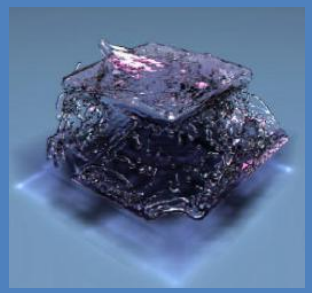
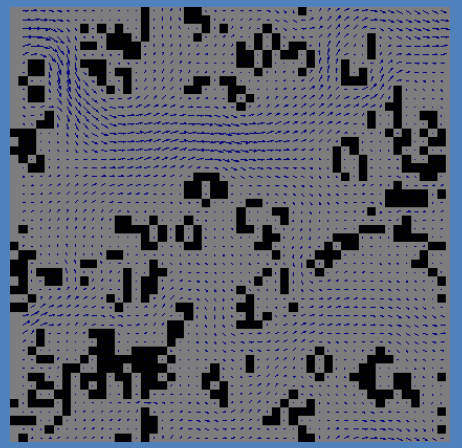


10th Indo-German Winter Academy 2011

Introduction to the Lattice Boltzmann Method

Abhijeet Tallavajhula
IIT Kharagpur
Tutors: Prof. U. Ruede, D. Bartuschat

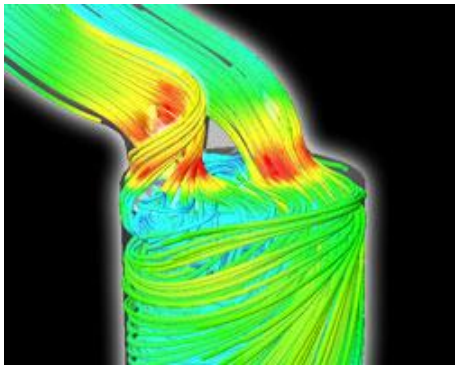


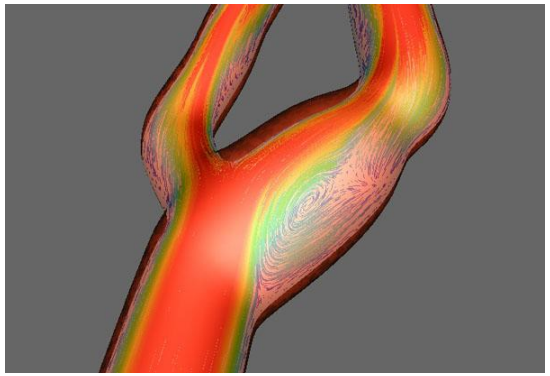
Overview of the presentation

- Development
- Derivation of the Lattice Boltzmann Equations
- Algorithm
- Advantages and Disadvantages of the Method
- Applications

Development

- Computational Fluid dynamics is the science of modeling various phenomena related to fluid mechanics. Simulation of fluid flow an essential aspect in many of today's engineering problems. A variety of flow types exist.
  - Different scales, e.g. wind turbine and flow in arteries
  - Different regimes, e.g. laminar and complex turbulent flow
  - Different physical behaviour, e.g. immiscible fluids and flows coupled with heat transfer





Development

- Established method- discretize the governing differential equations
  - mass conservation, the continuity equation
  - momentum conservation, the Navier-Stokes Equation

$$\frac{\partial}{\partial t}\boldsymbol{u} + (\boldsymbol{u} \cdot \operatorname{grad} \boldsymbol{u}) + \frac{1}{\rho}\operatorname{grad} p = \frac{\eta}{\rho}\Delta \boldsymbol{u} + \boldsymbol{g}$$

$$\operatorname{div} \boldsymbol{u} = 0$$

- The Lattice Boltzmann method is by contrast a bottom-up approach.
- They are a serious candidate to overcome the limitations of traditional techniques.

Development-Cellular Automata Modeling

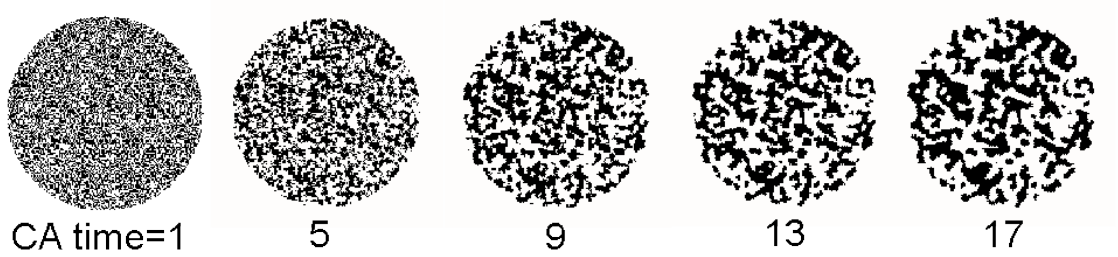
- Cellular Automata invented to model a self-replicating system, an idea of von Neumann that dates to 1940s. Defined as
  - a regular lattice in a discrete space called cells
  - the instantaneous state of each is a Boolean set.
  - The state of each cell, $\Phi_i(r_i,t)$ is updated synchronously at the next iteration by homogenous rules,

$$\Phi_i(r_i,t+1) = R_i(\Phi(r_i,t),\Phi(r_i+\delta_1,t),\ldots\Phi(r_i+\delta_N,t))$$

- Observed that even simple CA show complex behaviour
  - analogous to dynamical systems,
  - arise due to the interacting with one another.

Development-Cellular Automata Modeling

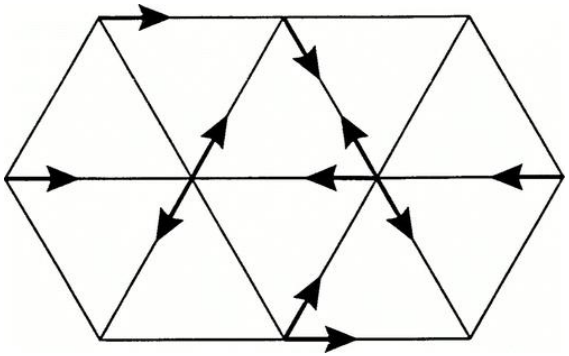
- Different levels of observation
  - macroscopic behaviour of a system might not depend on the details of the microscopic interactions, e.g. with the NS equation.
- "Everything should be made as simple as possible but not simpler"- Einstein, reflects the philosophy of modeling via CA.
  - Forest fires, road traffic, ant colonies have been simulated.



CA simulation of annealing. The two states (black & white) can be thought of as immiscible phases.

Development-Lattice Gas Automata

- A CA like rule to model gas dynamics.
  - Cells in a hexagonal FHP model.
  - Six valued state for each node, indicating incoming particle, $n_i(\mathbf{r},t)$
  - System evolved in two stages. In the streaming step, particles simply crossover to other sites,



$$n_i(\mathbf{r}+\lambda c_i, t+\tau) = n_i(\mathbf{r},t)$$

- But particles can collide as well, and a collision operator is needed.

$$n_i(\mathbf{r}+\lambda c_i, t+\tau) - n_i(\mathbf{r},t) = \Omega_i(n_i(\mathbf{r},t))$$

Development-Lattice Gas Automata

- From microdynamics to macrodynamics
  - Define quantities of interest

$$\rho = \sum_i n_i, \qquad \rho \mathbf{u} = \sum_i n_i v_i$$

  - Perform an ensemble average over the equations to get probabilities N_i

$$N_i(\mathbf{r} + \lambda c_i, t + \tau) - N_i(\mathbf{r}, t) = < \Omega_i(n_i(\mathbf{r}, t)) >$$

- Further steps to obtain equations for momentum and density include
  - Boltzmann hypothesis of molecular chaos. $< \Omega_i(n_i(\mathbf{r}, t)) > = \Omega_i(N_i(\mathbf{r}, t))$
  - Taylor expansion of the RHS.

Development-Lattice Gas Automata

- Further steps (contd.)
  - Chapman-Enskog expansion. The N_i are expanded about an equilibrium distribution with scale ε.
  - Multiscale expansion: $t = (t_1 / \varepsilon) + (t_2 / \varepsilon^2), \mathbf{r} = \mathbf{r}_1 / \varepsilon$

- The NS equations are recovered in the incompressible limit.
- The equations contain terms such as lattice viscosity
  - arise due to the discrete nature and have no physical counterpart.

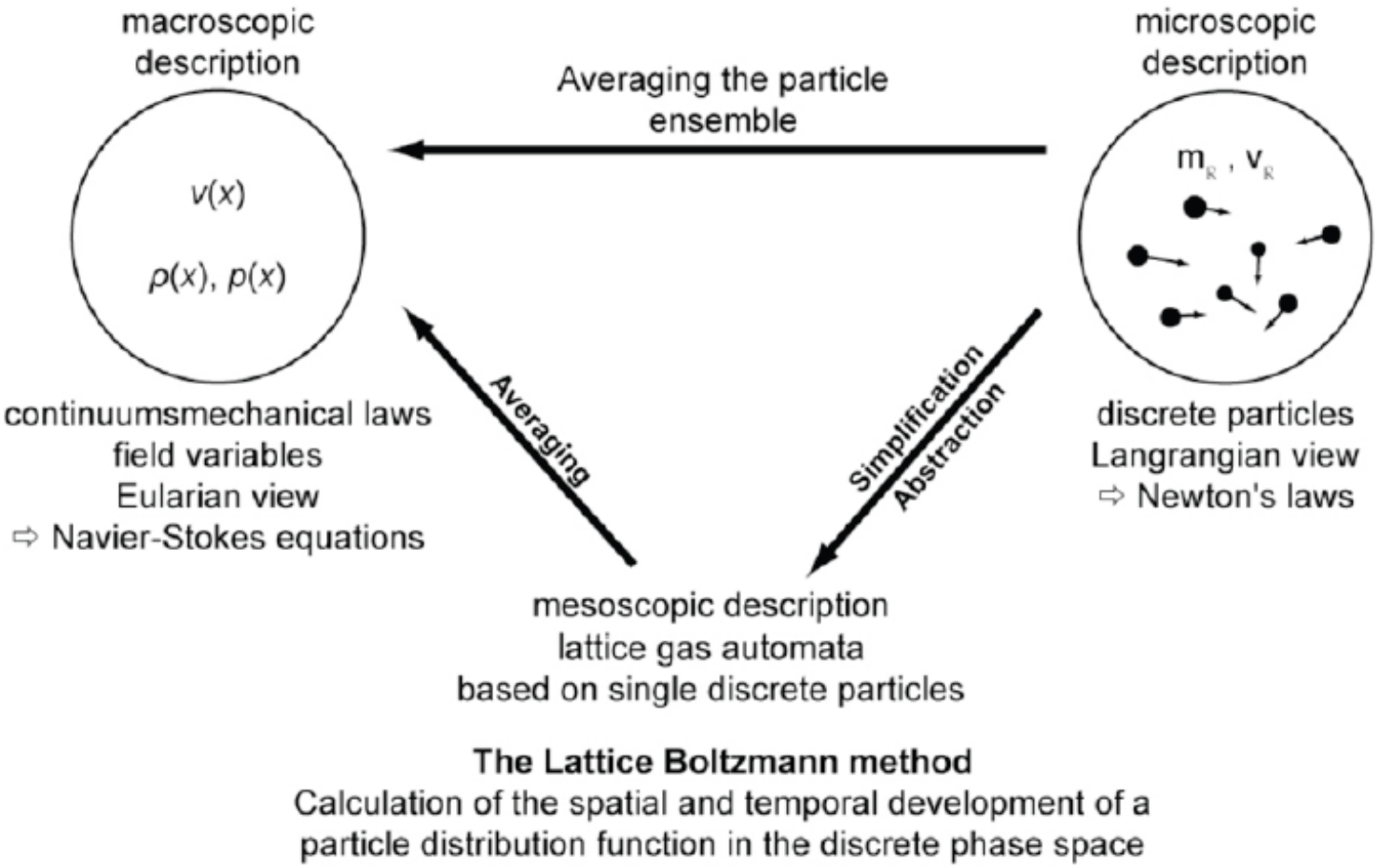
Development-From LGA to LBM

- However, LGA method has drawbacks
  - Simulation can be very noisy.
  - To obtain macroscopic behaviour, need to average over cells and time steps. Computational cost rises.
  - Due to Boolean nature, tuning of parameters not easy.
  - Not invariant to Galilean transformations.

- Simulate lattice Boltzmann equation directly- idea behind the Lattice Boltzmann Method.

$$N_i(\mathbf{r} + \lambda c_i, t + \tau) - N_i(\mathbf{r}, t) = \Omega_i(N_i(\mathbf{r}, t))$$

Development-From LGA to LBM



The Lattice Boltzmann method
Calculation of the spatial and temporal development of a particle distribution function in the discrete phase space

Derivation of LB Equations-Boltzmann equation

• The Boltzmann equation describes dynamics in terms of probability functions f in phase space:

$$\frac{\partial f}{\partial t} + \xi \nabla_x f + K \nabla_\xi f = Q(f, f), \quad f = f(t, x, \xi)$$

- ξ: microscopic velocities
- Probability functions f : defined such that $f(t,x)dxd\xi$ are the number of particles with velocity ξ at position x at time t.
- The third term on the LHS accounts for body forces that may be present.

• Solving the equation can be difficult due to the complicated collision term Q.

Derivation of LB Equations-BGK equation

- Collision term approximated by a linear expression. The resulting equation (ignoring external forces) is called the BGK (Bhatnagar, Gross, Krook) equation.

$$\frac{\partial f}{\partial t} + \xi \nabla_x f = -\frac{1}{\tau}(f - f^{(0)})$$

- RHS contains the equilibrium distribution function, and can be thought of as an expression that drives the system towards equilibrium.
- The term τ is a relaxation time, e.g. τ=1 would set the distribution to the equilibrium value at each step.

Derivation of LB Equations-Discretization

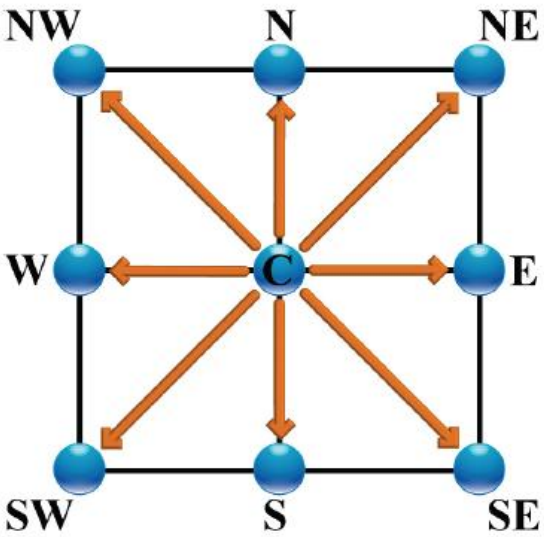
- The BGK equation is continuous in the phase variables *x* and *ξ*.
- The LB equations, though having continuous *f*, retain the discrete nature of LGA methods.
- Spatial discretization via cells- regular array of points in space.

$$\frac{\partial f_i}{\partial t} + \xi \nabla_x f_i = -\frac{1}{\tau}(f_i - f_i^{(0)})$$

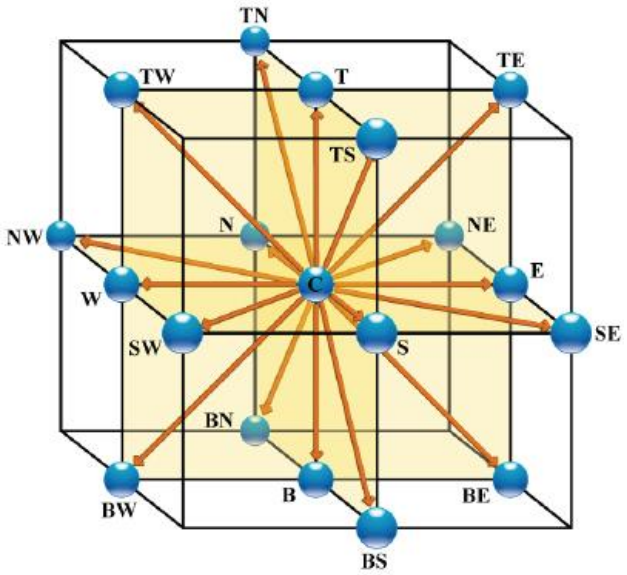
- Discretizing the velocity space is more involved. Without required symmetry
  - anisotropic effects will be observed.
  - NS equations will not be obtained in macroscopic limit.

Derivation of LB Equations-Discretization

• A FCHC model in 4 dimensions is considered and projected onto 3 dimensional space. The general type of lattice is denoted by DXQY, where X is the dimension and Y is the number of velocity directions.



D2Q9 model



D3Q19 model

Derivation of LB Equations-Discretization

• Time discretization is performed next, using an explicit forward Euler scheme. The result is the discrete lattice Boltzmann equation

$$f_i(x + c_i\Delta t, t + \Delta t) - f_i(x, |t) = -\frac{1}{\tau}(f_i - f_i^{eq})$$

• Macroscopic quantities of interest are density and momentum , calculated as

$$\rho = \int f(\vec{x}, \vec{\xi}, t) d\vec{\xi}$$

$$\rho\vec{u} = \int \xi f(\vec{x}, \vec{\xi}, t) d\vec{\xi}$$

In discrete space:

$$\rho = \sum_{i=0}^{N-1} f_i$$

$$\rho u = \sum_{i=0}^{N-1} f_i c_i$$

Derivation of LB Equations-Equilibrium solution

- f^{eq} is the local equilibirum function
  - Maxwellian distribution.
  - Parametrized by the conserved quantity density, speed and temperature T.
  - We will consider an isothermal case.

- The local equilibrium is reached when $\Omega(f^e, f^e)$ vanishes. In three dimensions, in continuous phase space, the distribution is

$$f^M = \rho \left(\frac{m^2}{2\pi RT} \right)^{3/2} e^{\frac{-(\vec{\xi}-\vec{u})^2 m^2}{2RT}}$$

Derivation of LB Equations-Equilibrium solution

- Taylor expansion upto third order used as approximation. It is sufficient in the case of low Mach number.

$$f^{(eq)} = \frac{\rho}{(2\pi RT)^{D/2}} e^{-\frac{\vec{\xi}^2}{2RT}} \left(1 + \frac{\vec{\xi}\cdot\vec{u}}{RT} + \frac{(\vec{\xi}\cdot\vec{u})^2}{2(RT)^2} - \frac{\vec{u}^2}{2RT}\right)$$

- Definitions for density and momentum in terms of *f* used.
- Integration over velocity space approximated by a quadrature formula.

$$f_i^{eq} = f_i^{eq}(\rho, u) = t_i \rho \left(1 + \frac{3}{c^2} c_i u + \frac{9}{2c^4}(c_i u)^2 - \frac{3u^2}{2c^2}\right)$$

Derivation of LB Equations-Equilibrium solution

- Weighting factor for D2Q9 model:

$$
\begin{aligned}
t_i &= 4/9 \quad \text{for} \quad i = C \\
t_i &= 1/9 \quad \text{for} \quad i = N, E, S, W \\
t_i &= 1/36 \quad \text{for} \quad i = NW, NE, SW, SE
\end{aligned}
$$

- Weighting factor for D3Q19 model:

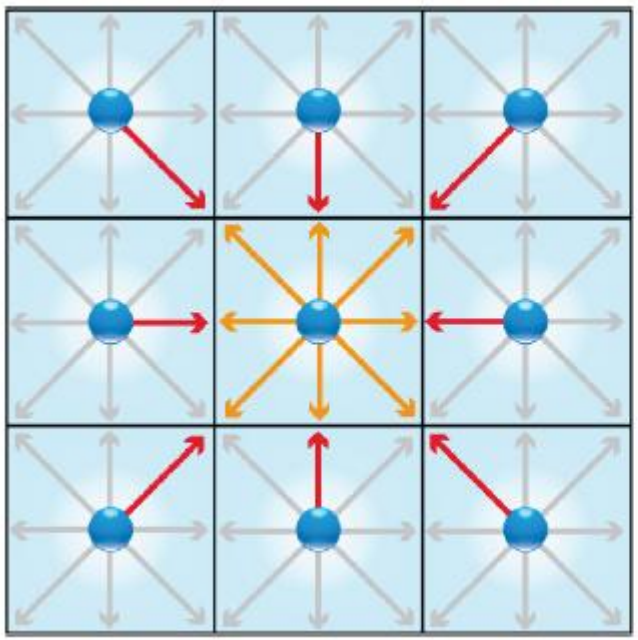
$$
\begin{aligned}
t_i &= 1/3 \quad \text{for} \quad i = C \\
t_i &= 1/18 \quad \text{for} \quad i = N, E, S, W, T, B \\
t_i &= 1/36 \quad \text{for} \quad i = \textit{all } 12 \textit{ others}.
\end{aligned}
$$

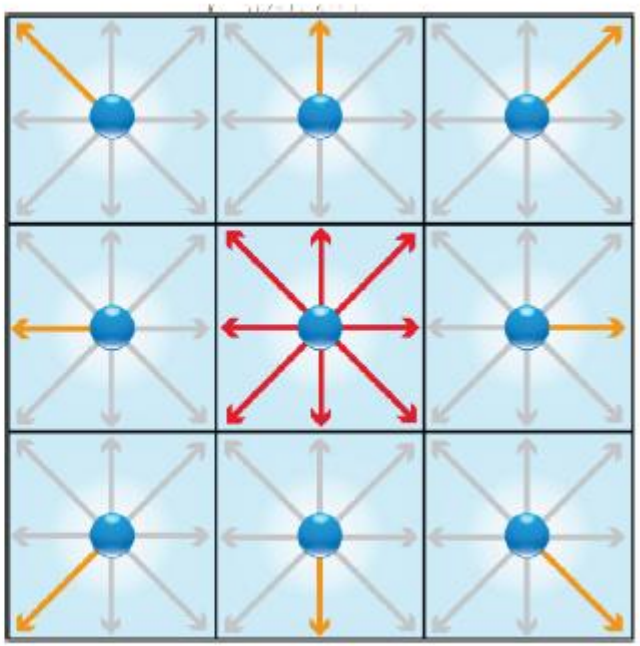
Derivation of LB Equations-Other features

- Discretization must be consistent, $v_i=c_i/\Delta t$
- Reynolds number is controlled by the particle mean free path l_{mfp}. Kinematic viscosity can be arbitrarily adjusted by varying parameter τ.
- Two working-regimes
  - adiabatic regime $l_{mfp} << l_d$, the dissipative length scale
  - numerically resolved, $a << l_d$
- $l_{mfp} << a << l_d$ for the NS equations to be valid. Adiabaticity is ensured by numerical resolution, but the converse is not true. Multiscale expansion breaks down before the limit of zero viscosity is reached.

Algorithm-Streaming step

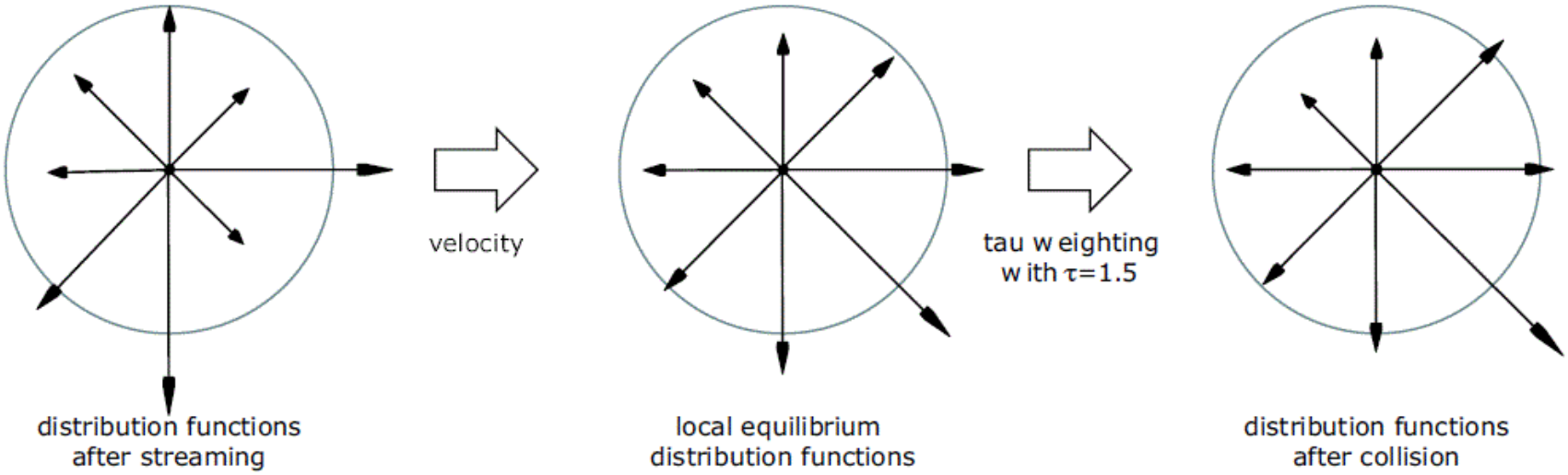
• In the streaming step, particles are simply shifted in the direction of motion to the adjacent nodes.





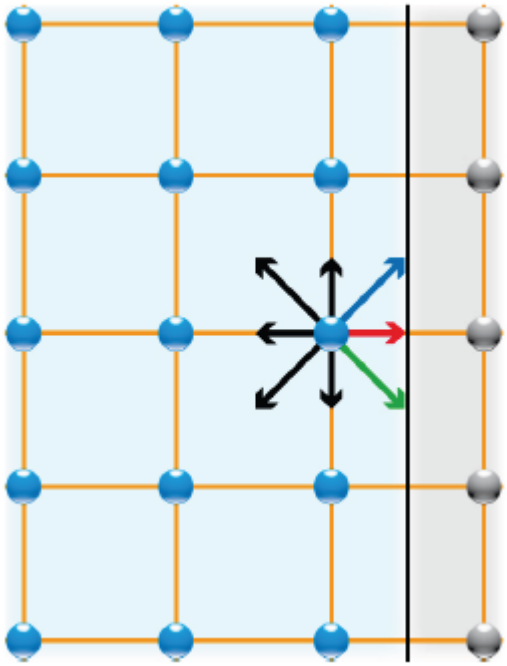
Algorithm-Collision step

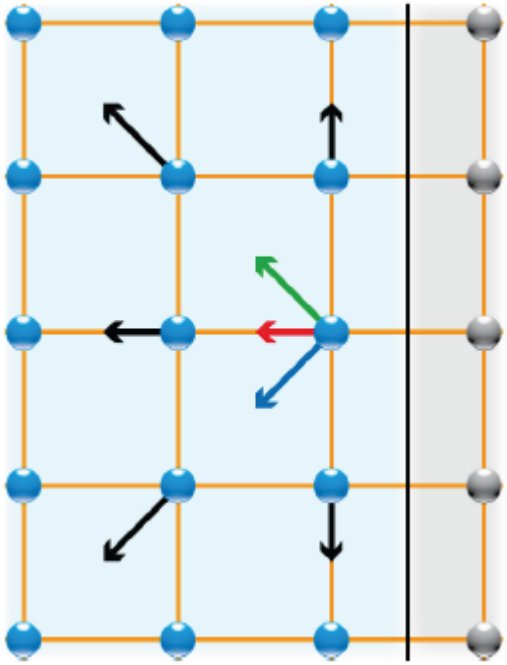
• The collision step models the interactions between particles. The factor τ controls the tendency of the system to return to equilibrium.



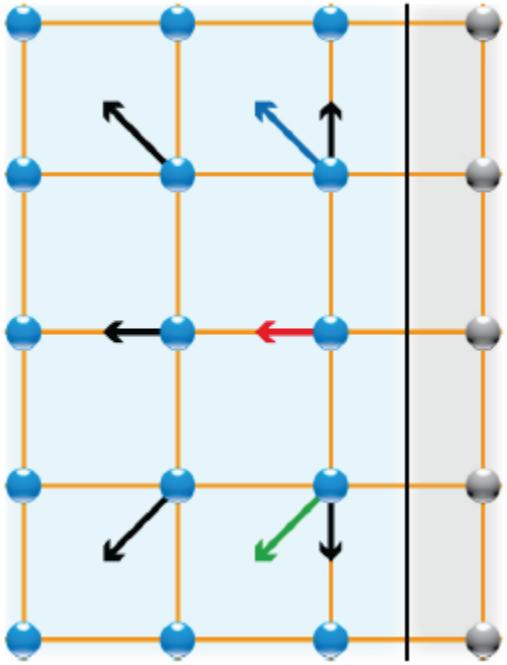
Algorithm-Boundary Conditions

- LBM allows intuitive and clear specification of BCs.
- A flag array can be used to distinguish bulk and boundary cells. Two common BCs are:





No slip- velocity at wall is zero.



Free slip- velocity normal to wall is zero.

Algorithm-Boundary Conditions

• Moving walls cause change of momentum due to friction. Change in momentum is modeled by a term in the no-slip condition.

$$f_{\bar{\alpha}}(x,t) = f_{\alpha}(x,t) - 2t_i\rho\frac{3}{c^2}c_{\alpha}u_w$$

α :direction towards wall, $\bar{\alpha}$:direction from wall, u_w: wall velocity

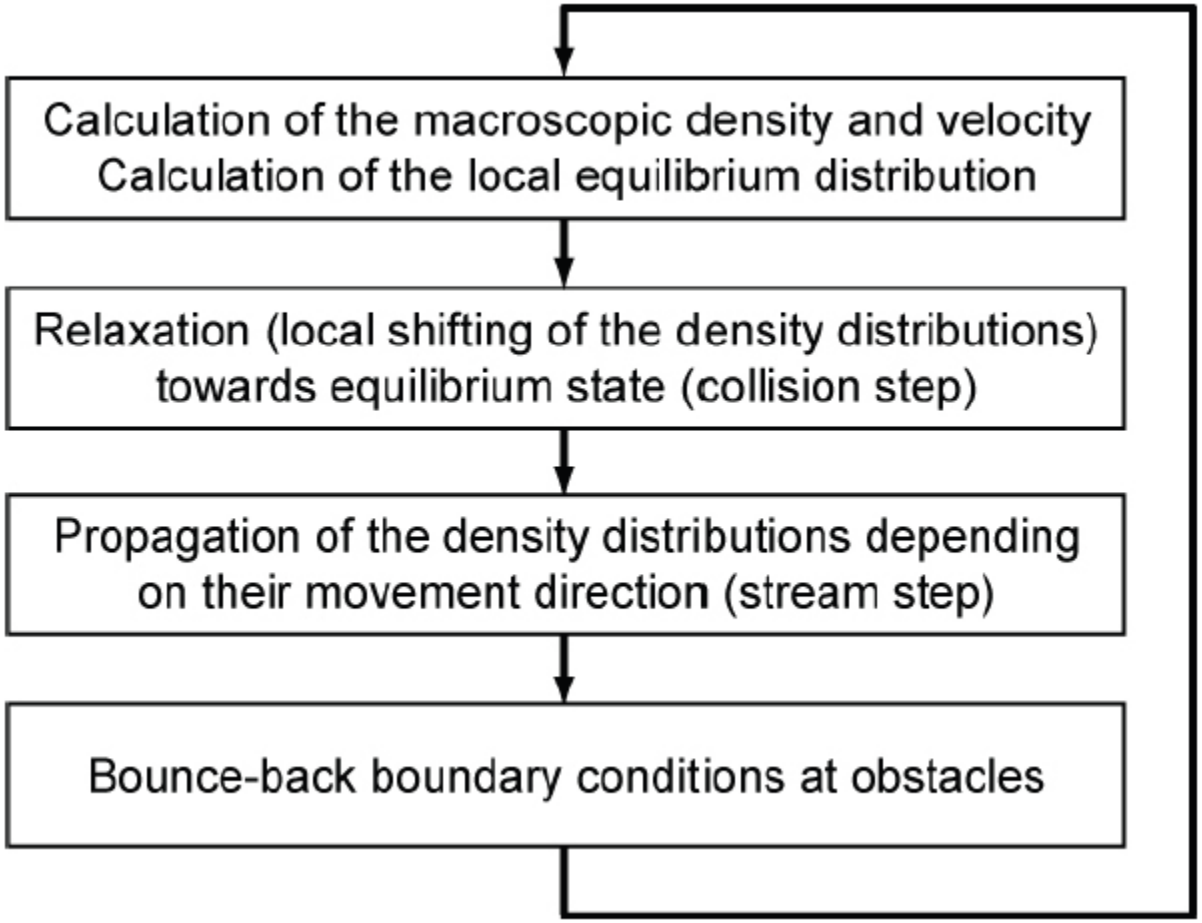
• Treating boundaries that are inclined to the direction of velocities: a curved boundary may be approximated by step-wise segments.

Algorithm-Other Conditions

- When do not want to observe the effect of free surfaces, Periodic Boundary Conditions used.
  - Wraparound condition. Particles that exit one wall re-enter from the opposite wall.
  - Mass and momentum are conserved.

- Body forces can be included. A constant acceleration can be modeled by a statement like u_x=-a. The particle distribution will be seen to respond to the force.

Algorithm


Calculation of the macroscopic density and velocity
Calculation of the local equilibrium distribution
Relaxation (local shifting of the density distributions) towards equilibrium state (collision step)
Propagation of the density distributions depending on their movement direction (stream step)
Bounce-back boundary conditions at obstacles

Advantages

- Compared to NS equations
  - NS equations are second-order PDEs. LBM consists of only first-order PDEs. This makes discretization and programming simpler.
  - NS solvers deal with the nonlinear convective term $\mathbf{u}.\nabla\mathbf{u}$. In LBM this term becomes simple advection.
  - To obtain pressure, CFD solvers use the Poisson equation. In LBM, calculated locally via an equation of state.
  - The Boltzmann equation is kinetic-based, and small-scale details can be dealt with in this method. Boundary conditions can be intuitively specified.

Advantages

- Compared to LGA
  - Statistical noise avoided.
  - Galiliean invariance can be incorporated.
  - Flow parameters like kinematic viscosity can be tuned.

- The scheme being local in space and explicit in time, LBM is scalable for parallel computing.
  - Cells interact only with their immediate neighbours. Computation workload shared by dividing the lattice into equal blocks. In practice, nature of the simulation also considered.
  - Each cell is updated synchronously.

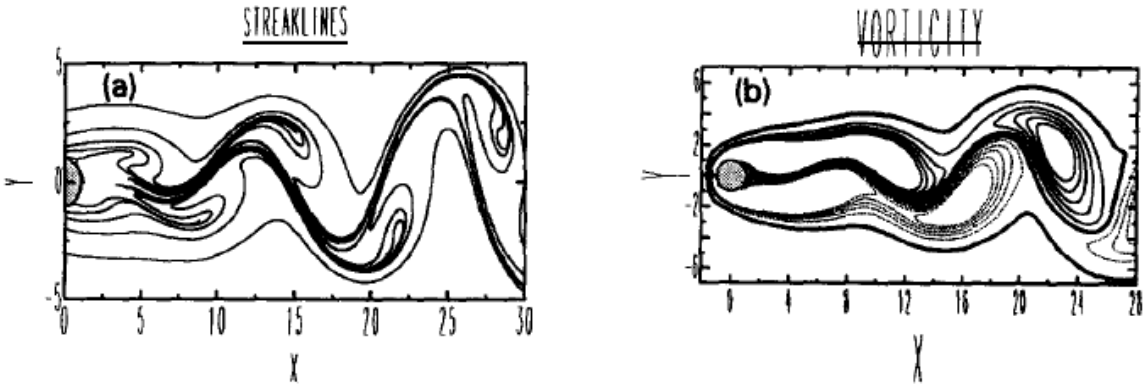
Disadvantages

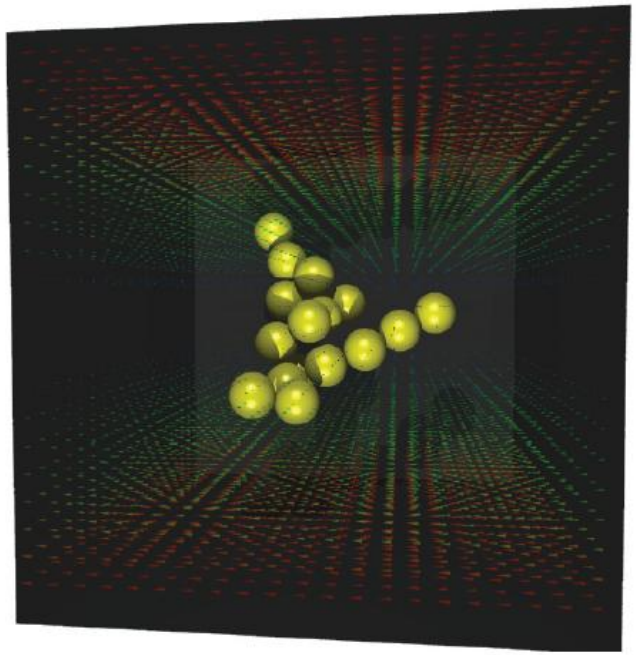
- Compared to NS equations
  - Regular square grids are a limitation. Combination of high and low resolution area, or application of curved grids is difficult.
  - Only a few commercial softwares have been developed.

- Subject to numerical instabilities, which are found to develop when the viscosity becomes small.
  - A flow speed sets up locally- local violation of Mach number.
  - Strong gradients are generated- local violation of the Knudsen number.

Applications

- Found application in many complex flows
  - Turbulent flows. Results have been validated against other methods like pseudo-spectral methods.





  - Flows in complex geometries, such as porous media. Above: moderate Reynolds number flow across a cylinder. Right: flow in the presence of particle agglomerates.

Applications

- Can be further generalized
  - Well suited to model multiphase and multicomponent flows. A state number, ‘colour’, added. It may be conserved, simulating phase-separation phenomena. Or might be redistributed in an attempt to model chemical change.
  - Can be extended to treat magnetohydrodynamics, which is the study of electrically conducting fluids. Examples are plasmas and electrolytes.
  - In order to deal with non-uniform spacing, two grids may be introduced- a fine, uniform grid hosts LBE dynamics and a coarse, non-uniform grid is a control for evaluation of fluid quantities.

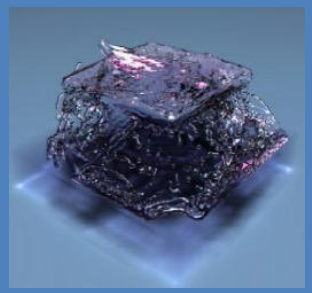
Conclusion

We have looked at

- Development of the Lattice Boltzmann Method from and the similarities with Cellular Automata and Lattice Gas Automata methods.
- Derivation of the Lattice Boltzmann Equations. The first-order Boltzmann equation and a linear collision operator was discretized in phase space and time to obtain the required equation. The equilibrium distribution was discussed.
- Algorithm of the method. The streaming, collide steps and different boundary conditions.
- Advantages and disadvantages compared to traditional CFD methods and the issue of numerical stability.
- Some areas of application, especially complex flows and extensions to the method.

References

- Cellular Automata Modeling of Physical Systems, Bastien Chopard and Michel Droz
- A single-phase free-surface Lattice Boltzmann Method, Diplomarbeit, Nils Thürey
- Lattice Boltzmann Simulation of Flow around moving Particles, Master Thesis, Klaus Igleberger
- The Lattice Boltzmann Equation: Theory and Application, R. Benzi, S. Succi, M. Vergassola



Thank You