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LATTICE GAS AUTOMATON

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Historical development of lattice Botzmann method

HPP model (Hardy, Pomeau and Pazzis) 1973

Original form of the lattice gas automaton

FHP model (Frisch, Hasslacher and Pomeau) 1986

Hexagonal grid, FHP-I: 6 neighbor nodes, FHP-II: 6 neighbor nodes and rest particles, FHP-III: 6 neighbor nodes, one rest particle and complete collision

FCHC model (Face centered hypercubid) 1986

FHP type 3D lattice gas model

Two color FCHC model (multiphase model on the basis of FHP-III) 1988

Two types of (colored) fluid phases (red and blue). Phase separation occur via introduction of color gradient vector

Lattice Boltzmann model (single phase) 1988

Particle distribution function instead of Boolean number, collision matrix

Lattice Boltzmann with Bhatnagar-Gross-Krook relaxation, 1992

Assumption of equilibrium distribution function

Multiphase LBGK model, 1993-1995

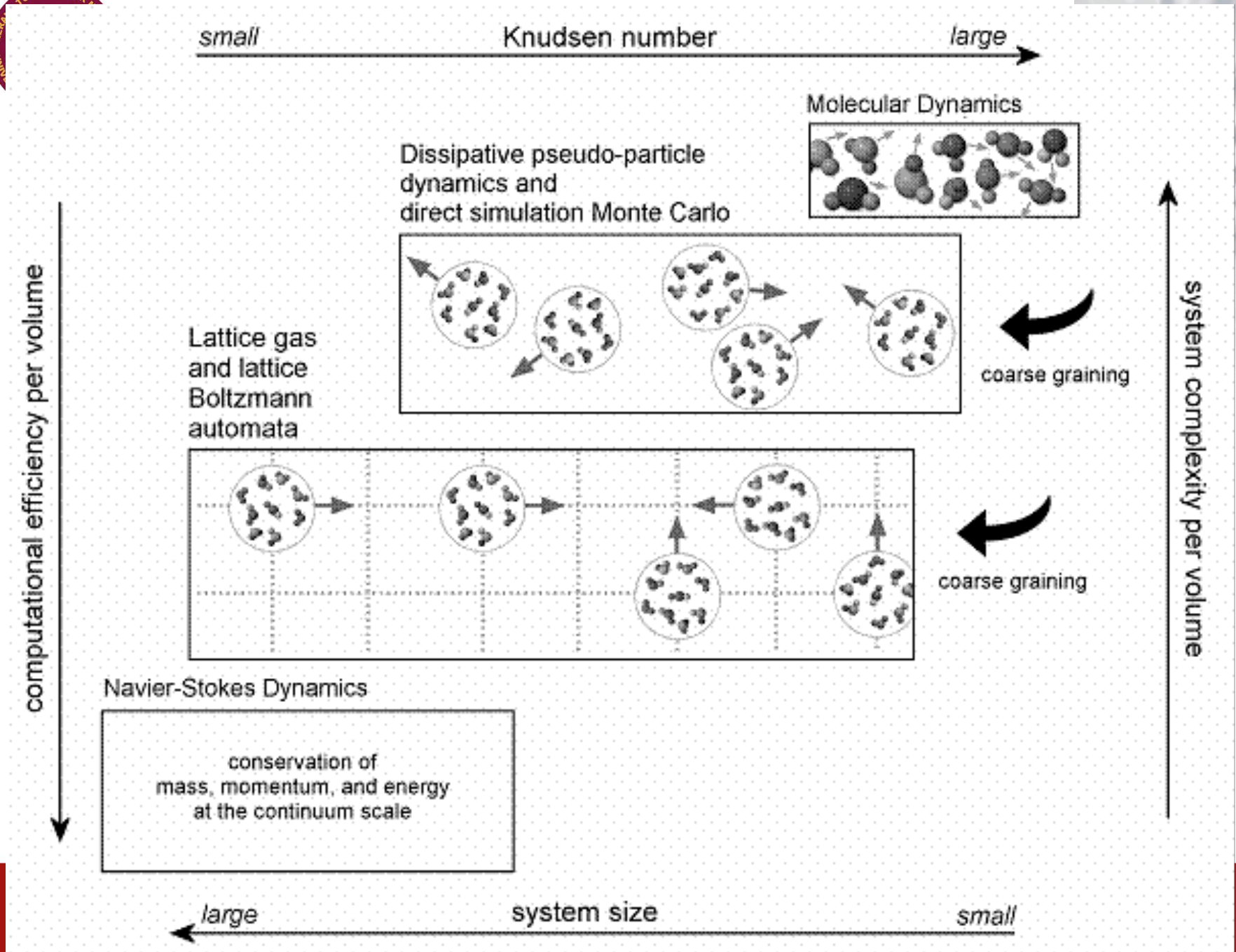
Shan-Chen model, Shan and Doolen model

Motivation for the use of Lattice Gas Automaton

Why LGA

- **The form of the hydrodynamics macroscale equation is in fact quite insensitive to microscopic details.**
- **Change in molecular interaction (collision) laws can affect parameters such as viscosity, but do not alter the basic form of the macroscopic equations (universality).**
- **The viscosity coefficient decrease as increasing number of collision.**
- **As a result, the overall behavior of fluids can be found without accurately reproducing the details of microscopic molecular dynamics.**
- **Navier-stokes formulation theoretically do not apply under condition characterized by large Knudsen number (mean free path divided by characteristic length scale. Limitation for the simulation of nano and miro flows.**

CFD with range of applicability



Various approaches to computational fluid dynamics together with their preferred range of applicability.

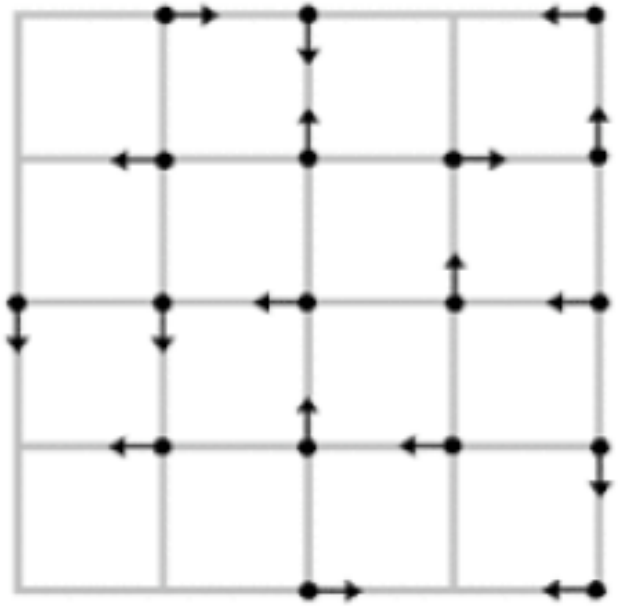
- *Molecular dynamics methods* integrate Newton's equations of motion for a set of molecules on the basis of an inter-molecular potential.

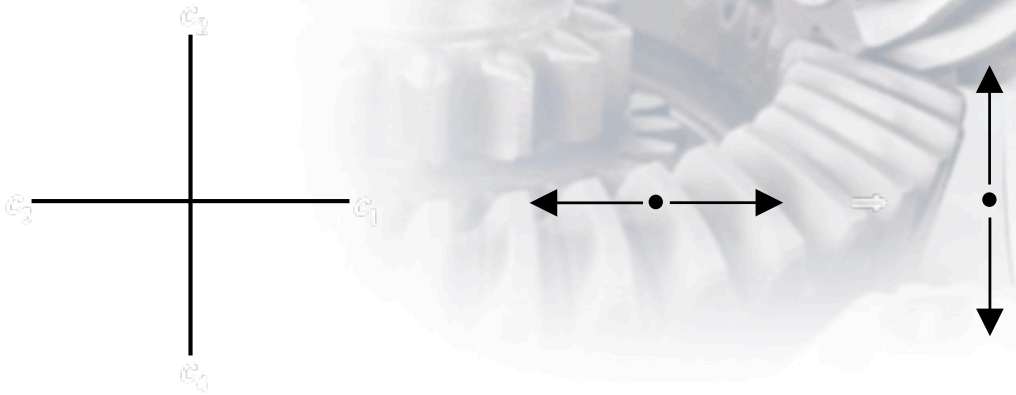
- *Dissipative particle dynamics and direction simulation Monte Carlo* are off-lattice pseudo-particle methods in conjunction with Newtonian dynamics.

- *Lattice gas and lattice Boltzmann methods* treat flows in terms of coarse grained fictive particles which reside on a mesh and conduct translation as well as collision steps entailing overall fluid-like behavior.

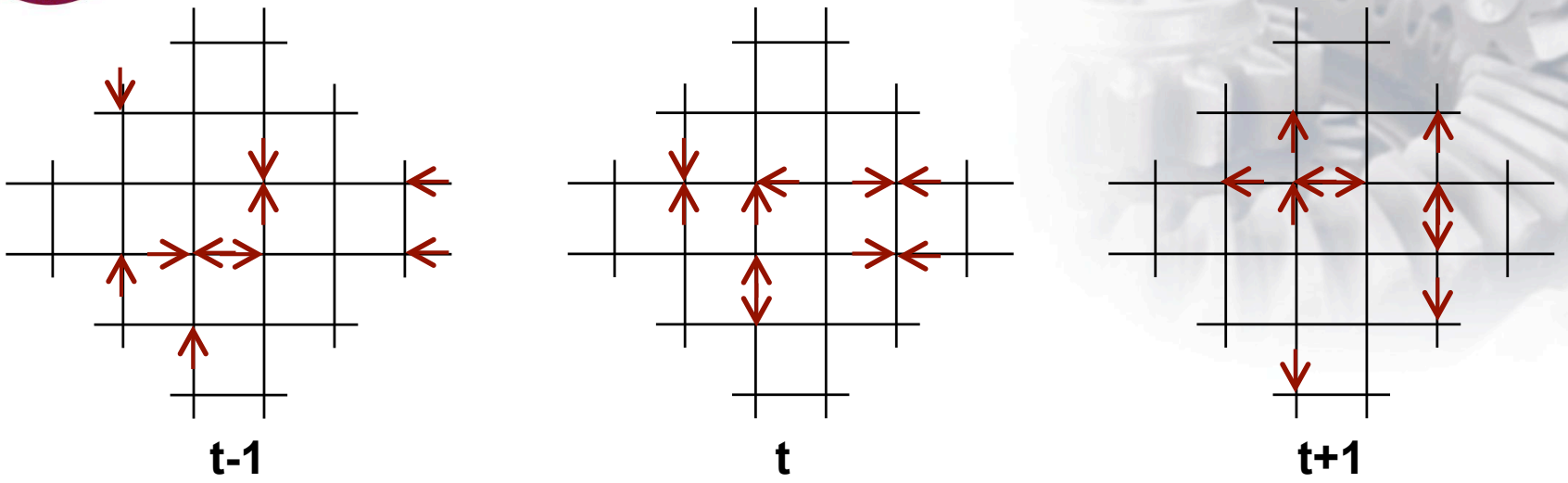
- *Navier-Stokes approaches* solve continuum-based partial differential equations which account for the local conservation of mass, momentum, and energy.

These three methods have their respective strength at different Knudsen numbers (ratio between the mean free molecule path and a characteristic length scale representing mesoscopic system)





- The first lattice gas model was first introduced by Frisch et al. (1986). (HPP)
- Only one particle is allowed to travel in each direction along a link (exclusion/ Pauri principle).
- Each particle have the same unit mass and travels at unit speed so it moves from one lattice to its neighboring site in each time step.



- There are two steps in lattice gas method.
- The moving step, also called the propagation or free-streaming step. Each particle moves one lattice unit along the direction of its velocity.
- The scattering step or collision step. If two and only two arrive at the same site, then they collide.

- When the particles arrive at the site, they collide according to the collision rules.
- When two particles arrive at the site from opposite directions (head-on collision), they immediately leave the site in the two other, previously unoccupied directions.
- The collision obeys the law that both the number of particles and the momentum at each site is conserved and thus the total particle number and total momentum are also conserved.
- However, HPP model unable to give isotropic momentum advection tensor up to fourth order (unable to reproduce Navier-Stokes equation).

FHP (Frisch, Hasslacher, Pomeau

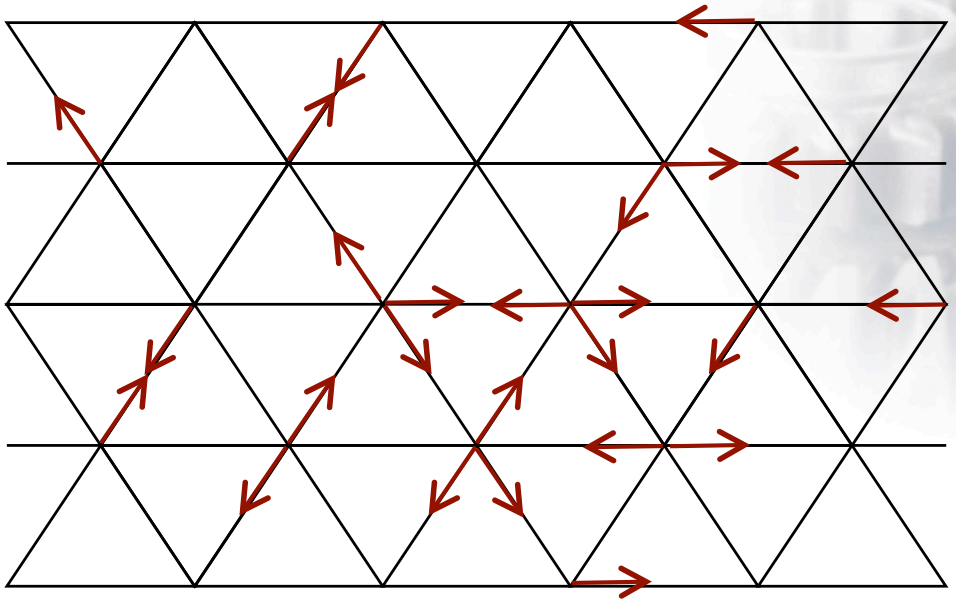


Fig. 3. FHP model

- **Model introduced by Frisch, Hasslacher and Pomeau (FHP) based on a hexagonal grid.**
- **Apply the same concept as HPP model which consist of free-streaming and collision steps.**
- **There are three version of FHP model, FHP-I, FHP-II and FHP-III.**

FHP Model

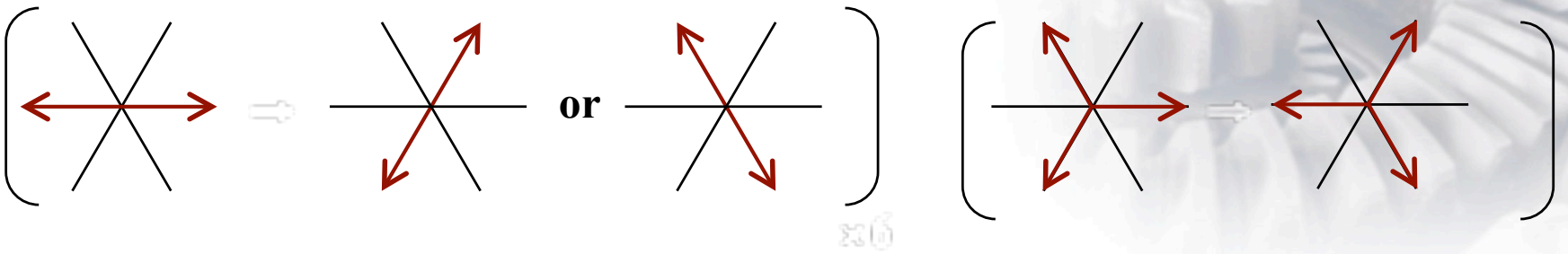
- FHP-I is the simplest of the FHP models which there are no rest particles.
- The particles collide according to the rules of group 1.
- This gives a total of 5 collisions out of 64 possible in-states.

- FHP-II model introduces a rest particles and allows the particles to collide according to the rules of group 1 and group 2.
- This gives 22 possible interactions out of a possible total of 128.

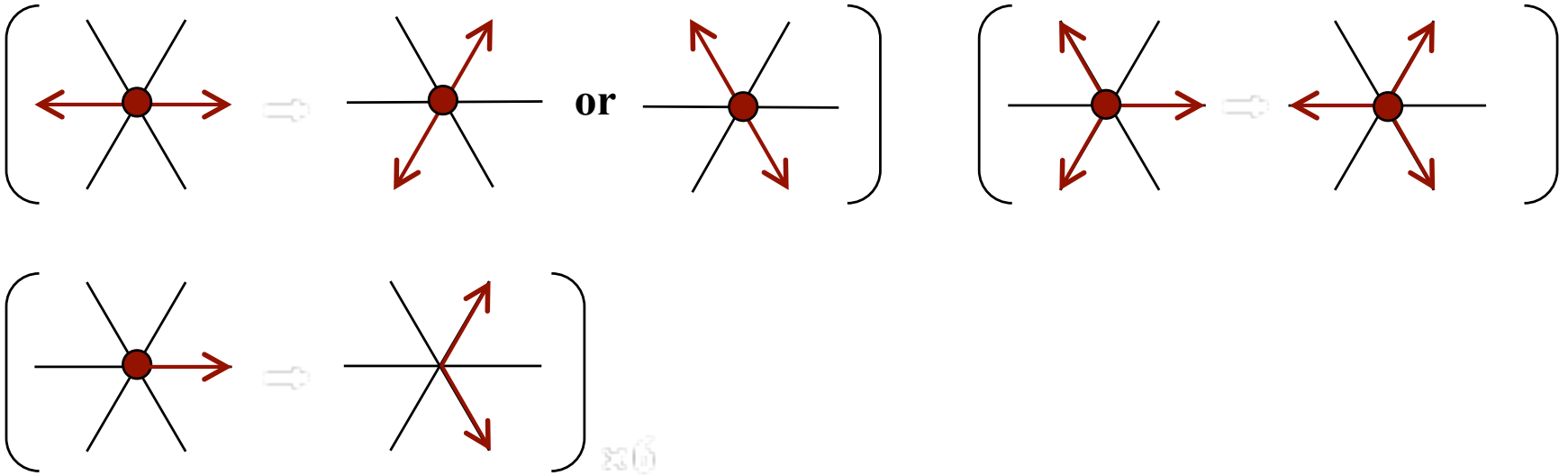
- FHP-III is an extension which allows all collision (rules of group 1,2 and 3) which conserve mass and momentum at each site.
- There are 76 possible collisions.

FHP Collision Model

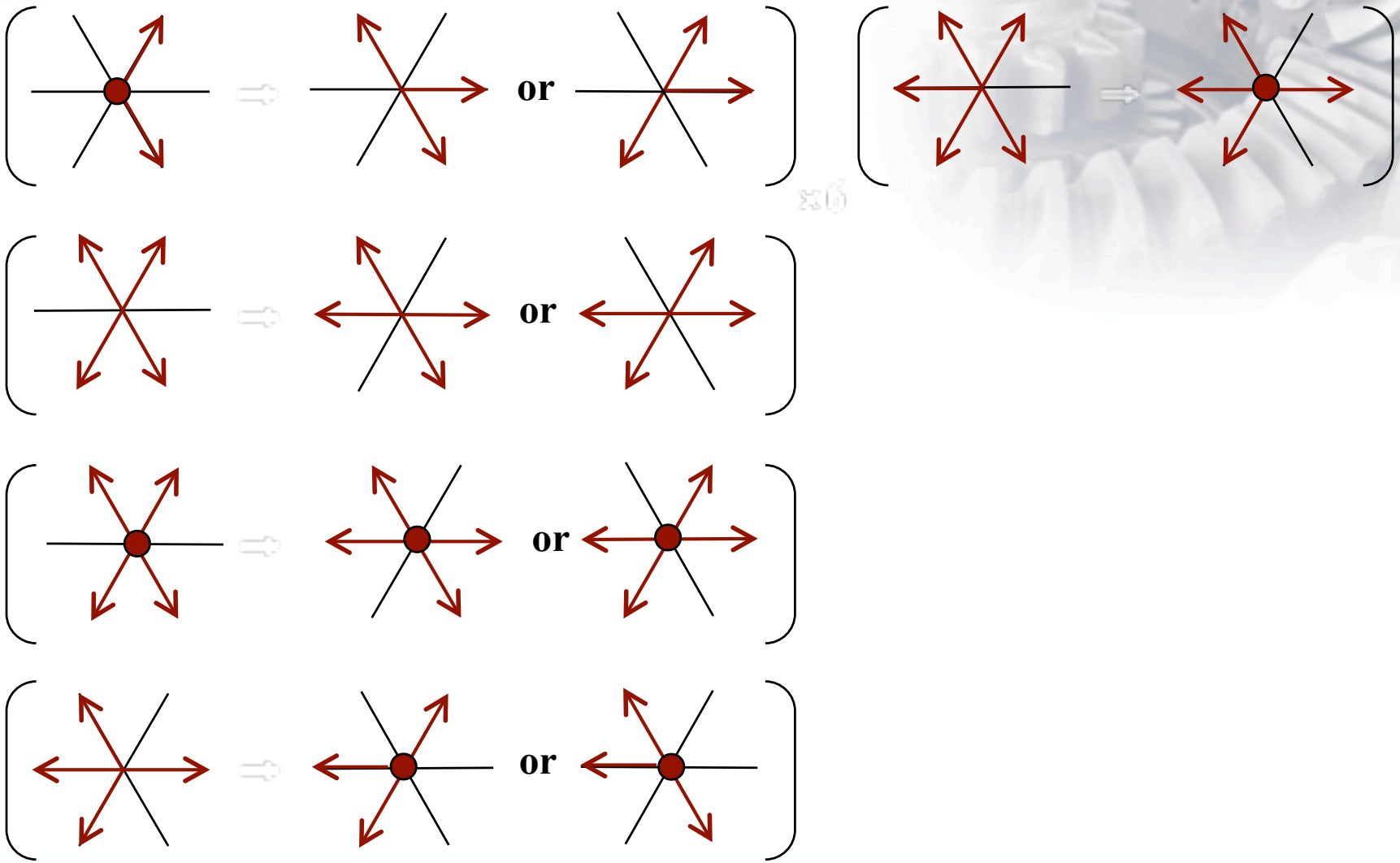
Group 1



Group 2

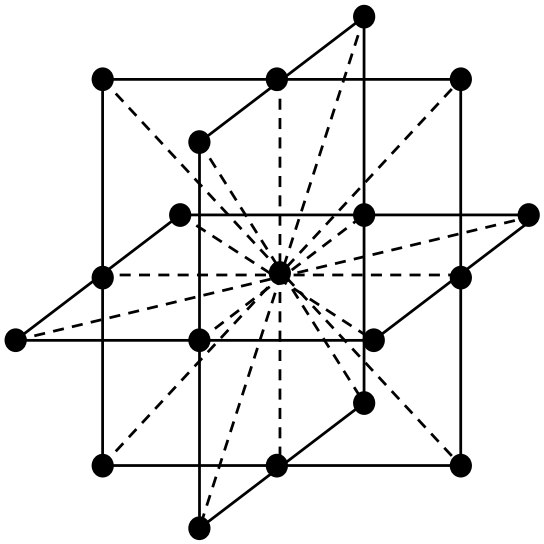


Group 3



FCHC 3-D Models

- The multi-speed three dimensional model was introduced by d'Humieres et al.
- It uses a regular cubic lattice and has particles traveling with three different velocities: zero, unity and .
- It has been found that three-dimensional lattice do not have enough symmetry to ensure macroscopic isotropy. This has been overcome by introducing a multi-speed model on a cubic lattice.



Drawbacks of Lattice Gas Model

Lattice gas models use quite simple concepts and the evolutions of particles lead to the mass and momentum conservation, but there are several disadvantages of this model;

1.Spurious conservation laws. (HPP model)

2.Lack of chiral invariance. (FHP model).

3.Unphysical velocity dependence of pressure.

4.Lack of Galilean invariants due to the density dependence on advection term.

5.Noisy.

Drawbacks of Lattice Gas Model

Spurious conservation law.

- **In addition to the mass and momentum conservation, there is a spurious conservation law.**
- **In addition to total particle number, the difference of particle numbers in any pair of opposite directions.**
- **One way to remove this spurious conservation is by introducing triple collisions.**
- **The simplest set of collisions rules with no spurious conservation law, is called FHP-I, involves only binary head collisions and triple collisions.**

Drawbacks of Lattice Gas Model

Lack of chiral invariance. (mirror symmetry)

- **There are deterministic and nondeterministic rules for the collision rules.**
- **Deterministic collision rules is when two particles arrive at a node from different direction, they immediately leave the node in the two other, previously unoccupied. (HPP model)**
- **Pre-collisional FHP input state can land into more than one (two) post collisional output state compliant with conservation laws.**
- **Consequently, unlike HPP, the time evolution of the FHP automaton is no longer deterministic.**
- **The resulting lack of chiral invariance is disposed of by choosing either collision with equal probabilities.**

Equations for the lattice gas model.

The lattice gas equation can be written as follow;

$$n(\mathbf{x}+\mathbf{c},t+1) = n(\mathbf{x},t) + \Delta(\mathbf{x},t)$$

$n(\mathbf{x},t)$ **is the occupation numbers of the links where,**

$$n(\mathbf{x},t) = \begin{cases} 1 & \text{occupied} \\ 0 & \text{otherwise} \end{cases}$$

The collision function $\Delta(\mathbf{x},t)$ **is defined as follow;**

$$\Delta(\mathbf{x},t) = \begin{cases} 1 & \text{Particle is added to the link} \\ 0 & \text{No change to the link} \\ -1 & \text{Particle is removed from the link} \end{cases}$$

The density and velocity defined as

$$\rho = \sum_i n_i$$

$$\rho \mathbf{u} = \sum_i n_i \mathbf{c}$$

Macrodynamical equations

The equation obtained from lattice gas method differs from the standard Navier-Stokes equation in the following ways.

i. **Non unity density dependence function in convection term. (lack of Galilean invariants)**

ii. **Viscosity is a function of density.**

iii. **The pressure term has an extra term which is dependent on the density and the velocity.**

Macroscopic quantities.

The probabilistic approach, ensemble averaged, is used in considering the mean population

The larger the averaging cell, the less noisy the result will be.

The size of a cell is, however, restricted by the limits imposed on the overall grid size by computer memory and time restriction.

Consequently, the noise cannot be completely overcome.

Macroscopic quantities.

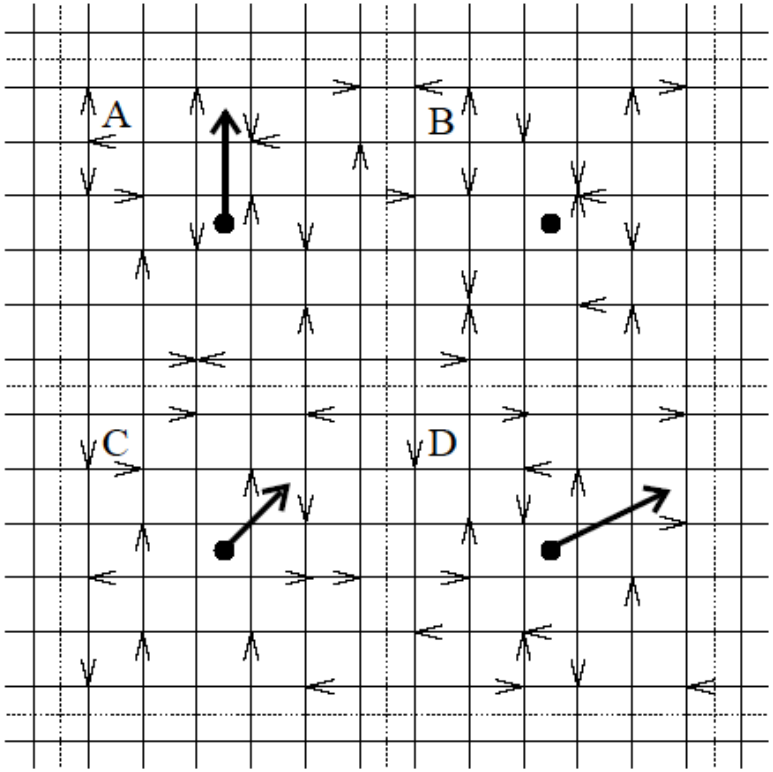


Fig. 7. An example of averaging on a section of square lattice with four averaging cells, shown by the dashed lines, superimposed over the grid. The individual particles are represented by the small arrows and the average velocities by the large arrows.

Cell	M_1	M_2	M_3	M_4	M	ρ	u_x	u_y	$\|\mathbf{u}\|$	θ
A	6	3	4	3	16	16/36	0	2/ ρ	2/ ρ	90
B	5	3	5	3	16	16/36	0	0	0	~
C	4	4	3	3	14	14/36	1/ ρ	1/ ρ	$\sqrt{2}/\rho$	45
D	4	5	3	3	15	15/36	2/ ρ	1/ ρ	$\sqrt{5}/\rho$	26.5

Fig. 8. The total number of particles M_i on link c_i, the x and y components of the averaged velocity u, its magnitude and inclination θ, the total number of particles M and the average density ρfor the four averaging cells shown in figure 7.