Introduction to Lattice Gas Cellular Automata

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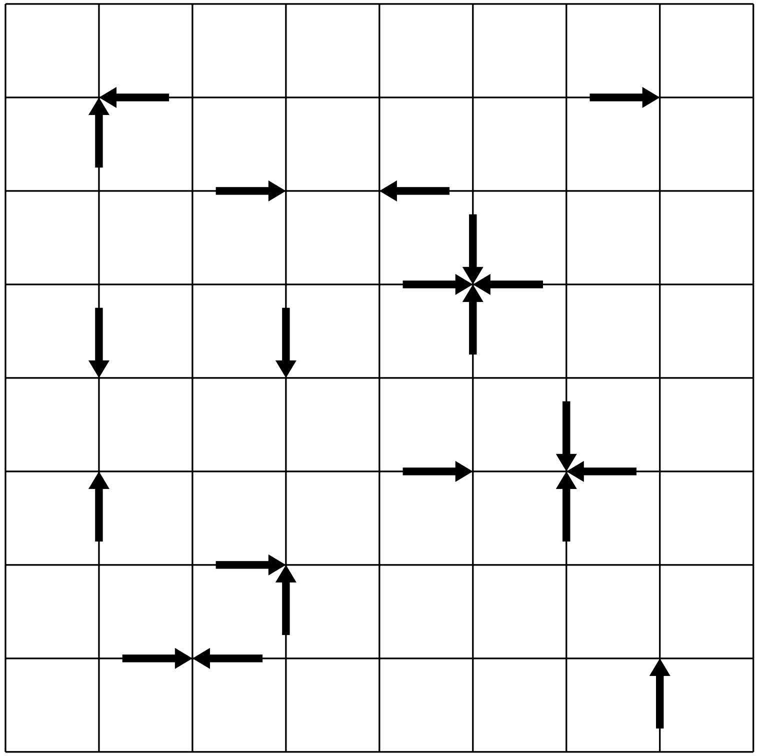
Concepts

- A LGA is a lattice of cells $\vec{r}$ so that:
- Each cell $\vec{r}$ contains typically $z+1$ quantities $n_i(\vec{r},t)$, $i=0,...z$,
- where z is the coordination number: all the neighbors of site $\vec{r}$ are obtained as $\vec{r}+\vec{v}_i$, where $\vec{v}_i$ are given vectors. By convention $\vec{v}_0=0$.
- The dynamics consist of two steps:
  - **Interaction step:** The quantities n_i "collide" locally and new values n'_i are computed at each lattice site, according to a pre-defined collision operator $\Omega_i(n)$
  - **Propagation step:** The quantitiy $n'_i(\vec{r})$ is sent to the neighboring site along lattice direction $\vec{v}_i$.

Example on a square lattice



Here, $n_i \in \{0, 1\}$. The arrows indicate the sites with $n_i = 1$, interpreted as the presence of an entering particle. The lattice direction are $\vec{v}_1 = (1, 0)$, $\vec{v}_2 = (0, 1)$, $\vec{v}_3 = (-1, 0)$ and $\vec{v}_4 = (0, -1)$

Exclusion principle

- It is convenient to choose n_i as a **Boolean** variable: this called the **exclusion principle**.
- n_i is interpreted as an occupation number: presence ($n_i = 1$) or absence ($n_i = 0$) of a physical particle entering a given site along direction $\vec{v}_i$.
- The quantities v_i can be though of as the admissible particle velocities.
- There is a finite number ($2^{(z+1)}$) of possible input configurations and the output of the collision can be pre-computed for all input states.

Microdynamics

- collision: $n_i^{out}(\vec{r}, t) = n_i^{in}(\vec{r}, t) + \Omega_i(n^{in}(\vec{r}, t)$
- propagation: $n_i^{in}(\vec{r} + \vec{v}_i \Delta t, t + \Delta t) = n_i^{out}(\vec{r}, t)$

where Δt carry the time units and $\vec{v}_i$ has the unit of a velocity.

Particle with velocity n_i travels in direction $\vec{v}_i$ and will thus reach lattice site $\vec{r} + \vec{v}_i$, still with velocity $\vec{v}_i$.

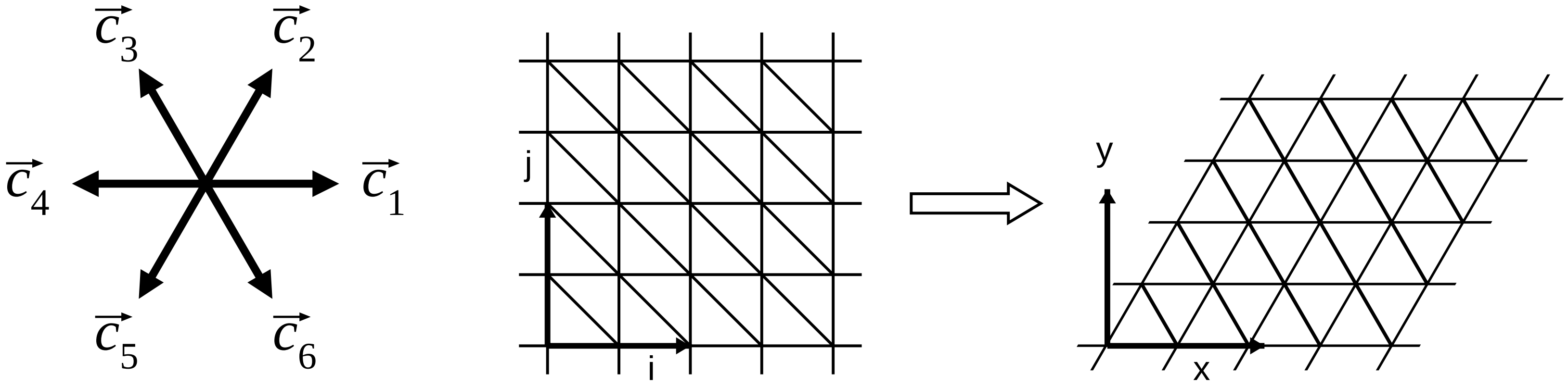
More compact formulation

$$n_i(\vec{r} + \vec{v}_i \Delta t, t + \Delta t) = n_i(\vec{r}, t) + \Omega_i(n(\vec{r}, t)$$

where $n_i \equiv n_i^{in}$

Note: if $\Omega_i = 0$, we obtain a free particle motion

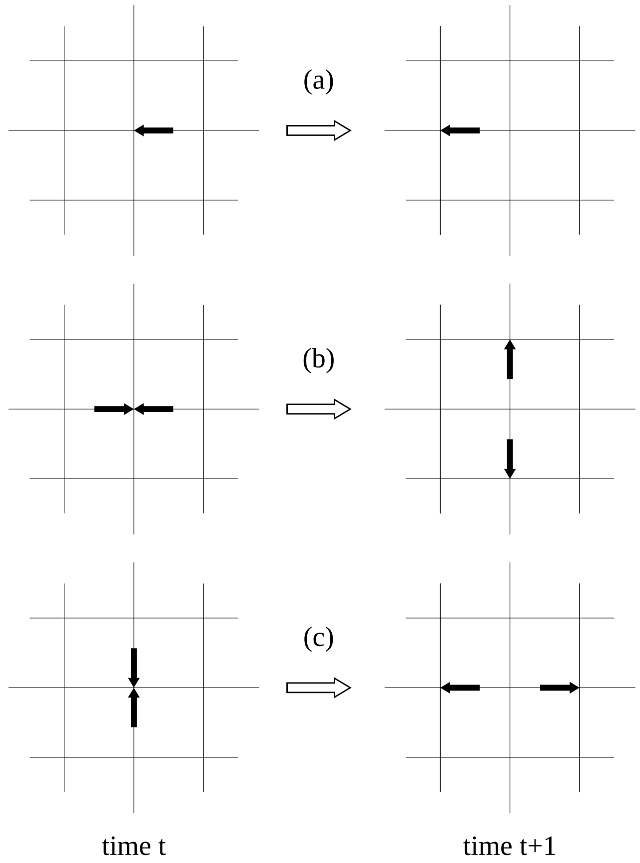
The hexagonal lattice



Simple LGA fluid models

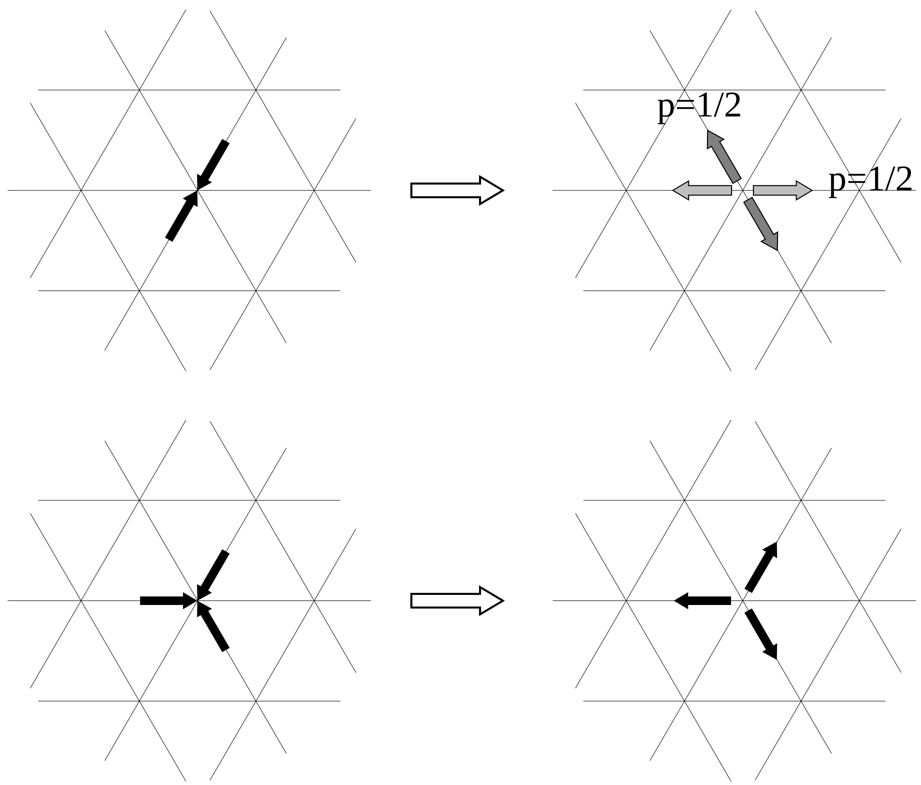
- HPP: Hardy, Pomeau, de Pazzis, 1971: kinetic theory of point particlse on the D2Q4 lattice
- FHP: Frisch, Hasslacher and Pomeau, 1986: first LGA reproducing a (almost) correct hydrodynamic behavior (Navier-Stokes eq.)

HPP model: collision rules



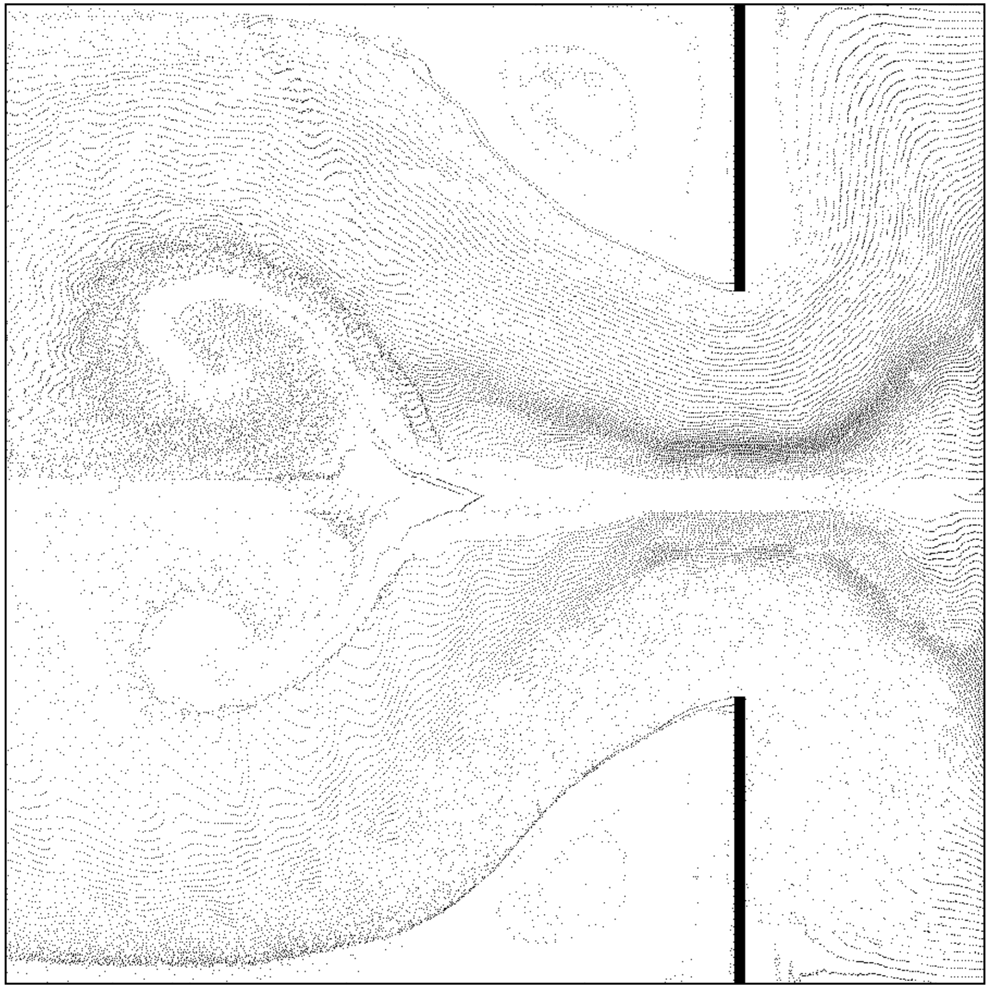
Conservation of mass and momentum.

FHP model: collision rules



Stochastic rule with Conservation of mass and momentum.

Flow past an obstacle (FHP)



Some demos

- Sound wave propagation: isotropy of HPP and FHP
- Exact calculation and time reversibility.
- Snow transport by wind

Spurious invariants

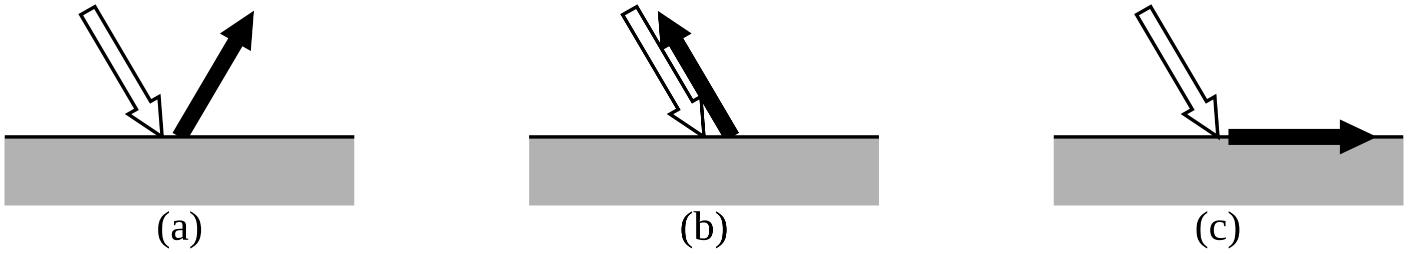
- momentum along each line
- momentum along each column
- Checkerboard invariant

Key Ingredient to build a LGA fluid

- Enforce the right conserved quantities in the collision rule
- Use a lattice with enough symmetry

Boundary Conditions

Bounce Back rule:



(a) Specular reflection, (b) bounce back condition and (c) trapping wall condition

HPP microdynamics

$$\begin{aligned} n_i(\vec{r}+\Delta t\vec{v}_i, t+1) &= n_i(\vec{r}, t) \\ &-n_i n_{i+2}(1-n_{i+1})(1-n_{i+3}) \\ &+n_{i+1}n_{i+3}(1-n_i)(1-n_{i+2}) \end{aligned}$$

Mass conservation:

$$\sum_i n_i^{out} = \sum_i n_i^{in}$$

Momentum conservation:

$$\sum_i n_i^{out}\vec{v}_i = \sum_i n_i^{in}\vec{v}_i$$

Computer Implementation

Calculation on the fly:

$n_i^{out} = n_i - n_i n_{i+2}(1 - n_{i+1})(1 - n_{i+3}) + n_{i+1} n_{i+3}(1 - n_i)(1 - n_{i+2})$

and

$$n_i(\vec{r}) = n_i^{out}(\vec{r} - \vec{v}_i)$$

Lookup table:

define $k = n_1 + 2n_2 + 4n_3 + 8n_4$. Precompute a lookup table $L(k)$ with $L(k) = k$ if $k \neq 5$ or $k \neq 10$ and

$$L(5) = 10 \qquad L(10) = 5$$

Density distributions and macroscopic quantities

Density distribution function for velocity $\vec{v}_i$:

$$N_i(\vec{r}, t) =< n_i(\vec{r}, t) >\in [0, 1]$$

Average over ensemble of block of cells, or over time intervals.

Macroscopic quantities:

Particle density and velocity (momentum)

$$\rho(\vec{r}, t) = \sum_i N_i \qquad \rho(\vec{r}, t)\vec{u}(\vec{r}, t) = \sum_i N_i \vec{v}_i$$

The (lattice) Boltzmann equation

Molecular chaos assumption:

$$< \Omega_i(n) >= \Omega_i(< n >) = \Omega_i(N)$$

That is $< n_i n_j >= N_i N_j$ if $i \neq j$. Note that $< n_i n_i >=< n_i >$ if n_i is Boolean.

Boltzmann equation (HPP):

$$\begin{aligned} N_i(\vec{r} + \Delta t \vec{v}_i, t+1) - N_i(\vec{r}, t) = & - & N_i N_{i+2}(1 - N_{i+1})(1 - N_{i+3}) \\ & + & N_{i+1} N_{i+3}(1 - N_i)(1 - N_{i+2}) \end{aligned}$$

Macroscopic limit I

The lattice spacing Δr and time step Δt goes to zero, with $\Delta r/\Delta t = v$.

Taylor expansion:

$$
\begin{aligned}
\partial_t N_i + \vec{v}_i \cdot \mathrm{grad} N_i &= \frac{1}{\Delta t}\Omega_i(N) \\
&= -\frac{1}{\Delta t} N_i N_{i+2}(1 - N_{i+1})(1 - N_{i+3}) \\
&\quad +\frac{1}{\Delta t} N_{i+1} N_{i+3}(1 - N_i)(1 - N_{i+2})
\end{aligned}
$$

Note: we should expand to second order in Δt !!!!

Terminology

- Greek indices label the spatial components of d-dimensional quantities: $v_{i\alpha}$ is the $\alpha = 1, 2, ..., d$ component of velocity vector $\vec{v}_i$.
- Summation over repeated indices is assumed. For instance $v_{i\alpha} u_\alpha = \vec{v}_i \cdot u$

Macroscopic limit II

Conservation laws:

$$\sum_i \Omega_i = 0 \qquad \sum_i \vec{v}_i \Omega_i = 0$$

for all values of N_i.

Zeroth order moments of microdynamics:

$$\partial_t \sum_i N_i + \partial_\alpha \sum_i v_{i\alpha} N_i = 0$$

where summation over repeated greek indices is assumed (Einstein convention).

Continutity equation:

$$\partial_t \rho + \partial_\alpha \rho u_\alpha = 0$$

Momentum equation

First order moments of microdynamics:

$$\partial_t \sum_i N_i v_{i\alpha} + \partial_\beta \sum_i v_{i\beta} v_{i\alpha} N_i = 0$$

We define the momentum tensor

$$\Pi_{\alpha\beta} = \sum_i N_i v_{i\alpha} v_{i\beta}$$

“Navier-Stokes” equation:

$$\partial_t \rho u_\alpha + \partial_\beta \Pi_{\alpha\beta} = 0$$

Chapman-Enskog expansion (1)

Goal: obtain $\Pi = \Pi(\rho, \vec{u})$

For this, we compute $N_i = N_i(\rho, \vec{u})$ so as to get

$$\Pi_{\alpha\beta}(\rho, \vec{u}) = \sum_i N_i(\rho, \vec{u}) v_{i\alpha} v_{i\beta}$$

Chapman-Enskog expansion:

$$N_i = N_i^{(0)} + \Delta t N_i^{(1)} + (\Delta t)^2 N_i^{(2)} + ...$$

where Δt is small (compared to the typical time variation of N_i; it is a Knudsen number expansion).

Note: in the multiscale Chapman-Enskog expansion, the space and time derivative are also expanded. Here we simplify!

Chapman-Enskog expansion (2)

Let's substitute $N_i = N_i^{(0)} + \Delta t N_i^{(1)}$ into the microdynamics $\partial_t N_i + \vec{v}_i \cdot \mathrm{grad} N_i = \frac{1}{\Delta t}\Omega_i(N)$.

We have (Taylor expansion):

$$\frac{1}{\Delta t}\Omega_i(N^{(0)} + \Delta t N^{(1)}) = \frac{1}{\Delta t}\Omega_i(N^{(0)}) + \sum_j \frac{\partial \Omega_i(N^{(0)})}{\partial N_j} N_i^{(1)}$$

and

$$\partial_t N_i + \vec{v}_i \cdot \mathrm{grad} N_i = \partial_t N_i^{(0)} + \vec{v}_i \cdot \mathrm{grad} N_i^{(0)} + O(\Delta t)$$

Chapman-Enskog expansion (3)

The terms with equal Δt order give

$$O(\Delta t^0): \qquad \Omega_i(N^{(0)}) = 0$$

and $O(\Delta t)$:

$$\partial_t N_i^{(0)} + \vec{v}_i \cdot \mathrm{grad} N_i^{(0)} = \sum_j \frac{\partial \Omega_i(N^{(0)})}{\partial N_j} N_i^{(1)}$$

Thus we can first compute $N^{(0)}$ and then $N^{(1)}$.

Chapman-Enskog expansion (4)

The matrix $\partial\Omega/\partial N$ is not invertible because of the conservation laws:

$$\sum_i \Omega_i = \sum_i \vec{v}_i \Omega_i = 0$$

Thus, there are linear combinations of the columns of $\partial\Omega/\partial N$ which are zero.

Fortunately, if we impose that

$$\rho = \sum_i N_i^{(0)} \qquad \rho\vec{u} = \sum_i N_i^{(0)} \vec{v}_i$$

and

$$\sum_i N_i^{(1)} = \sum N_i^{(1)} \vec{v}_i = 0$$

we will obtain a solution anyway.

Case of the HPP model (1)

The equation $\Omega_i(N^{(0)}) = 0$ gives

$$N_i^{(0)} N_{i+2}^{(0)} (1 - N_{i+1}^{(0)})(1 - N_{i+3}^{(0)}) = N_{i+1}^{(0)} N_{i+3}^{(0)} (1 - N_i^{(0)})(1 - N_{i+2}^{(0)})$$

or

$$\tilde{N}_i \tilde{N}_{i+2} = \tilde{N}_{i+1} \tilde{N}_{i+3}$$

where we have introduced

$$\tilde{N}_i = \frac{N_i^{(0)}}{1 - N_i^{(0)}}$$

Case of the HPP model (2)

Thus, taking the log, we get

$$\log \tilde{N}_1 - \log \tilde{N}_2 + \log \tilde{N}_3 - \log \tilde{N}_4 = 0$$

This is one equation with 4 unkown. We write

$$\log \tilde{N}_i = A + \vec{B} \cdot \vec{v}_i$$

where A and $\vec{B}$ are 3 unknown.

We then obtain

$$\tilde{N}_i = \exp(A + \vec{B} \cdot \vec{v}_i) \qquad N_i^{(0)} = \frac{1}{1 - \exp(A + \vec{B} \cdot \vec{v}_i)}$$

Case of the HPP model (3)

$$N_i^{(0)} = \frac{1}{1 - \exp(A + \vec{B} \cdot \vec{v}_i)}$$

is called the **local equilibrium** distribution (because it is a zero of the collision term).

Here $N_i^{(0)}$ is a Fermi-Dirac distribution (exclusion principle).

The quantities A and B are function of the density ρ and velocity $\vec{u}$ because:

$$\rho = \sum_i N_i^{(0)} \qquad \rho\vec{u} = \sum_i N_i^{(0)} \vec{v}_i$$

Case of the HPP model (4)

With $A = A(\rho, \vec{u})$ and $\vec{B} = \vec{B}(\rho, \vec{u})$ we obtain, to order $O(u^2)$ (low Mach number expansion) an expression for $N_i^{(0)}$

$$N_i^{(0)} = \rho \left[\frac{1}{4} + b\vec{u} \cdot \vec{v}_i + e(\vec{u} \cdot \vec{v}_i)^2 + hu^2 \right]$$

where a, b, e and h can be computed from the last two equations.

The FHP local equilibrium

Following the same derivation, we obtain, for the FHP model

$$N_i^{(0)} = \rho \left[\frac{1}{6} + \frac{1}{3} \vec{u} \cdot \vec{v}_i + G(\rho) v_{i\alpha} v_{i\beta} u_\alpha u_\beta + \frac{G(\rho)}{2} u^2 \right]$$

with

$$G(\rho) = \frac{2(3-\rho)}{3(6-\rho)}$$

Calculation of the momentum tensor

We can now compute $\Pi^{(0)}_{\alpha\beta} = \sum_i N_i^{(0)} v_{i\alpha} v_{i\beta}$. This amounts to computing quantities such as

$$\sum_{i=0}^{z} 1, \qquad \sum_{i=0}^{z} \vec{v}_i, \qquad \sum_{i=0}^{z} v_{i\alpha} v_{i\beta}$$

and

$$\sum_{i=0}^{z} v_{i\alpha} v_{i\beta} v_{i\gamma}, \qquad \sum_{i=0}^{z} v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta}$$

Isotropy problem with HPP

For a square lattice, such as that used in the HPP model, the fourth order tensor

$$\sum_{i=0}^{z} v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta}$$

is **not isotropic**. Its value depends on the specific orientation of the vector $\vec{v}_i$.

Therefore, HPP is not an acceptable physical model because physical quantities “see” the underlying lattice.

Second order tensor in HPP

On the other hand, the 2nd order tensor

$$\sum_{i=0}^{z} v_{i\alpha} v_{i\beta} = 2v^2 \delta_{\alpha\beta}$$

because $\vec{v}_1$ and $\vec{v}_2$ (or $\vec{v}_3$ and $\vec{v}_4$) form a orthogonal basis.

Any vector $\vec{a}$ can be written as

$$v^2 \vec{a} = (\vec{a} \cdot \vec{v}_1)\vec{v}_1 + (\vec{a} \cdot \vec{v}_2)\vec{v}_2$$

Thus, in components

$$v^2 a_\alpha = a_\beta v_{1\beta} v_{1\alpha} + a_\beta v_{2\beta} v_{2\alpha}$$

therefore

$$v_{1\beta} v_{1\alpha} + v_{2\beta} v_{2\alpha} = v^2 \delta_{\alpha\beta}$$

Lattice properties

Thus, the microscopic velocity vectors must obey some isotropy properties,

Each lattice direction can possibly weighted by a quantity m_i.

- Zeroth order tensor: $\sum_{i=0}^{z} m_i = C_0$
- First order tensor: $\sum_{i=0}^{z} m_i \vec{v}_i = 0$
- Second order tensor: $\sum_{i=0}^{z} m_i v_{i\alpha} v_{i\beta} = v^2 C_2 \delta_{\alpha\beta}$
- Third order tensor: $\sum_{i=0}^{z} m_i v_{i\alpha} v_{i\beta} v_{i\gamma} = 0$
- Fourth order:

$$\sum_{i=0}^{z} m_i v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta} = v^4 C_4 (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$$

Terminology

- Greek indices label the spatial components: $v_{i\alpha}$ is the $\alpha = 1, 2, ..., d$ component of velocity vector $\vec{v}_i$.
- The function $\delta_{\alpha\beta}$ is the Kronecker function: it is 0 if $\alpha \neq \beta$, and 1 otherwise.
- The quantity v is the ratio of the lattice spacing to the time step Δt.

DdQq topologies

Several lattices can be considered. They are identified by their spatial dimension d and the amount of velocity vectors $q = z$ or $q = z + 1$.

- D2Q4: square lattice (4th order tensor is not isotropic)
- D2Q7: hexagonal lattice with one rest particle
- D2Q9: square lattice + diagonal + rest particle
- D3Q19: cubic lattice with diagonals and rest particle
- D4Q24: cubic lattice in 4D

The lattice coefficients

model	slow velocities	fast velocities	C_0	C_2	C_4
D1Q3	$\lvert v_i \rvert = v$, $m_i = 1$		2	2	2/3
D2Q9	$\lvert v_i \rvert = v$, $m_i = 4$	$\lvert v_i \rvert = \sqrt{2}v$, $m_i = 1$	20	12	4
D2Q7	$\lvert v_i \rvert = v$, $m_i = 1$		6	3	3/4
D3Q15	$\lvert v_i \rvert = v$, $m_i = 1$	$\lvert v_i \rvert = \sqrt{3}v$,$m_i = 1/8$	7	3	1
D3Q19	$\lvert v_i \rvert = v$, $m_i = 2$	$\lvert v_i \rvert = \sqrt{2}v$,$m_i = 1$	24	12	4

$m_0 = 1$ for all models.

Calculation of the non-equilibrium distributions (1)

Once $N_i^{(0)}$ is known, we can return to the second step of the Chapman-Enskog expansion and compute $N_i^{(1)}$ as

$$\sum_j \frac{\partial \Omega_i(N^{(0)})}{\partial N_j} N_i^{(1)} = \partial_t N_i^{(0)} + \vec{v}_i \cdot \mathrm{grad} N_i^{(0)}$$

There is however an extra subtility to ensure that the above equation has a solution (remember that $\partial \Omega / \partial N$ is not invertible).

Calculation of the non-equilibrium distributions (2)

The idea is to express the time derivative $\partial_t N_i^{(0)}$ as

$$\partial_t N_i^{(0)} = \frac{\partial N_i^{(0)}}{\partial \rho} \partial_t \rho + \frac{\partial N_i^{(0)}}{\partial \rho u_\alpha} \partial_t \rho u_\alpha$$

and use the equations of conservation for $\partial_t \rho$ and $\partial_t \rho u_\alpha$

$$\partial_t \rho = -\mathrm{div} \rho \vec{u} \qquad \partial_t \rho u_\alpha = -\partial_\beta \Pi_{\alpha\beta}^{(0)}$$

Calculation of the non-equilibrium distributions (3)

After such a calculation, $N^{(1)}$ contains first spatial derivative of ρ and $\vec{u}$. That is how the viscous term $\nu \nabla^2 \vec{u}$ appears in the equation for $\partial_t \vec{u}$.

Note that for the HPP model, the non-equilibrium distributions are anisotropic and the viscosity is no longer a scalar.

This calculation is tedious (matrix inversion) and will be performed in the case of the Lattice Boltzmann methods where it is much simpler.

Case of FHP

For FHP, a full derivation (multiscale, second order) gives

$$N_i^{(1)} = -\frac{144\Delta t}{\rho(6-\rho)^3}(v_{i\alpha}v_{i\beta} - \frac{1}{2}\delta_{\alpha\beta})\partial_\beta \rho u_\alpha$$

and thus a built-in viscosity

$$\nu = \Delta t v^2 \left(\frac{1}{2\rho(1-\frac{\rho}{6})^3} - \frac{1}{8} \right)$$