Neumann (zero normal flux) boundary conditions for diffusion

We wish to have a boundary condition of the type

$$n \cdot u = 0$$

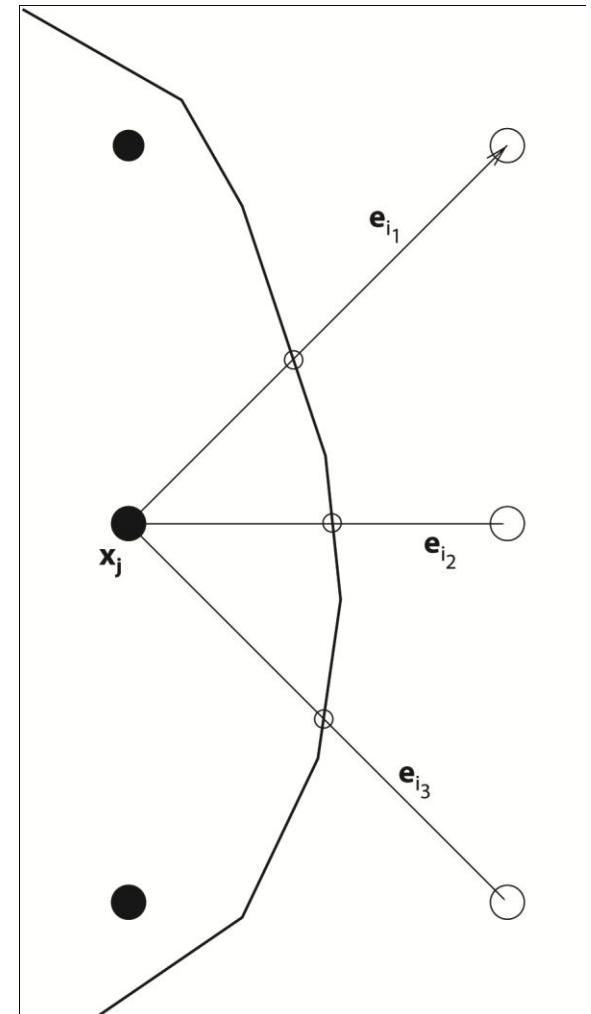
$$u = -D\nabla\rho + \rho v$$

i.e. zero flux across the boundary.

We need to assign values for the distribution function for the incoming velocities that intersect the boundary.

We assign an equilibrium distribution at the solid nodes:

$$f_i(x_j, t) = f_i^{\text{eq}}(\rho(x_j, t), u(x_j, t))$$



Neumann (zero normal flux) boundary conditions for diffusion

The unknown density and flux are computed using a mirror point

$$\tilde{x}_j = x_j + 2q_j n_j$$

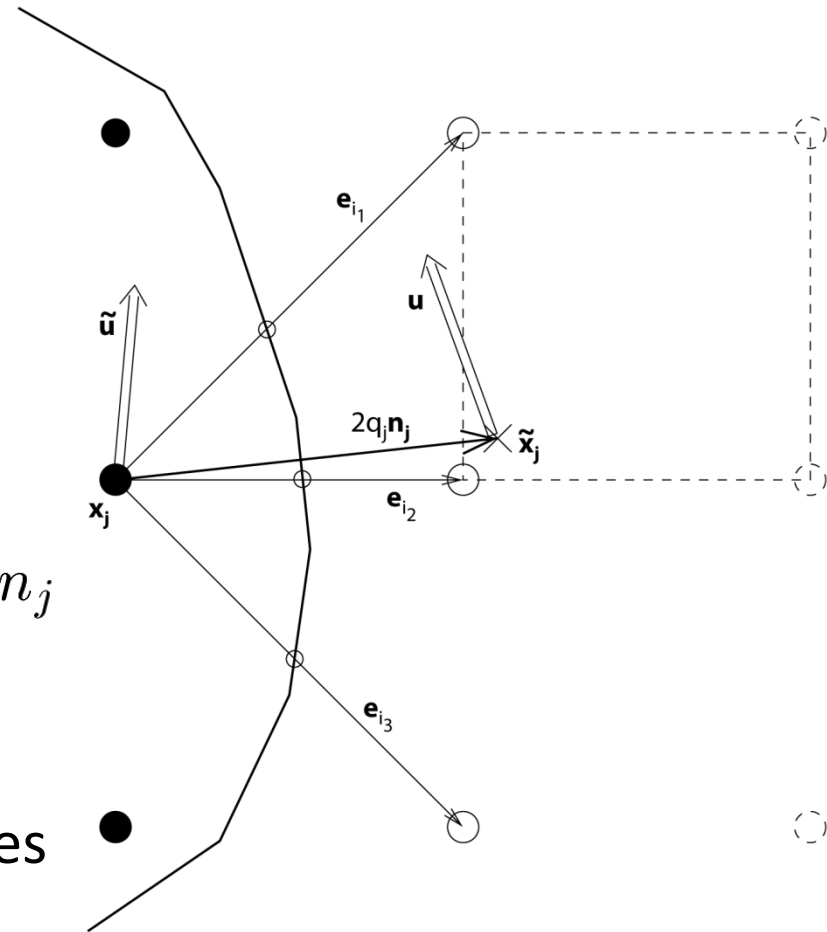
using a mirror rule for the flux

$$\rho(x_j) = \rho(\tilde{x}_j)$$

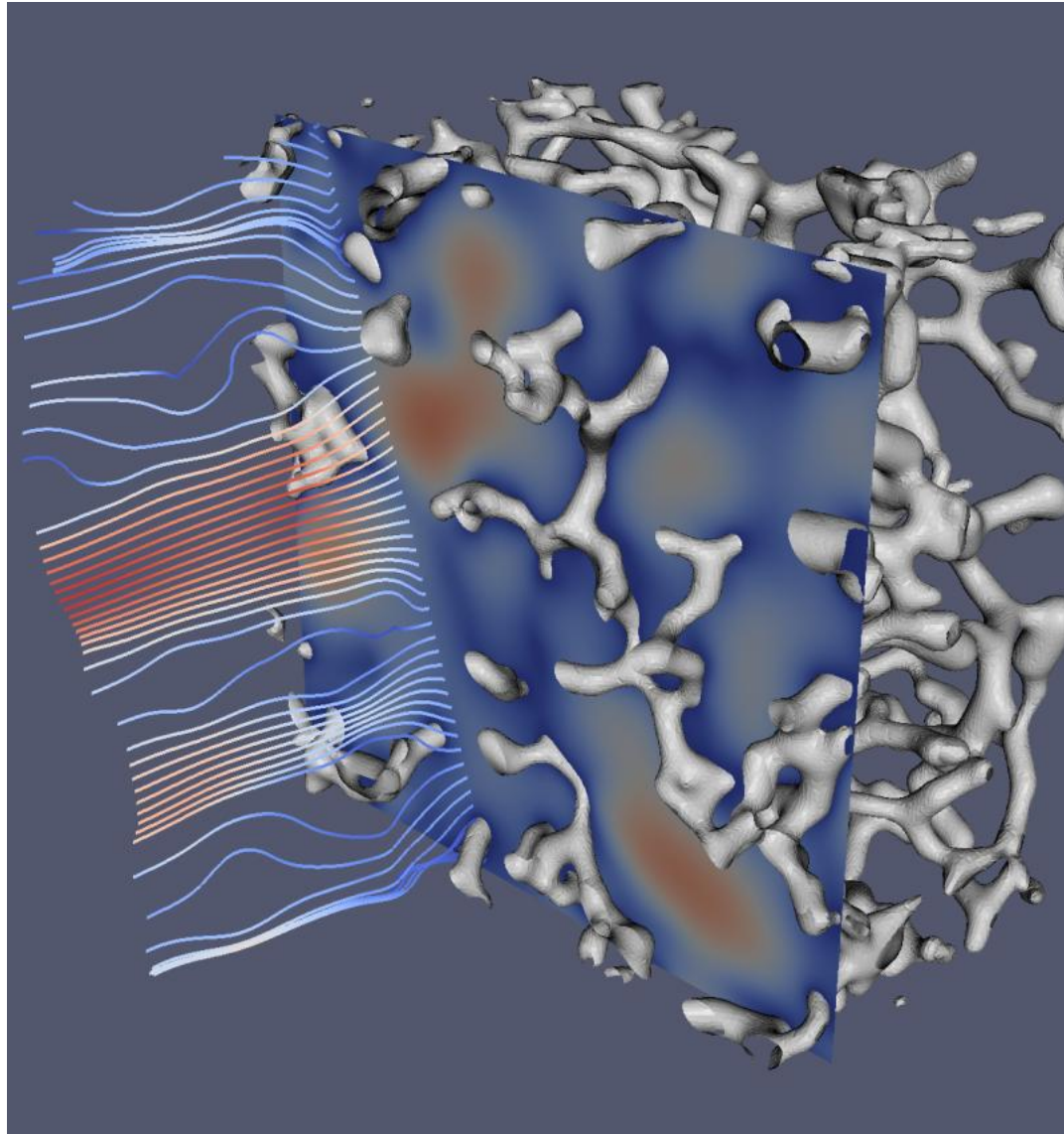
$$u(x_j) = \tilde{u}(\tilde{x}_j) = u(\tilde{x}_j) - 2(u(\tilde{x}_j) \cdot n_j)n_j$$

Values are interpolated to the mirror point from neighboring grid nodes.

Normals n_j and distances q_j are averages from intersection points.

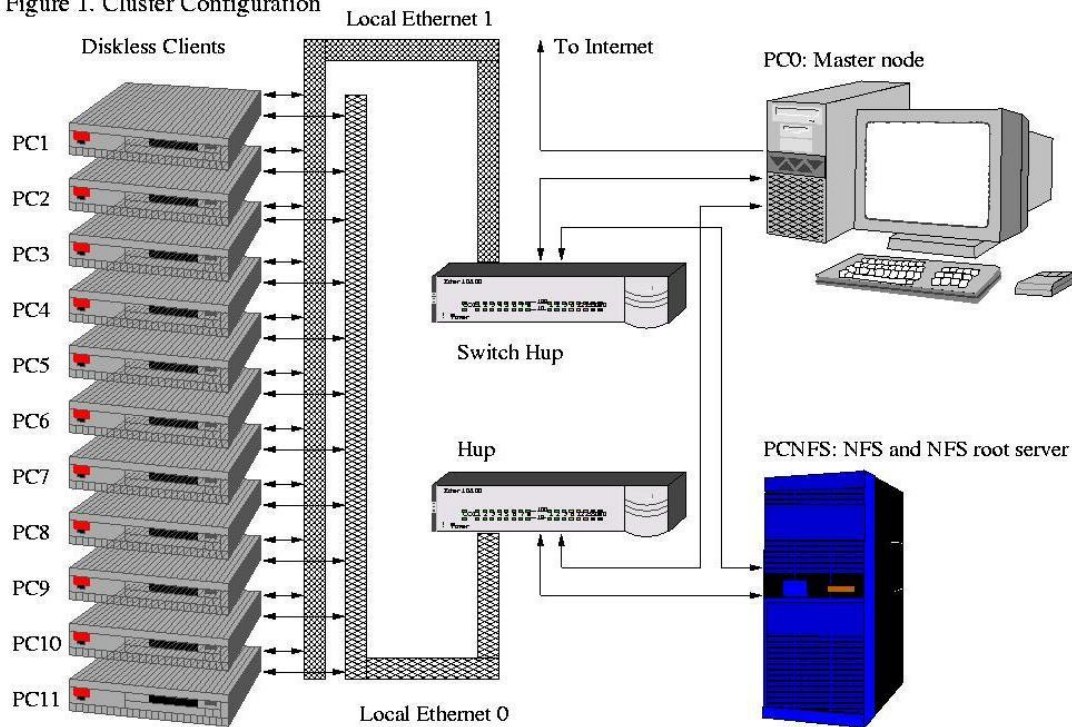


Example: flow through a gel structure



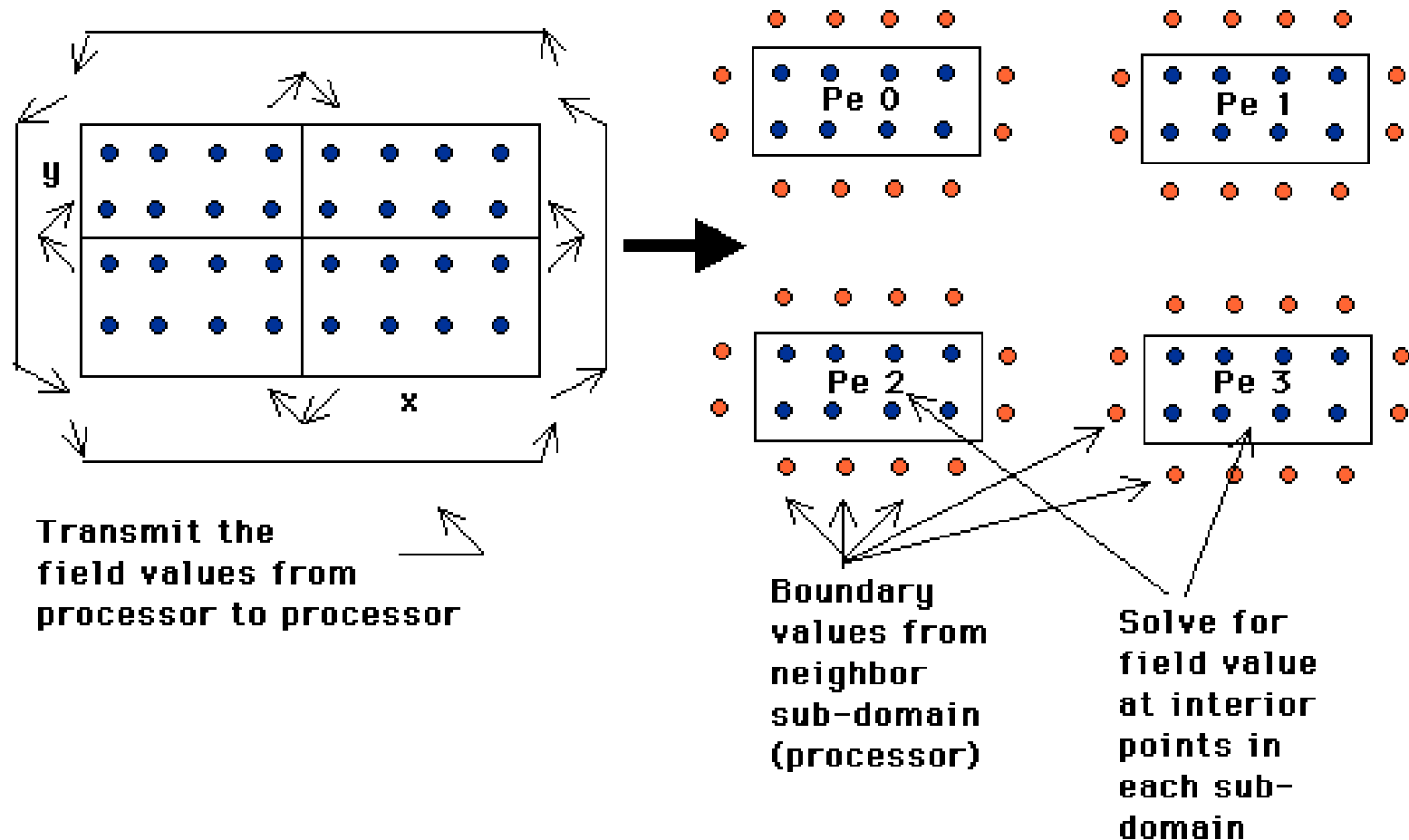
Parallel computations with Lattice Boltzmann by MPI

Figure 1. Cluster Configuration



Parallel computations by domain decomposition

Domain Decomposition - sub-domains & boundary values



Diffusion LBE. Diffusive scaling limit. (Hard calculations!)

$$f(n+1, j+\mathbf{c}, \mathbf{c}) - f(n, j, \mathbf{c}) = \frac{1}{\tau} [f^{eq} - f](n, j, \mathbf{c})$$

$$(n, j, \mathbf{c}) \text{ correspond to } (t_n(\epsilon), \mathbf{x}_j(\epsilon), \mathbf{c}) = (\epsilon^2 n, \epsilon j, \mathbf{c})$$

To make notations shorter we skip indexes after the discrete velocities \mathbf{c} of particles and indexes after f for distribution functions and write $f(\mathbf{c})$ instead.

Diffusive scaling means that we choose time scale:

$$\Delta t = \epsilon^2 = \Delta \mathbf{x}^2$$

The differential equation corresponding to the diffusive scaling is

$$\epsilon^2 \partial_t f + \epsilon \mathbf{c} \cdot \nabla f = \frac{1}{\tau} [f^{eq} - f]$$

To model diffusion we introduce the equilibrium function as: $f^{eq} = \omega(\mathbf{c}) [\rho]$

We introduce the asymptotic expansion $f = \sum_{m=0}^{\infty} \epsilon^m f^{(m)}$ to see the

connection between the Lattice Boltzmann equation and the diffusion equation for small $\Delta \mathbf{x} = \epsilon$ and will compute corresponding diffusion coefficient.

Diffusion LBE: continuum case.

Moments of $f^{(m)}$ are projections of $f^{(m)}$ on powers of discrete velocities \mathbf{c} :

$$\rho^{(m)} = \langle f^{(m)}, \mathbf{1} \rangle = \sum_{\mathbf{c}} f^{(m)}(\mathbf{c});$$

$$u_i^{(m)} = \langle f^{(m)}, \mathbf{c}_i \rangle = \sum_{\mathbf{c}} f^{(m)}(\mathbf{c}) \mathbf{c}_i;$$

We put the expansion $f = \sum_{m=0}^{\infty} \epsilon^m f^{(m)}$ into the equation

$$\epsilon^2 \partial_t f + \epsilon \mathbf{c} \cdot \nabla f = \frac{1}{\tau} [f^{eq} - f]$$

and collect terms of the same order, that gives equations for $f^{(m)}$:

$$\partial_t f^{(k)} + \mathbf{c} \cdot \nabla f^{(k+1)} = \frac{1}{\tau} [f^{eq(k+2)} - f^{(k+2)}]$$

Diffusion LBE: continuum case.

$$\begin{aligned}\partial_t f^{(k)} + \mathbf{c} \cdot \nabla f^{(k+1)} &= \frac{1}{\tau} [f^{eq(k+2)} - f^{(k+2)}] \\ &= \frac{1}{\tau} [\omega(\mathbf{c})\rho^{(k+2)} - f^{(k+2)}]\end{aligned}$$

This is an equation with respect to $f^{(k+2)}$ with right hand side dependent on lower terms in the expansion for f or in the abstract form:

$$\mathcal{L} f^{(k+2)} = \mathcal{B}$$

To have this equation solvable we must have the right hand side be orthogonal to the kernel of the operator \mathcal{L} consisting of constants. It implies:

$$\partial_t \rho^{(k)} + \nabla \cdot u^{(k+1)} = 0$$

Diffusion LBE: continuum case.

m=0: We observe that $f^{(0)} = \omega(\mathbf{c})\rho(t, \mathbf{x})$.

m=1: The equation for $f^{(1)}$ is:

$$\mathbf{c} \cdot \nabla f^{(0)} = \frac{1}{\tau} [\omega(\mathbf{c})\rho^{(1)} - f^{(1)}]$$

Multiplying scalarly the last equation by \mathbf{c} , we get, writing

$\omega(\mathbf{c}) = \omega$:

$$\sum_{\mathbf{c}} \omega \mathbf{c}_i \mathbf{c}_k \cdot \nabla_k \rho^{(0)} = \sum_{\mathbf{c}} \frac{1}{\tau} [\omega \mathbf{c}_i \rho^{(1)} - f_i^{(1)} \mathbf{c}_i] = -\frac{1}{\tau} [u_i^{(1)}]$$

$$u_i^{(1)} = -\tau \left(\sum_{\mathbf{c}} \omega \mathbf{c}_i^2 \right) \nabla_i \rho^{(0)}$$

$$[\omega(\mathbf{c})\rho^{(1)} - f^{(1)}] = \tau \mathbf{c} \cdot \nabla f^{(0)}$$

$$c_s^2 = \left(\sum_{\mathbf{c}} \omega |\mathbf{c}_i|^2 \right)$$

First order terms in the expansion

We solve the equation for $f^{(1)}$ by projecting

$\text{Pr } f = f - \langle \mathbf{1}, f \rangle$ on the subspace of functions orthogonal to constants in the discrete velocity space.

$$\begin{aligned}\text{Pr } f^{(1)} &= -\tau \text{Pr} \left(\mathbf{c} \cdot \nabla f^{(0)} \right) \\ &= -\tau \left(\omega \left(\mathbf{c} \cdot \nabla \rho^{(0)} \right) - \langle \mathbf{1}, \omega \left(\mathbf{c} \cdot \nabla \rho^{(0)} \right) \rangle \right)\end{aligned}$$

We arrive also to $\rho^{(1)} = 0$, $\langle \mathbf{1}, \omega \left(\mathbf{c} \cdot \nabla \rho^{(0)} \right) \rangle = 0$ because $\mathbf{c} \cdot \nabla f^{(0)}$, is odd and $\omega(\mathbf{c})$ is even with respect to the velocity variable and $f^{(1)}$ must be odd with respect to the velocity variable.

Therefore $f^{(1)} = \text{Pr } f^{(1)} = -\tau \omega \left(\mathbf{c} \cdot \nabla \rho^{(0)} \right)$ and $\rho^{(1)} = 0$.

Diffusion equation as a compatibility condition of second order

m=2: Equations in the next order look as

$$\partial_t f^{(0)} + \mathbf{c} \cdot \nabla f^{(1)} = \frac{1}{\tau} [\omega(\mathbf{c}) \rho^{(2)} - f^{(2)}]$$

with compatibility condition: $\langle \mathbf{1}, \partial_t f^{(0)} + \mathbf{c} \cdot \nabla f^{(1)} \rangle = 0$

It implies that $\text{Pr } f^{(2)} = -\tau \text{Pr} (\partial_t f^{(0)} + \mathbf{c} \cdot \nabla f^{(1)})$

and that the compatibility condition is the diffusion equation for $\rho^{(0)}$:

$$\partial_t \rho^{(0)} - (c_s^2 \tau) \Delta \rho^{(0)} = 0, \quad c_s^2 = \left(\sum_{\mathbf{c}} \omega |\mathbf{c}_i|^2 \right)$$

Diffusion LBE: discrete case

$$f(n+1, j+\mathbf{c}, \mathbf{c}) - f(n, j, \mathbf{c}) = \frac{1}{\tau} [f^{eq} - f](n, j, \mathbf{c}).$$

We introduce the asymptotic expansion $f = \sum_{m=0}^{\infty} \epsilon^m f^{(m)}$

The difference operator in the left hand side can be expressed by means of the Taylor expansion:

$$\begin{aligned} f^{(m)}(t_n + \epsilon^2, \mathbf{x}_j + \epsilon\mathbf{c}, \mathbf{c}) - f^{(m)}(t_n, \mathbf{x}_j, \mathbf{c}) = \\ \epsilon (\mathbf{c} \cdot \nabla) f^{(m)} + \epsilon^2 \left(\partial_t + \frac{1}{2}(\mathbf{c} \cdot \nabla)^2 \right) f^{(m)} \\ + \epsilon^3 (\mathbf{c} \cdot \nabla) \left(\partial_t + \frac{1}{6}(\mathbf{c} \cdot \nabla)^2 \right) f^{(m)} + \dots \end{aligned}$$

Diffusive limit. Discrete case (similar)

m=0: We observe that $f^{(0)} = \omega(\mathbf{c})\rho(t, \mathbf{x})$.

m=1: The equation for $f^{(1)}$ is: $\mathbf{c} \cdot \nabla f^{(0)} = \frac{1}{\tau} [\omega(\mathbf{c})\rho^{(1)} - f^{(1)}]$

$$u_i^{(1)} = -\tau \left(\sum_{\mathbf{c}} \omega |\mathbf{c}_i|^2 \right) \nabla_i \rho^{(0)} = -\tau c_s^2 \nabla_i \rho^{(0)}$$

$$f^{(1)} = -\tau \omega (\mathbf{c} \cdot \nabla \rho^{(0)})$$

m=2 The equation in the next order looks as:

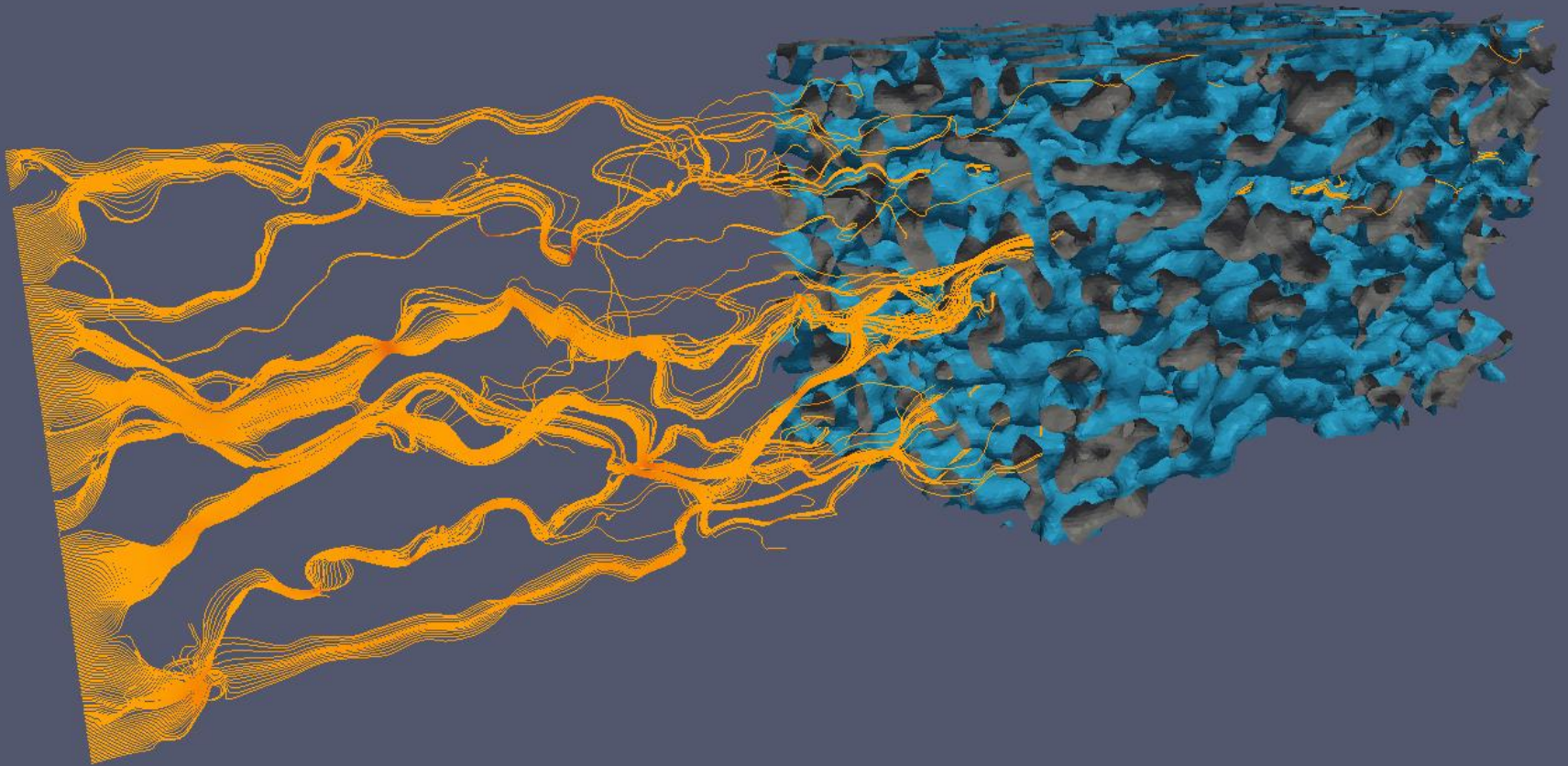
$$\partial_t f^{(0)} + \mathbf{c} \cdot \nabla f^{(1)} + \frac{1}{2} (\mathbf{c} \cdot \nabla)^2 f^{(0)} = \frac{1}{\tau} [\omega(\mathbf{c})\rho^{(2)} - f^{(2)}]$$

with compatibility conditions: $\partial_t \rho^{(0)} + \nabla \cdot u^{(1)} + \frac{1}{2} \sum_i \omega |\mathbf{c}_i|^2 \Delta \rho^{(0)} = 0$

$$\partial_t \rho^{(0)} + c_s^2 \left(\frac{1}{2} - \tau \right) \Delta \rho^{(0)} = 0 \quad \text{- diffusion equation}$$

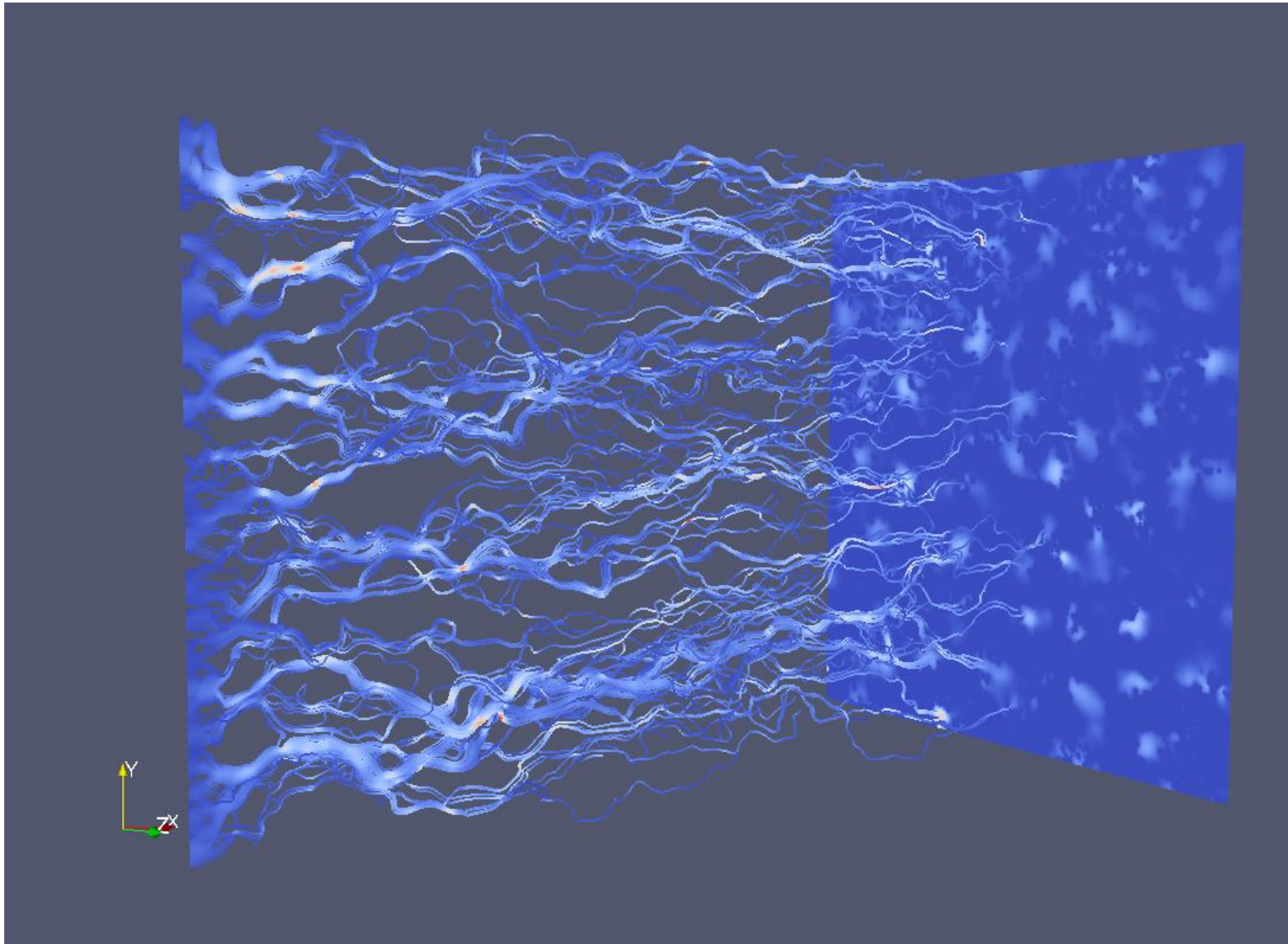
$$c_s^2 \left(\frac{1}{2} - \tau \right) \quad \text{- diffusion coefficient}$$

Example of diffusion



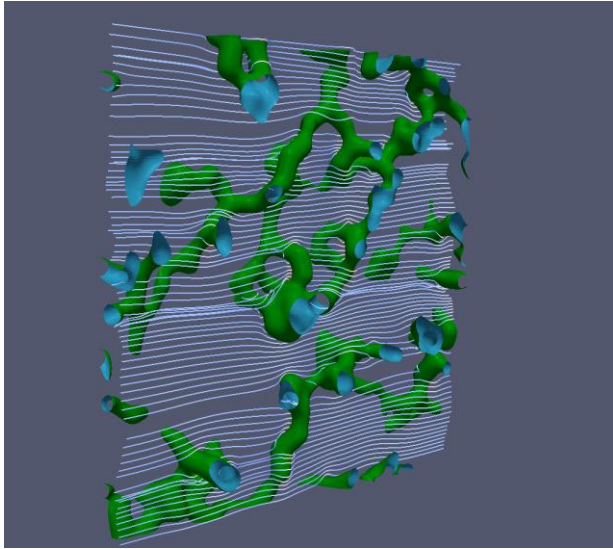
Diffusion through EC/HPC(30%) film

Example of flow

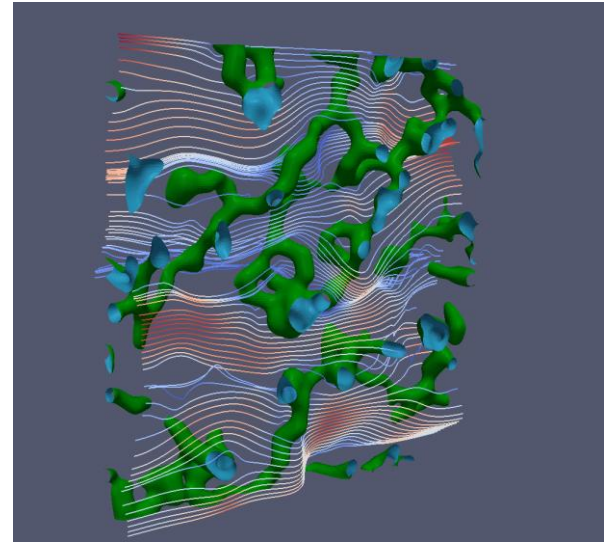


Flow through a sample of EC/HPC(30%) film

Diffusion and flow streamlines



Streamlines for diffusion



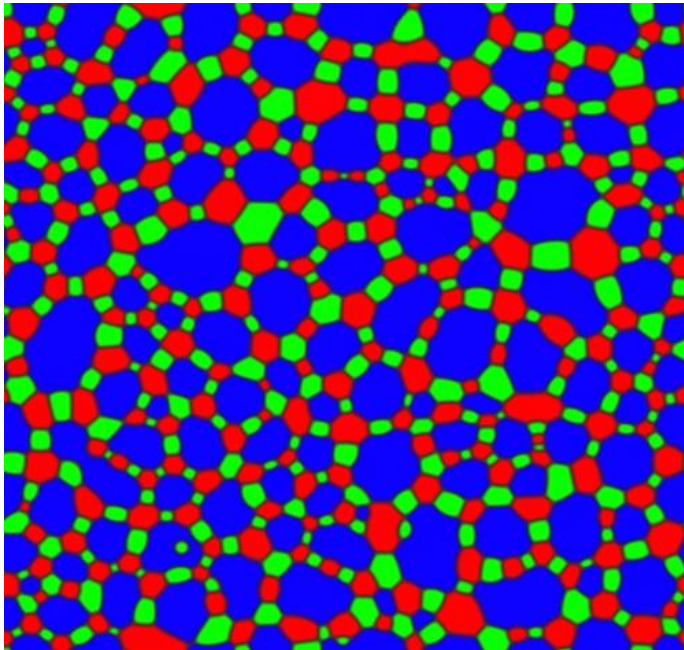
Streamlines for flow

As a result of computations we get a velocity field v for flow, and a flux field

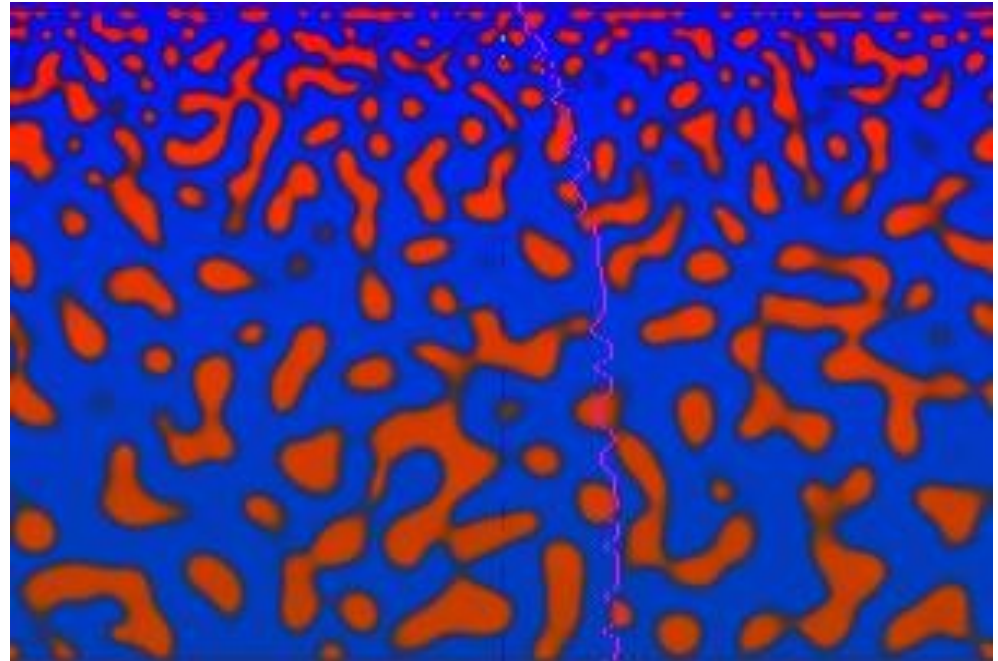
$$u = -D\nabla\rho + \rho v$$

for diffusion and for advection – diffusion. Velocity here is zero in the pure diffusion case. Streamlines are computed by integration of ODE along these vector fields and show the average paths of fluid particles for the flow case and solvent particles in the diffusion case.

Examples of multiphase flows.



Three phase flow



Two phase flow and
diffusion of the third phase

Multy-phase flows. Shan Chen model

$$f_i^\sigma(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i^\sigma(\mathbf{x}, t) - \frac{\Delta t}{\tau_\sigma} [f_i^\sigma(\mathbf{x}, t) - f_i^{\sigma,eq}(\mathbf{x}, t)],$$

$$f_i^{\sigma,eq}(\mathbf{x}, t) = w_i \rho_\sigma \left[1 + \frac{\mathbf{v}_i \cdot \mathbf{u}_\sigma^{eq}}{c_s^2} + \frac{(\mathbf{v}_i \cdot \mathbf{u}_\sigma^{eq})^2}{2c_s^4} - \frac{\mathbf{u}_\sigma^{eq^2}}{2c_s^2} \right]$$

$$\mathbf{u}_\sigma^{eq} = \mathbf{u}' + \frac{\tau_\sigma \mathbf{F}_\sigma}{\rho_\sigma}, \quad \mathbf{u}' = \frac{\sum_\sigma \frac{\rho_\sigma \mathbf{u}_\sigma}{\tau_\sigma}}{\sum_\sigma \frac{\rho_\sigma}{\tau_\sigma}} \quad \text{- is common velocity of phases}$$

$$\mathbf{F}_\sigma = \mathbf{F}_\sigma^{coh} + \mathbf{F}_\sigma^{ads} + \mathbf{F}_\sigma^b \quad \text{is the sum of forces acting between different phases}$$

\mathbf{F}_σ^{coh} is responsible for phase separation

\mathbf{F}_σ^{ads} is responsible for adhesion forces

Interphase forces in the Shan Chen model

$\mathbf{F}_\sigma = \mathbf{F}_\sigma^{coh} + \mathbf{F}_\sigma^{ads} + \mathbf{F}_\sigma^b$ is the sum of forces acting between different phases

For simple repulsion between different species the interactive force in a binary mixture can be chosen as:

$$\mathbf{F}_\sigma^{coh}(\mathbf{x}, t) = -\rho_\sigma(\mathbf{x}, t) G_\sigma^{coh} \sum_i w_i \rho_{\bar{\sigma}}(\mathbf{x} + \mathbf{v}_i \Delta t) \mathbf{v}_i$$

where σ and $\bar{\sigma}$ mark different phases. i

Similarly the adhesion between fluid particles and the solid boundary can be chosen :

$$\mathbf{F}_\sigma^{ads}(\mathbf{x}, t) = -\rho_\sigma(\mathbf{x}, t) G_\sigma^{ads} \sum_i w_i S_i(\mathbf{x} + \mathbf{v}_i \Delta t) \mathbf{v}_i$$

Where S_i is 1 if the node i is inside the solid and zero otherwise.

To model a mixture of wetting and non-wetting fluid G_σ^{ads} can be chosen positive for wetting fluid and $-G_\sigma^{ads}$ (negative with the same absolute value) for non-wetting fluid.

Macroscopic equations corresponding to the Shan Chen model of multiphase flows

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \nabla \cdot [\rho \nu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho \mathbf{g}$$

$$\rho = \sum_{\sigma} \rho_{\sigma}$$

$$\rho \mathbf{u} = \sum_{\sigma} \sum_i f_i^{\sigma} v_i + \frac{1}{2} \sum_{\sigma} \mathbf{F}_{\sigma}$$

Shan & Doolen (1995)

The parameter G^{coh} defines missible or immissible character of multiphase flows in the Shan Chen model. The thickness of the interface increases with decreasing G^{coh} and fluids mix together below certain threshold.

The difference of pressure inside and outside of a bubble satisfies the Young – Laplace law : it is proportional to the curvature of the bubble $1/R$.

$$\cos \theta = \frac{G_B^{ads} - G_A^{ads}}{G^{coh} \frac{\rho_A - \rho_B}{2}}$$

Huang *et al.* (2007)

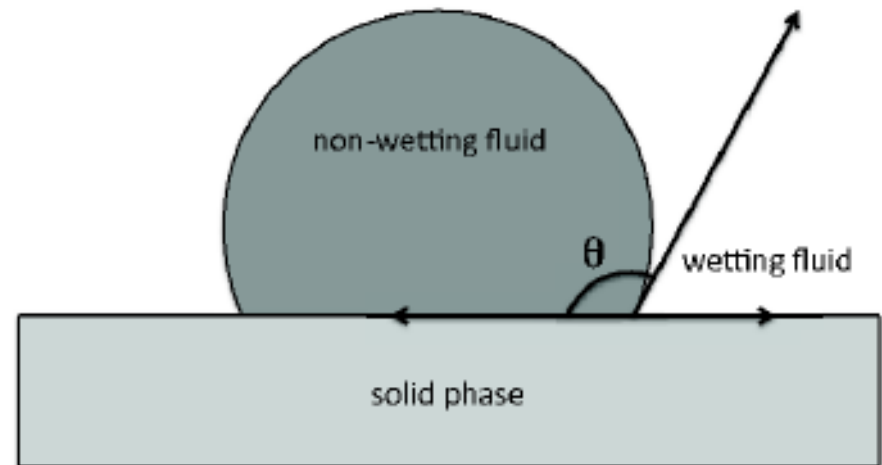


Figure 4.4: Sketch of contact angle θ .