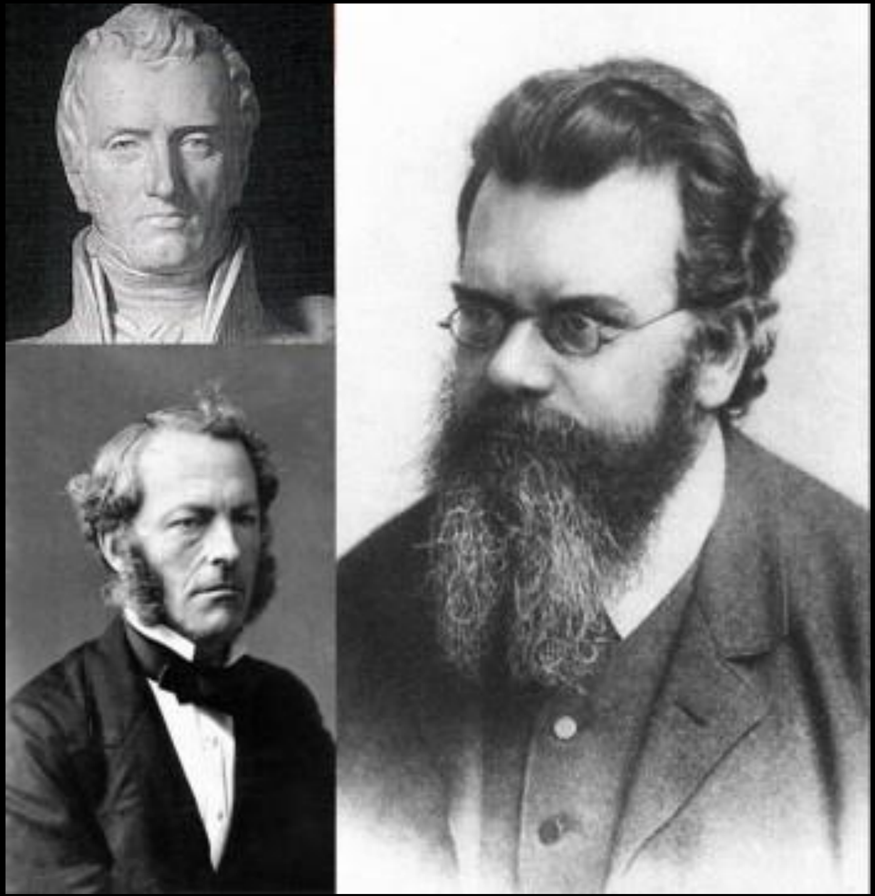
The Lattice Boltzmann Method

Bahman Sheikh and Nirjhor Chakraborty

Claude-Louis Navier



Sir George Stokes   Ludwig Boltzmann

Numerical Microscope for Fluid Mechanics

Microscopic Model

using

Mesoscopic Kinetic Equations

to solve

Macroscopic Fluid Mechanics

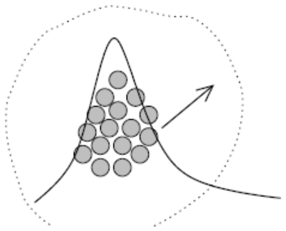
source: Michael C. Sukop

Introduction

Meso Scale

Lattice Gas Cellular Automata (LGCA)

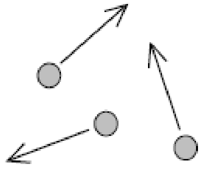
Lattice Boltzmann Method (LBM)



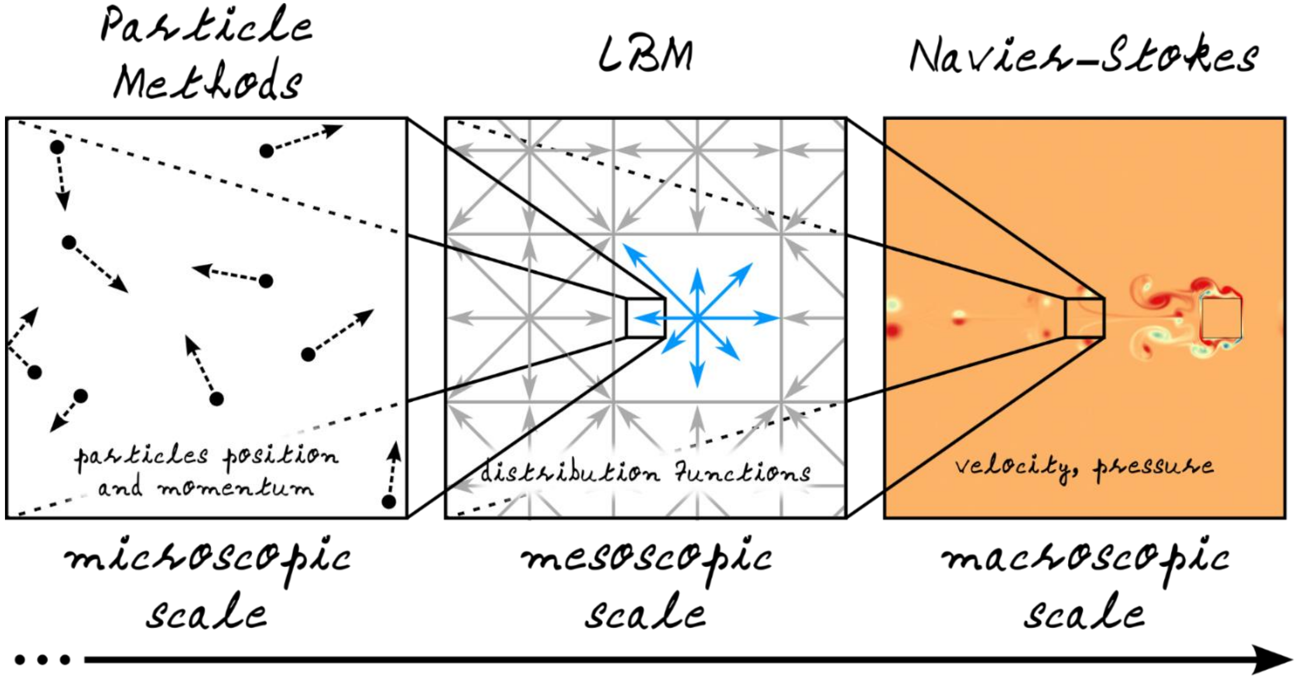
Micro Scale (Bottom Up)

Molecular Dynamics
(Hamilton’s Equation)

Direct Simulation Monte Carlo
(DSMC)

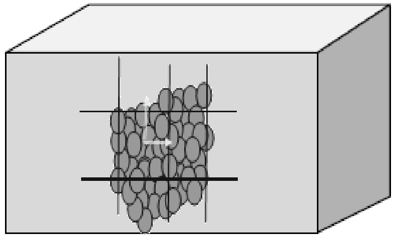


Modelling individual
molecules



Continuum (Top Down)

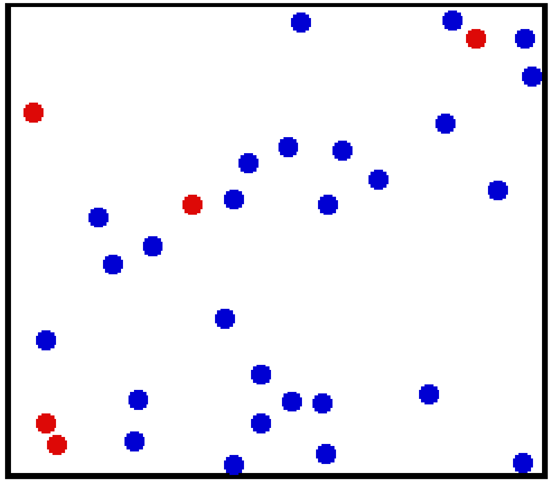
Finite Element
Finite Volume
Finite Difference
Spectral Methods



Solving PDE
Navier Stokes

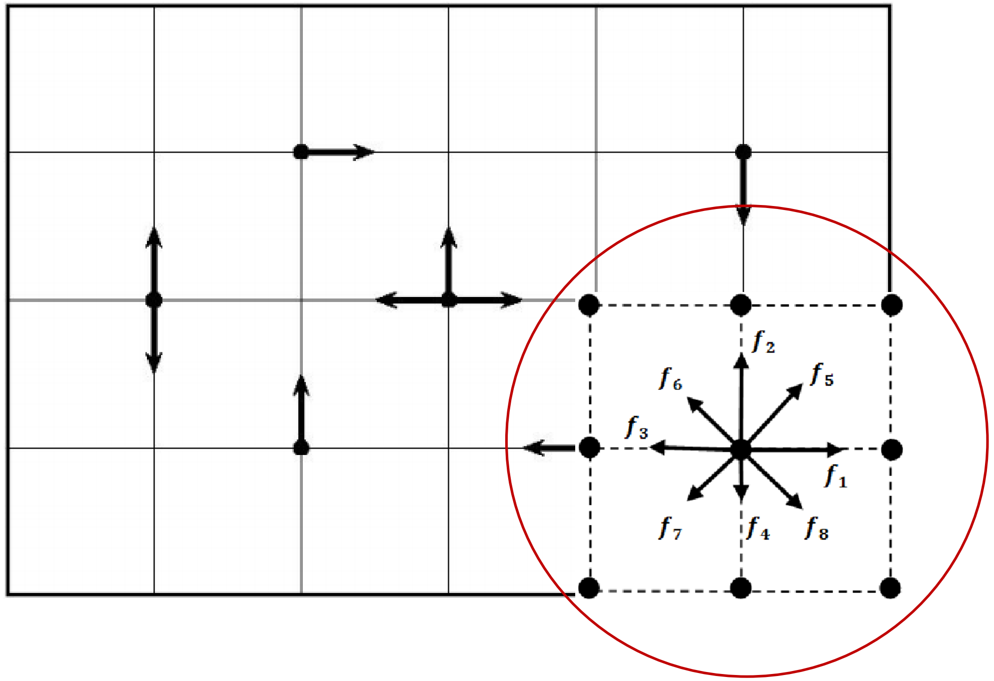
source: Mele 2013

General Principles

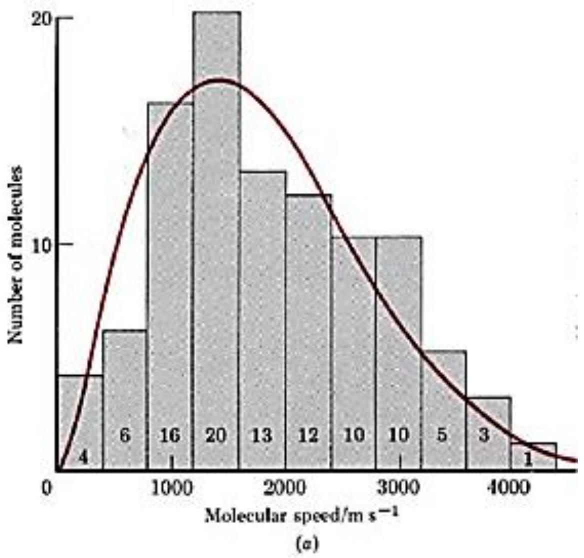


Molecular Behavior

Lattice Gas Automata



The Boltzmann Distribution



Boltzmann Kinetic Equation

$$\frac{\partial f}{\partial t} + \boldsymbol{e} \cdot \nabla f + \frac{\boldsymbol{F}}{m}\frac{\partial f}{\partial \boldsymbol{e}} = \Omega(f)$$

Lattice Boltzmann

$$f_i(x + e_i \Delta t, t + \Delta t) - f(x,t) = -\frac{\left[f_i(x,t) - f_i^{eq}(x,t)\right]}{\tau}$$

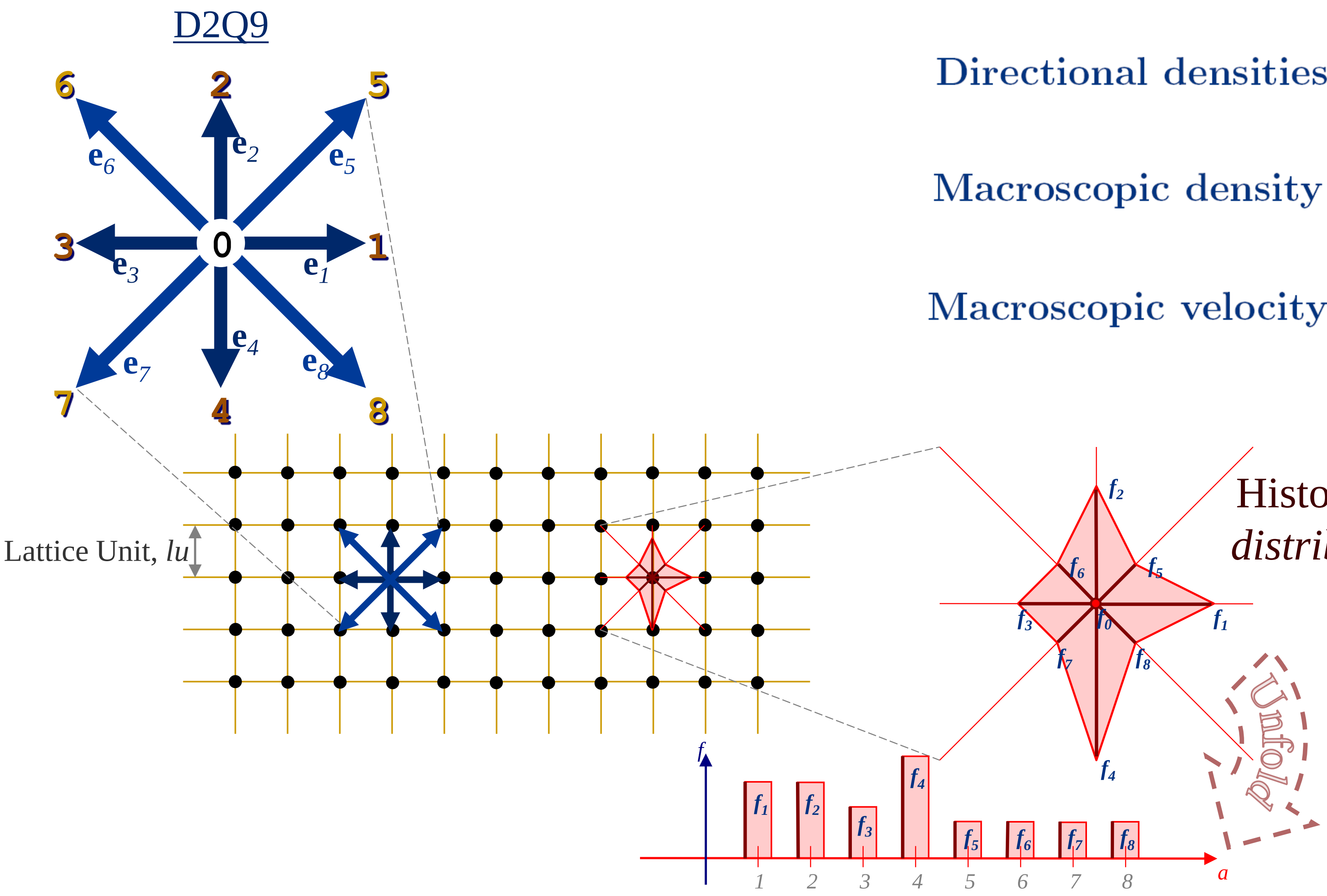
General Principles

Discrete Velocities $\mathbf{e}_a$

Directional densities f_a

Macroscopic density $\rho = \sum_{a=0}^{8} f_a$

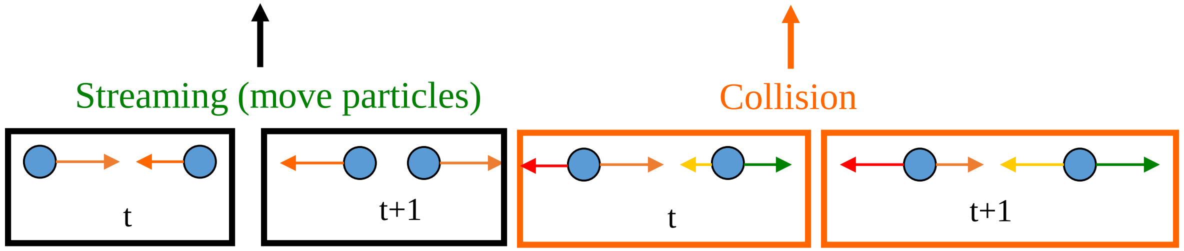
Macroscopic velocity $\mathbf{u} = \frac{1}{\rho} \sum_{a=0}^{8} f_a \mathbf{e}_a$

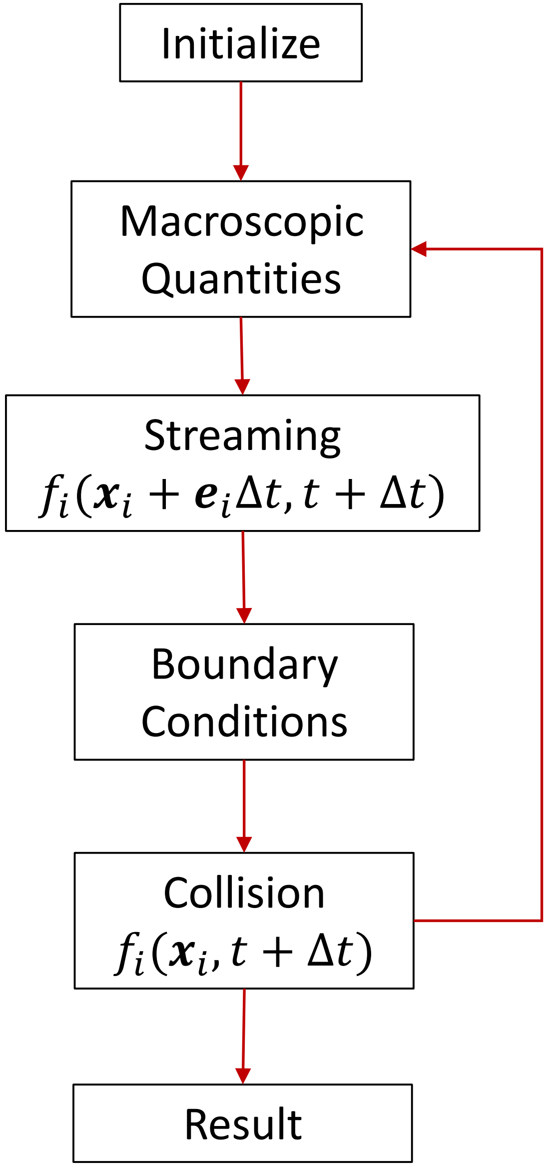


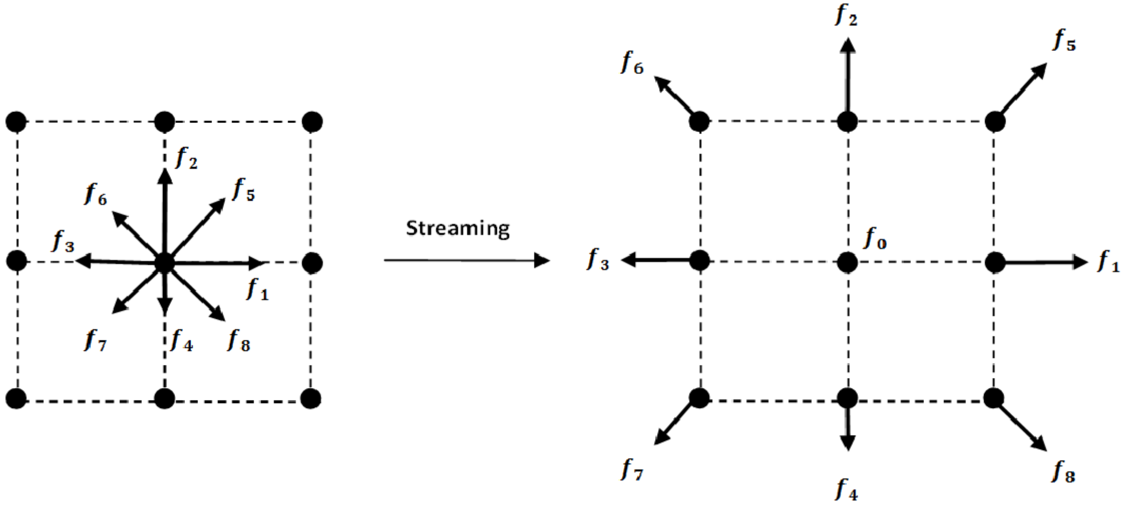
Histogram view of the *distribution function, f.*

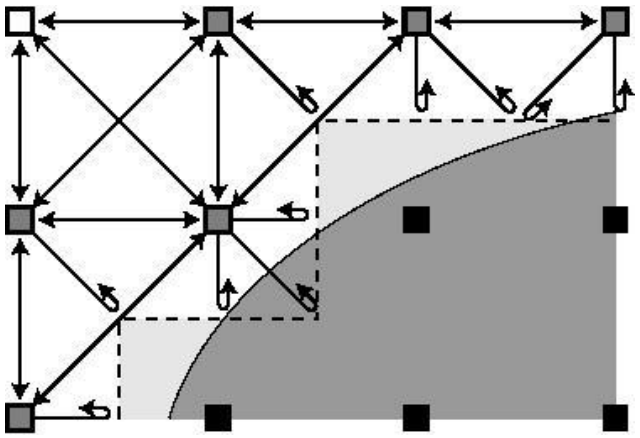
The Algorithm

$$f_i(x + e_i\Delta t, t + \Delta t) - f(x,t) = -\frac{[f_i(x,t) - f_i^{eq}(x,t)]}{\tau}$$









Source: Bao and Meskas 2011

History

Cellular Automata

- Stanislaw Ulam and John von Neumann 1940s

Lattice Gas Cellular Automata (LGCA)

- Hardy, de Pazzis, Pomeau 1973

Square grid, failed

- Frisch, Hasslacher, Pomeau 1986

Hexagonal grid, Recovered Navier-Stokes

Lattice Boltzmann Model

- McNamara and Zanetti 1988

Suggested Boltzmann Statistics, removed statistical noise

- Qian et al. 1992

Replaced collision matrix, Single relaxation time (BGK)

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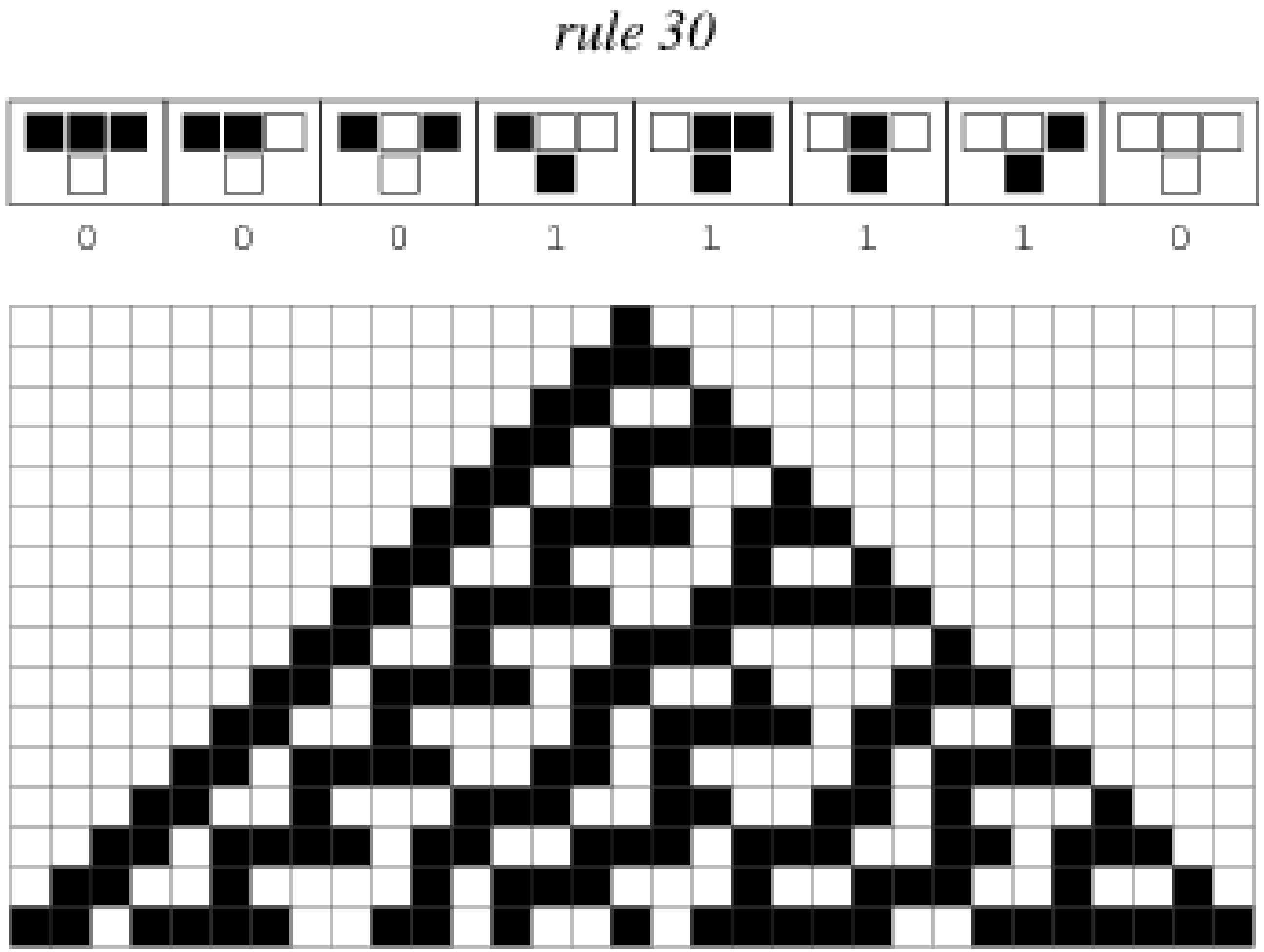

source: Wolfram Mathworld

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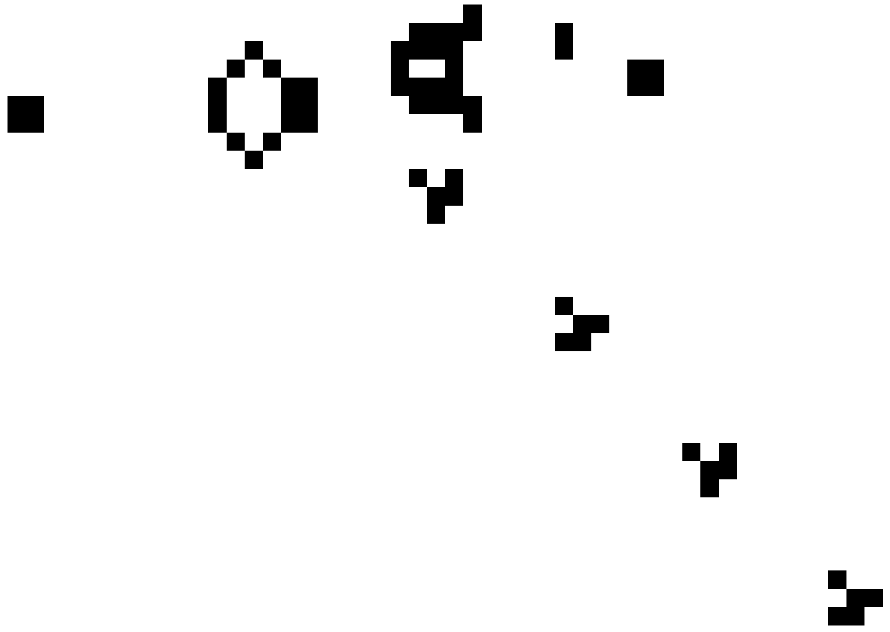

source: [Wikipedia-Cellular Automaton]

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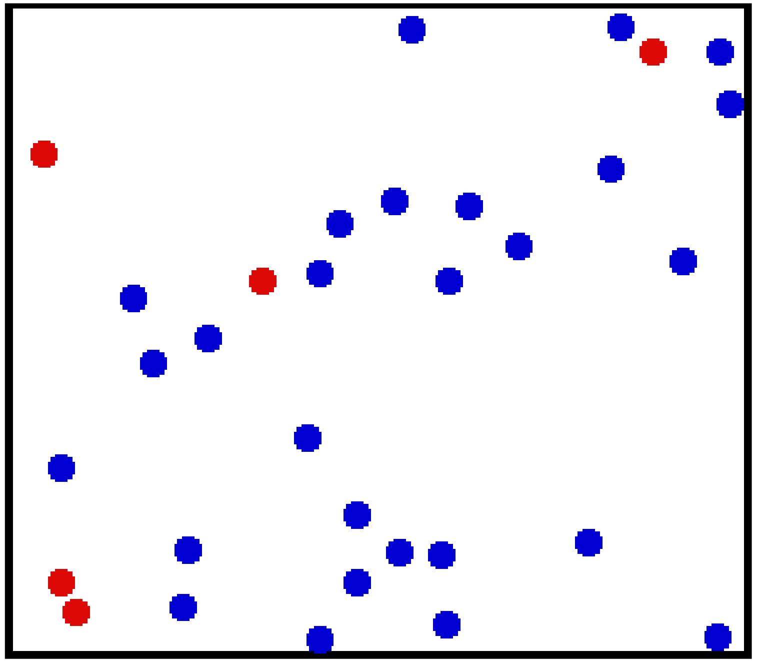

$$Re = \frac{vL}{\nu}$$

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Cellular Automata

- Stanislaw Ulam and John von Neumann 1940s

$$n_i(x + e_i\Delta t, t + \Delta t) - n_i(x, t) = \Omega_i$$

$$n_i = 0,1 \qquad \Omega_i = -1,0,1$$

Lattice Gas Cellular Automata (LGCA)

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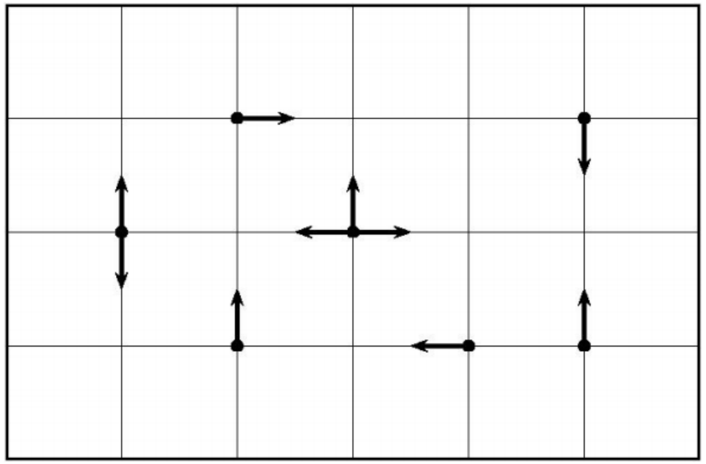

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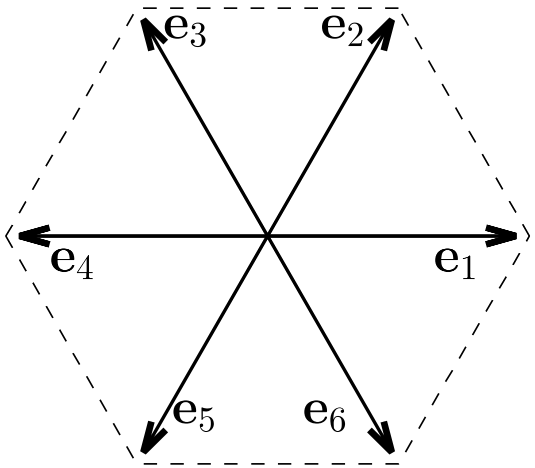

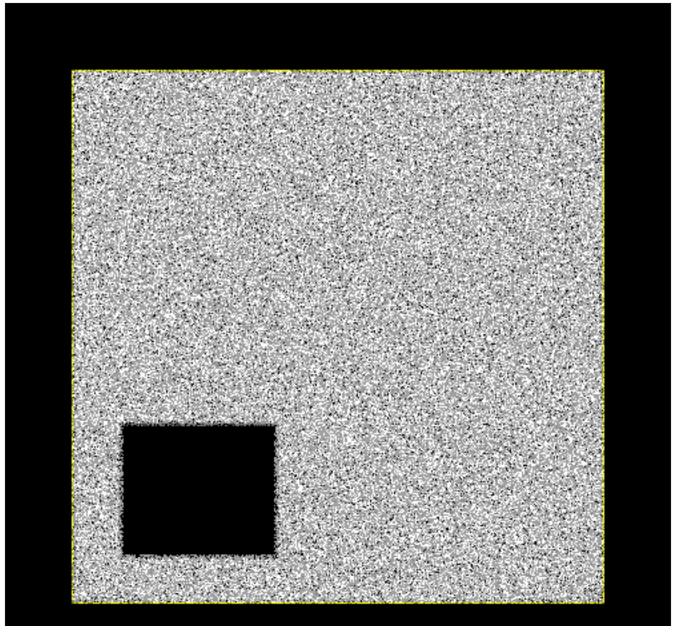

source: Wikipedia-Lattice Gas Automata

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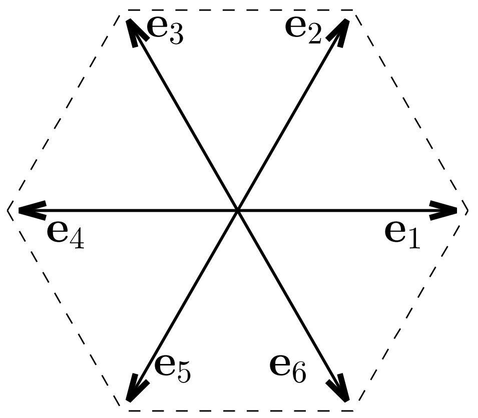

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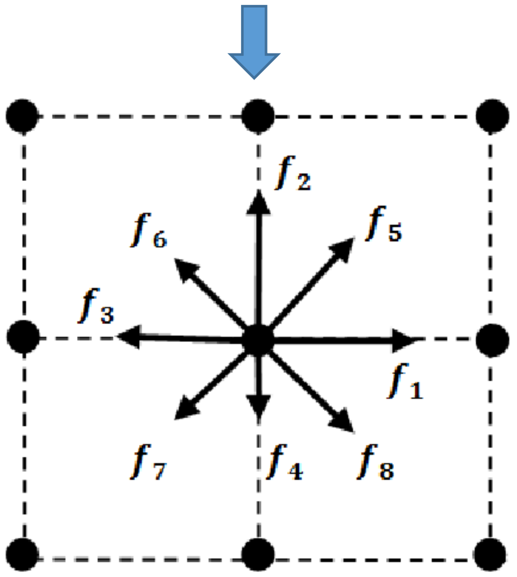

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Hexagonal grid, N-S

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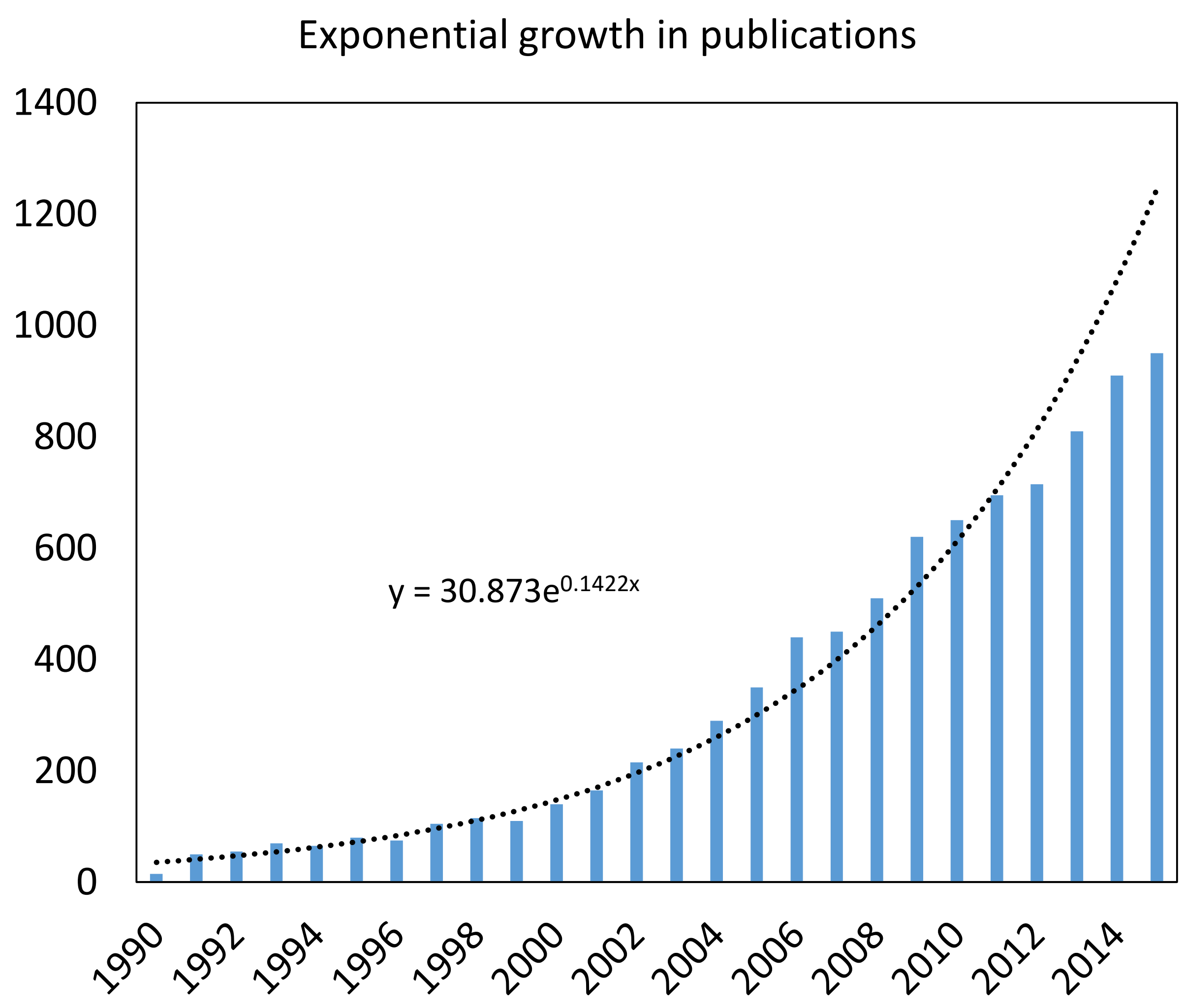


source: Web of Science

Advantages

vs. Lattice Gas Automata

- No statistical noise
- Flow parameters like viscosity can be tuned

vs. Navier Stokes

- Consists only of first order PDEs
- Simple to discretize
- No non-linear convective term to deal with
- No need to solve Poisson equation for pressure

Parallel Computing

- Near ideal (linear) scalability in parallel computing
- Cells interact only with immediate neighbors and computations done locally

Flexible Geometry

- Mesh-free
- Geometric complexity is not a challenge
- This includes the solid moving and domain deformation

Multi Phase

- Efficient inter-phase interaction handling for multiphase flow
- Phase interaction is inherently included in the particle collisions

Current Drawbacks

Lattice-Boltzmann Space – Real Space

- Hard to prescribe compressibility and permeability
- Thermo-hydrodynamics missing

Under Development

Computationally Expensive

- Uniform square grids
- Cannot combine high and low resolution regions

Only for Low Mach Number

- The f^{eq} in the BGK (Bhatnagar-Gross-Krook) collision operator is an expansion of the Maxwell-Boltzmann distribution function
- Particles can only move 1 lattice step per unit time

Numerical Instabilities

Cannot handle very low viscosity,

Unproven for high Knudsen number regimes

- Concept of viscosity unclear in micro-pore
- New ideas like multi-relaxation time (MRT) still to be tested for validity

Lattice Boltzmann Method

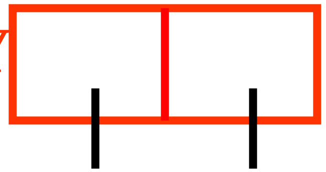
Boltzmann’s idea

LBM Nomination

Common lattice nomination:

Qian et al. (1992)

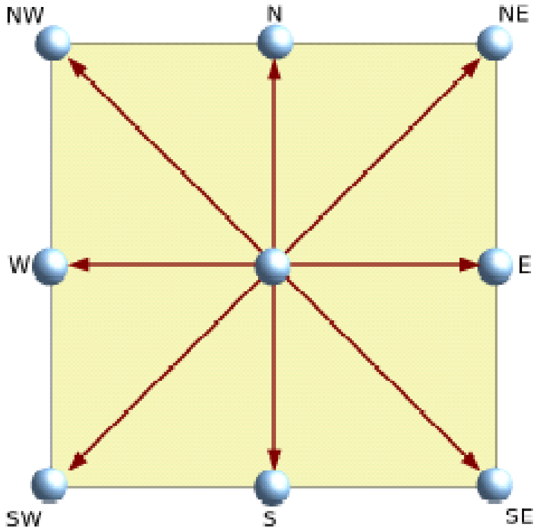
DXQY



number of dimensions

number of distinct lattice velocities

Model for two dimensions:



source: J.Götz 2006

D2Q9

- most common model in 2D
- 9 discrete velocity directions
- eight distribution functions with the particles moving to the neighboring cells
- one distribution function according to the resting particle

LBM Nomination

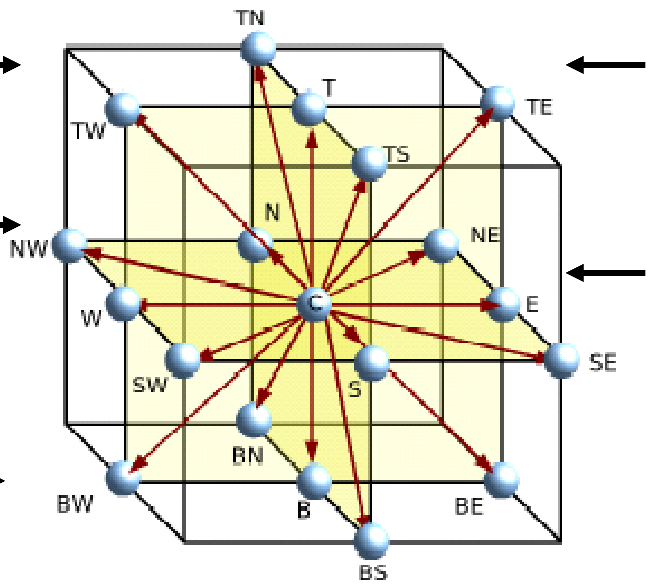
Models for three dimensions:

D3Q15	D3Q19	D3Q27
small range of stability	good compromise between the two models	highest computational effort

19 distribution functions →

one stationary velocity in the center for the particles at rest →

6 velocity directions along the Cartesian axes →



← 12 velocities combining two coordinate directions

← resting particles don`t move in the following time step, but: changing amount of resting particles due to collisions

source: J.Götz 2006

Streaming and Collision

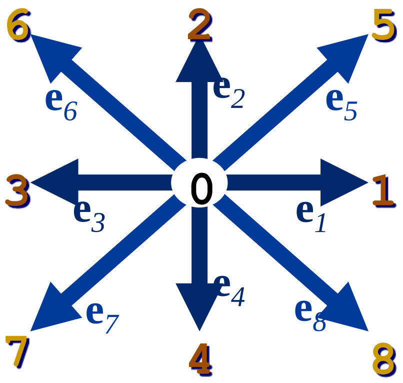
$$f_a(x + e_a \Delta t, t + \Delta t) = f_a(x,t) - \Omega$$

streaming

collision

Single relaxation time, Bhatnagar-Gross-Krook (BGK):

$$f_a(x + e_a \Delta t, t + \Delta t) = f_a(x,t) - \frac{f_a(x,t) - f_a^{eq}(x,t)}{\tau}$$



D2Q9

$a = 0 \; to \; 8$

$$f_a^{eq}(x) = w_a \rho(x)[1 + 3\frac{e_a.\boldsymbol{u}}{c^2} + \frac{9}{2}\frac{(e_a.\boldsymbol{u})^2}{c^4} - \frac{3}{2}\frac{\boldsymbol{u}^2}{c^2}]$$

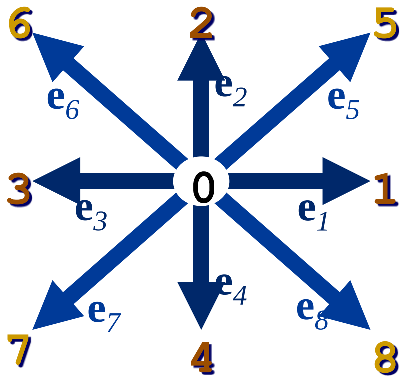
$$w_0 = \frac{4}{9}; \quad w_{1,2,3,4} = \frac{1}{9}, \quad w_{5,6,7,8} = \frac{1}{36} \qquad \rho = \sum_a f_a \qquad \boldsymbol{u} = \frac{1}{\rho}\sum_a e_a f_a$$

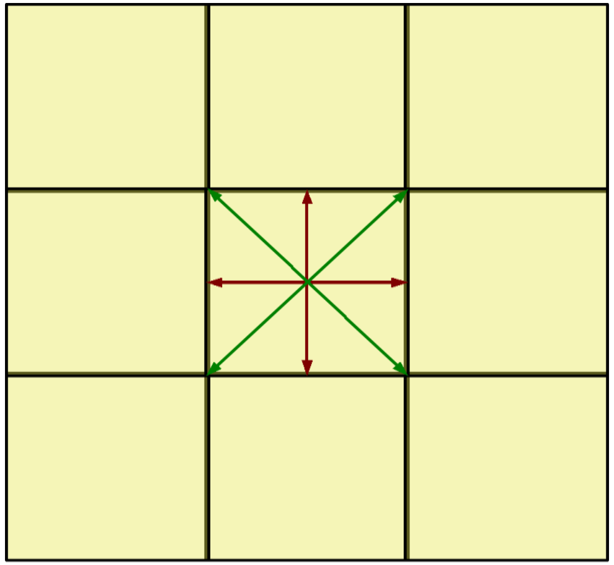
Streaming

Streaming step:

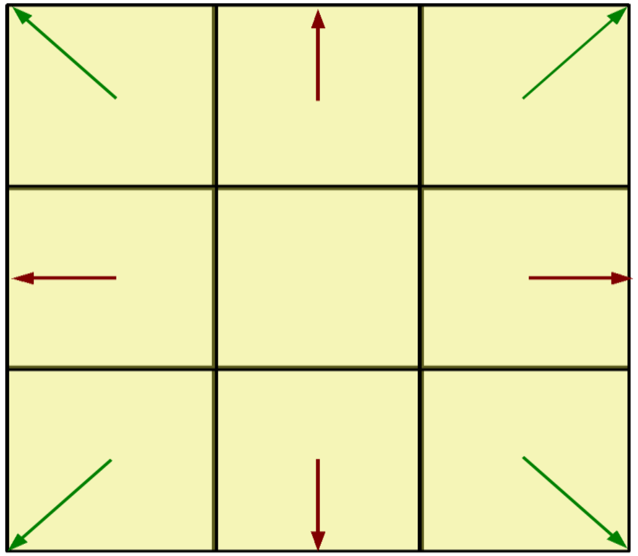
streaming of the particles to their neighboring cells according to their velocity directions.

$$f_a(x + e_a \Delta t, t + \Delta t) = f_a(x, t + \Delta t)$$



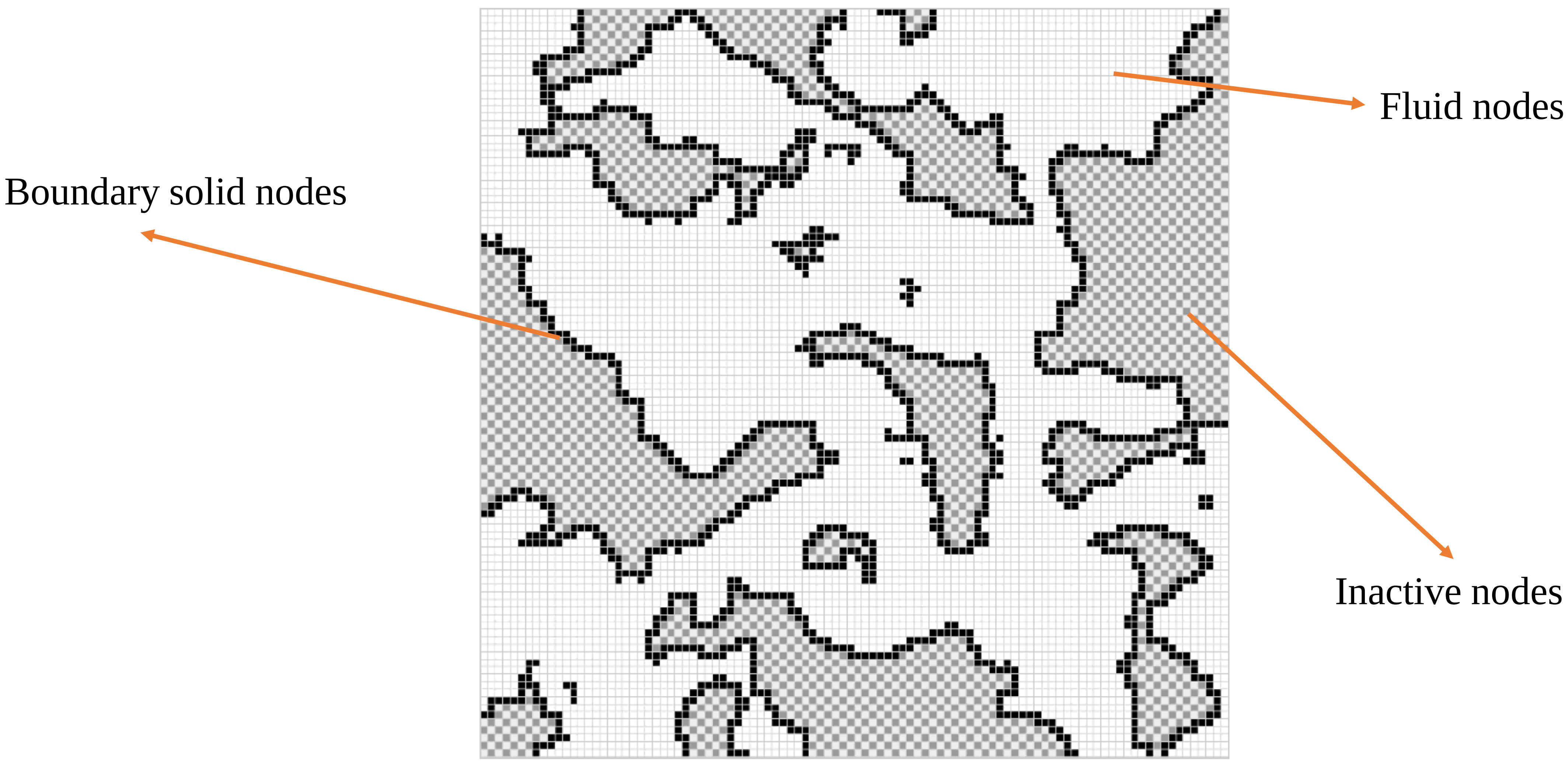


particle distribution before stream step

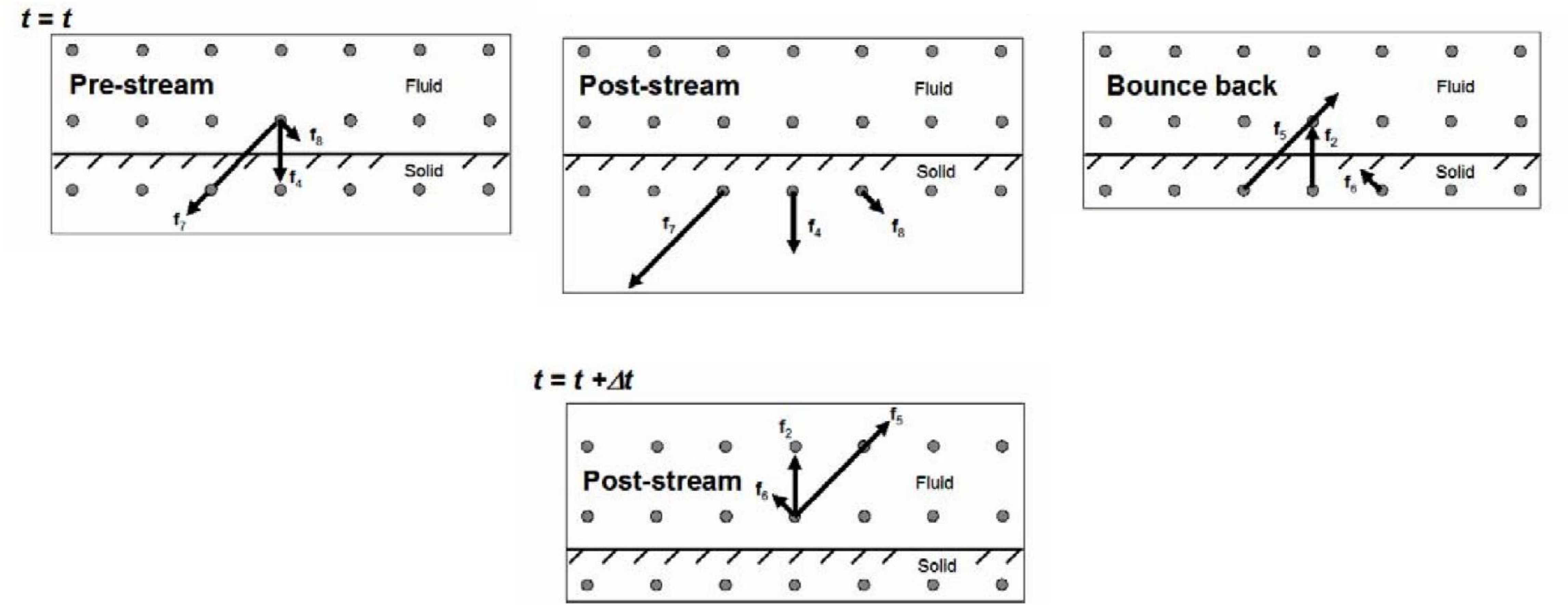


particle distribution after stream step

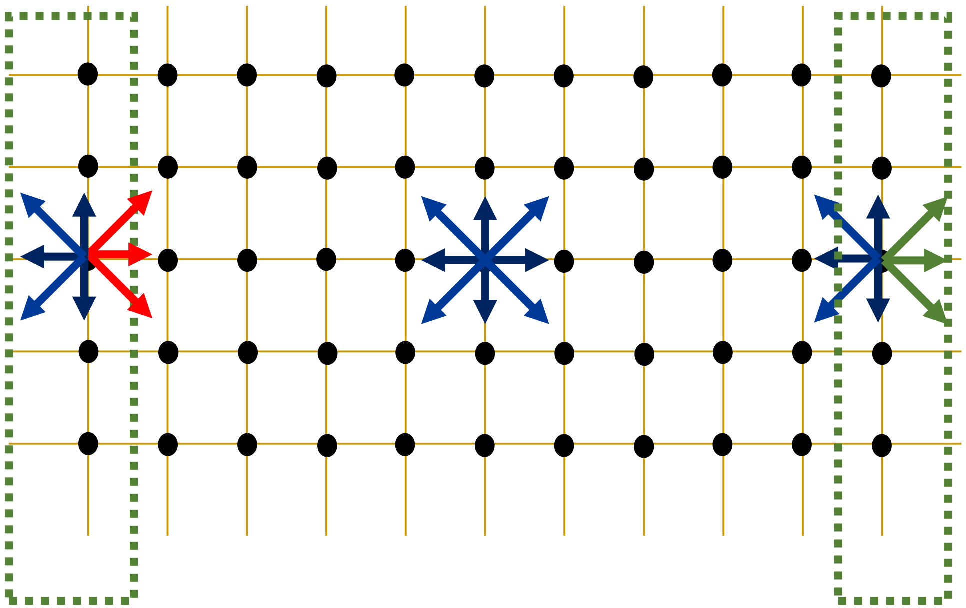
Bounceback Boundaries



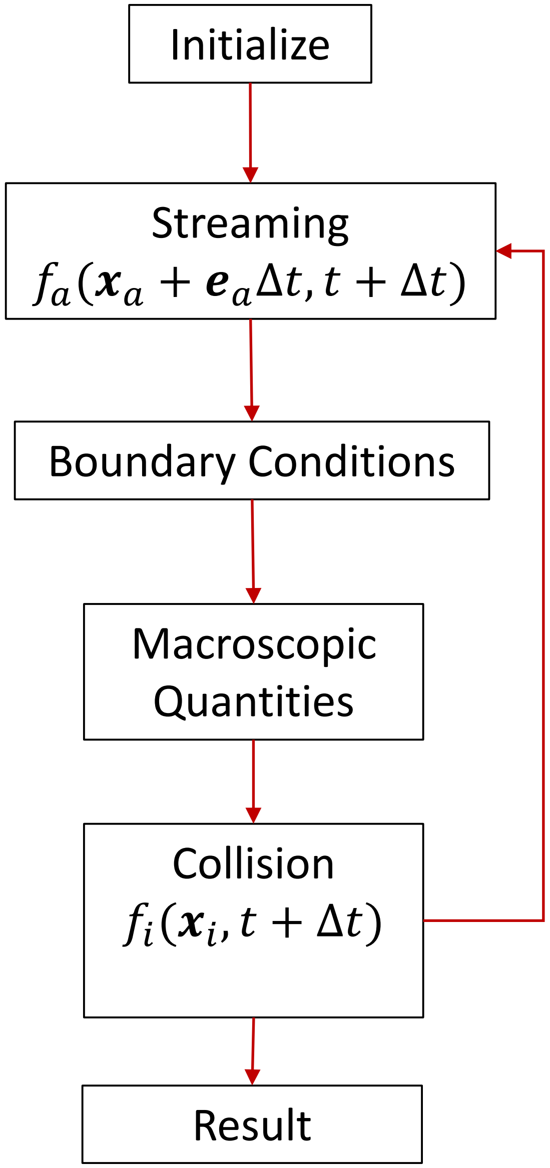
Bounceback Boundaries



Periodic Boundaries



LBM Algorithm



$$f_a(x + e_a\Delta t, t + \Delta t) = f_a(x, t + \Delta t)$$

$$\rho = \sum_a f_a \qquad \boldsymbol{u} = \frac{1}{\rho}\sum_a e_a f_a$$

$$f_a^{eq}(x) = w_a\rho(x)[1 + 3\frac{e_a.\boldsymbol{u}}{c^2} + \frac{9}{2}\frac{(e_a.\boldsymbol{u})^2}{c^4} - \frac{3}{2}\frac{\boldsymbol{u}^2}{c^2}]$$

$$f_a(x + e_a\Delta t, t + \Delta t) = f_a(x, t) - \frac{f_a(x, t) - f_a^{eq}(x, t)}{\tau}$$

Two Phase Lattice Boltzmann Method

Two phase lattice Boltzmann methods

- Gunstensen et al. (1991),
- Shan & Chen (1993, 1994)
- Free energy by Swift et al. (1995, 1996)
- …

➢ Nourgaliev et al. (2005)

Shan-Chen Two Phase Formulation

- Fluid-Fluid forces:

$$F_{c,\sigma} = -G_c \rho_\sigma(x,t) \sum_m w_m \rho_{\bar{\sigma}}(x + e_m \Delta t, t) e_m$$

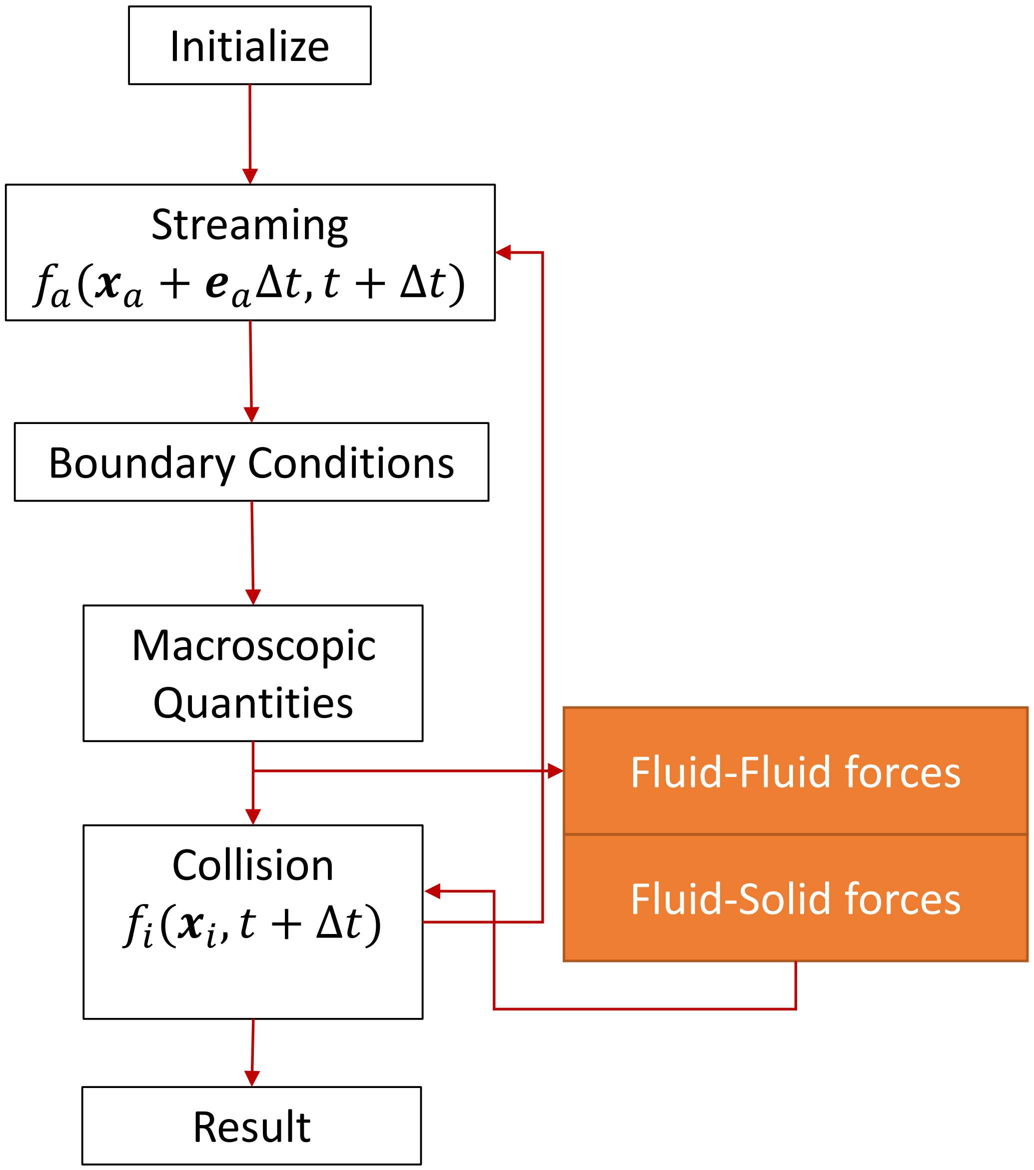
- Solid-Fluid forces:

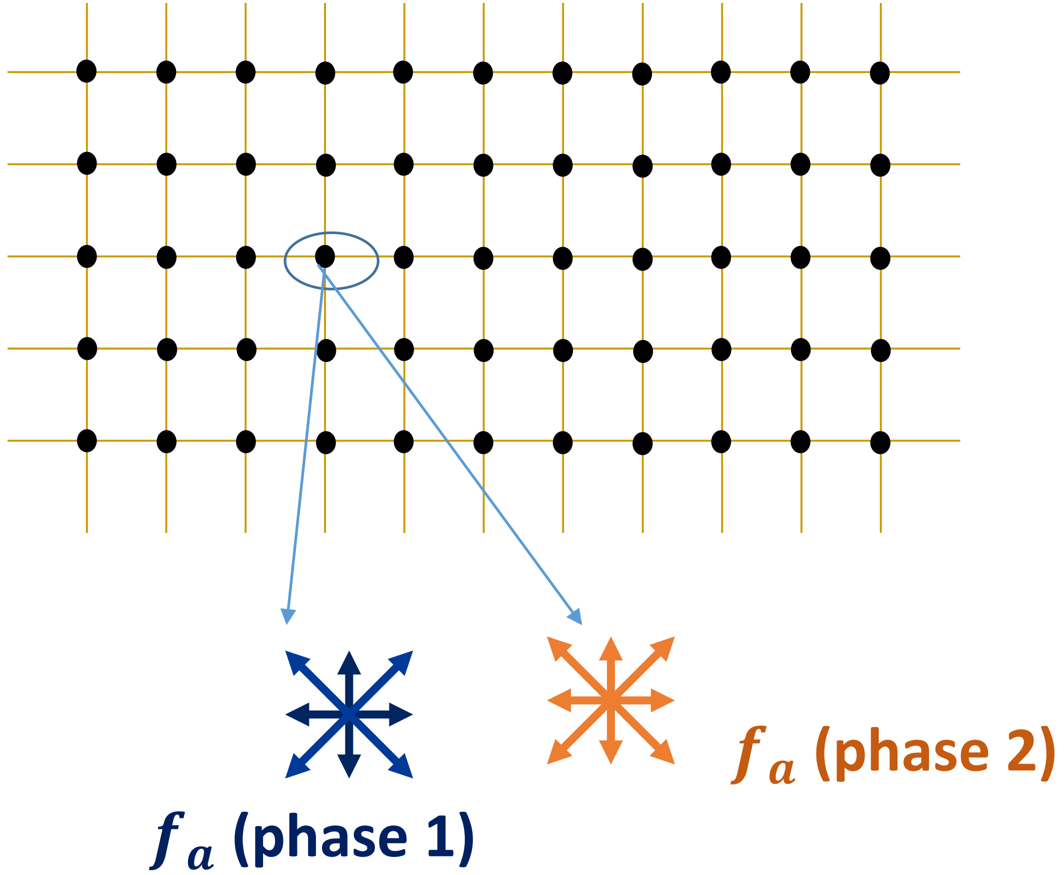
$$F_{a,\sigma} = -G_{a,\sigma} \rho_\sigma(x,t) \sum_m w_m s(x + e_m \Delta t, t) e_m$$

- Incorporating external forces on each phase

$$\vec{u}' = \frac{\sum_\sigma \left(\sum_m \frac{f_m^\sigma \vec{e}_m}{\tau_\sigma} \right)}{\sum_\sigma \frac{\rho_\sigma}{\tau_\sigma}} \qquad \vec{u}_\sigma^{eq} = \vec{u}' + \frac{\tau_\sigma F_\sigma}{\rho_\sigma}$$

LBM Algorithm (two-phase)





Calculation Example

Problem Description

- D2Q9 model
- 9 lattices
- Channel flow from left to right
- Bounce back and periodic boundary
- Initial parameter

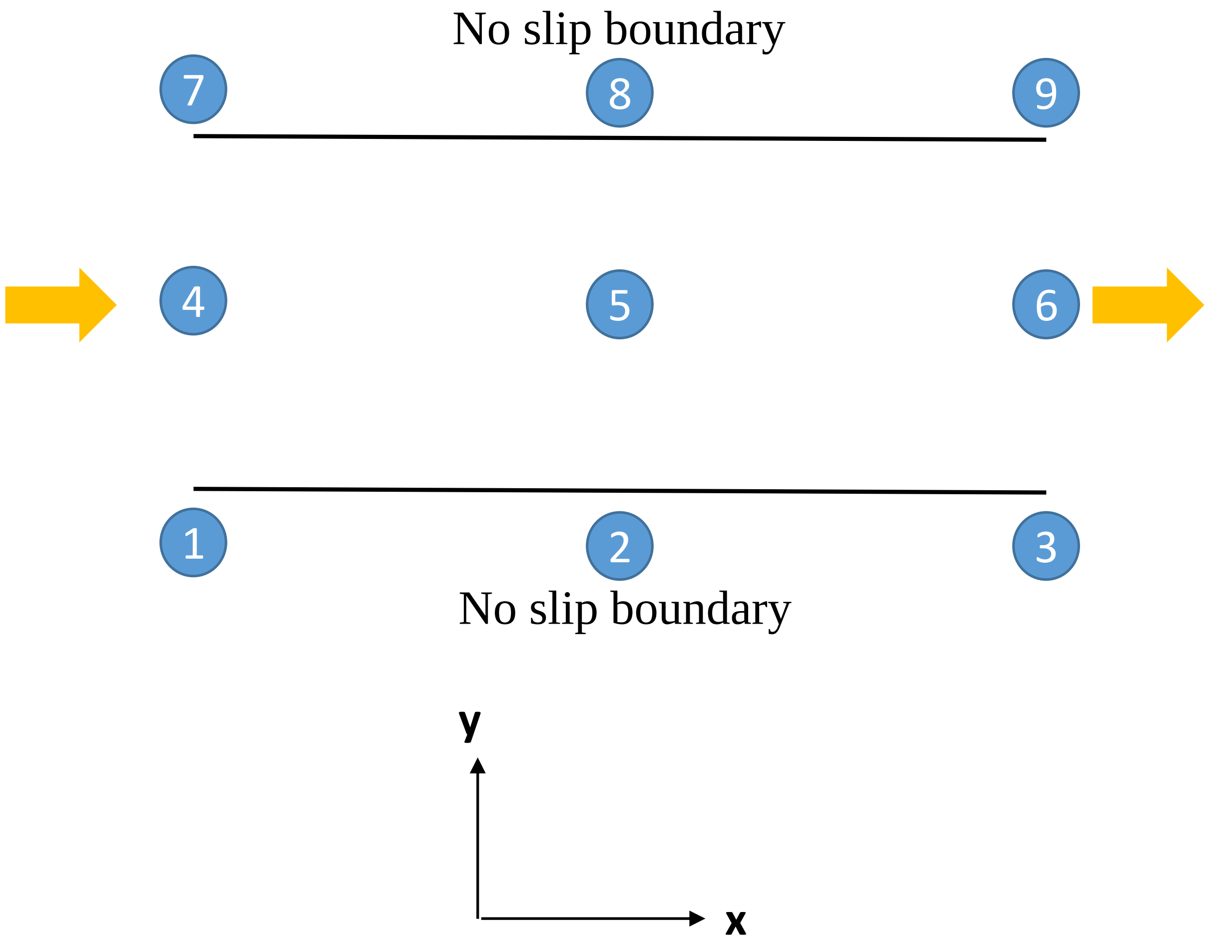
$$\rho = 1.0\ \frac{\text{gr}}{cm^3}$$

$$a = 0.001\ \text{cm/s}$$

$$initial\ velocity = 0.0$$

$$\tau = 1.0$$

$$c = 1.0$$



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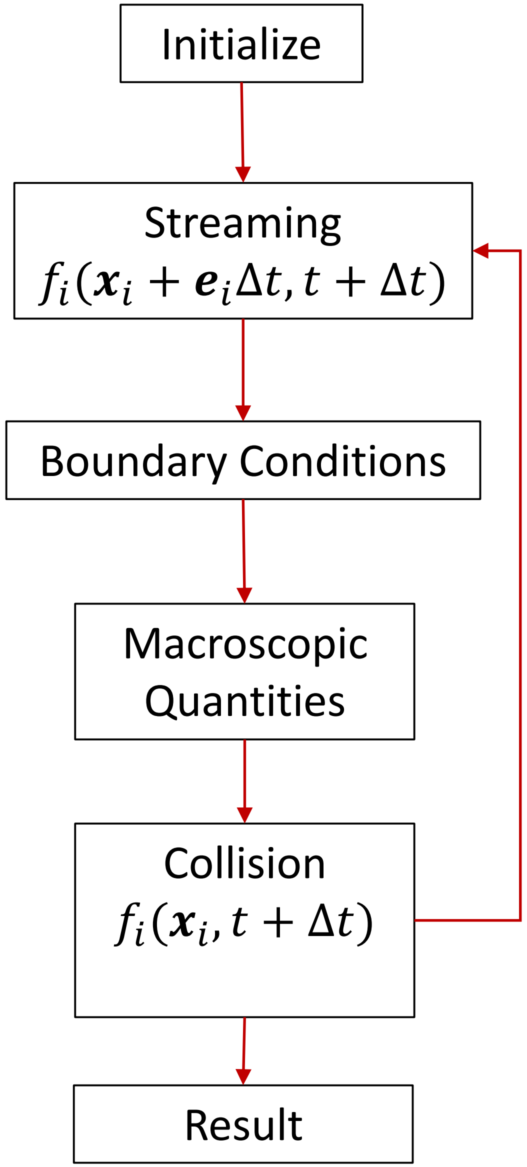
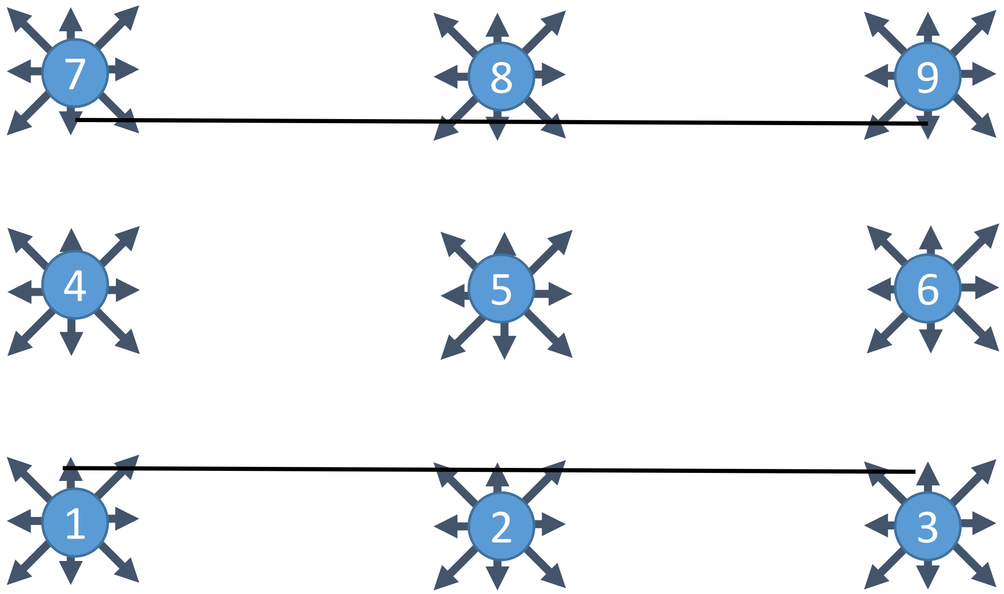


Calculation Example: Initialization



$$f_a\ (x) = w_a \rho(x)\left[1 + 3\frac{e_a.\boldsymbol{u}}{c^2} + \frac{9}{2}\frac{(e_a.\boldsymbol{u})^2}{c^4} - \frac{3}{2}\frac{\boldsymbol{u}^2}{c^2}\right]$$

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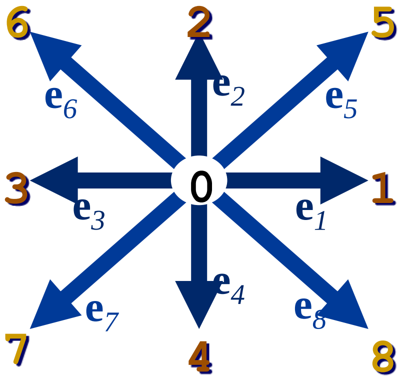


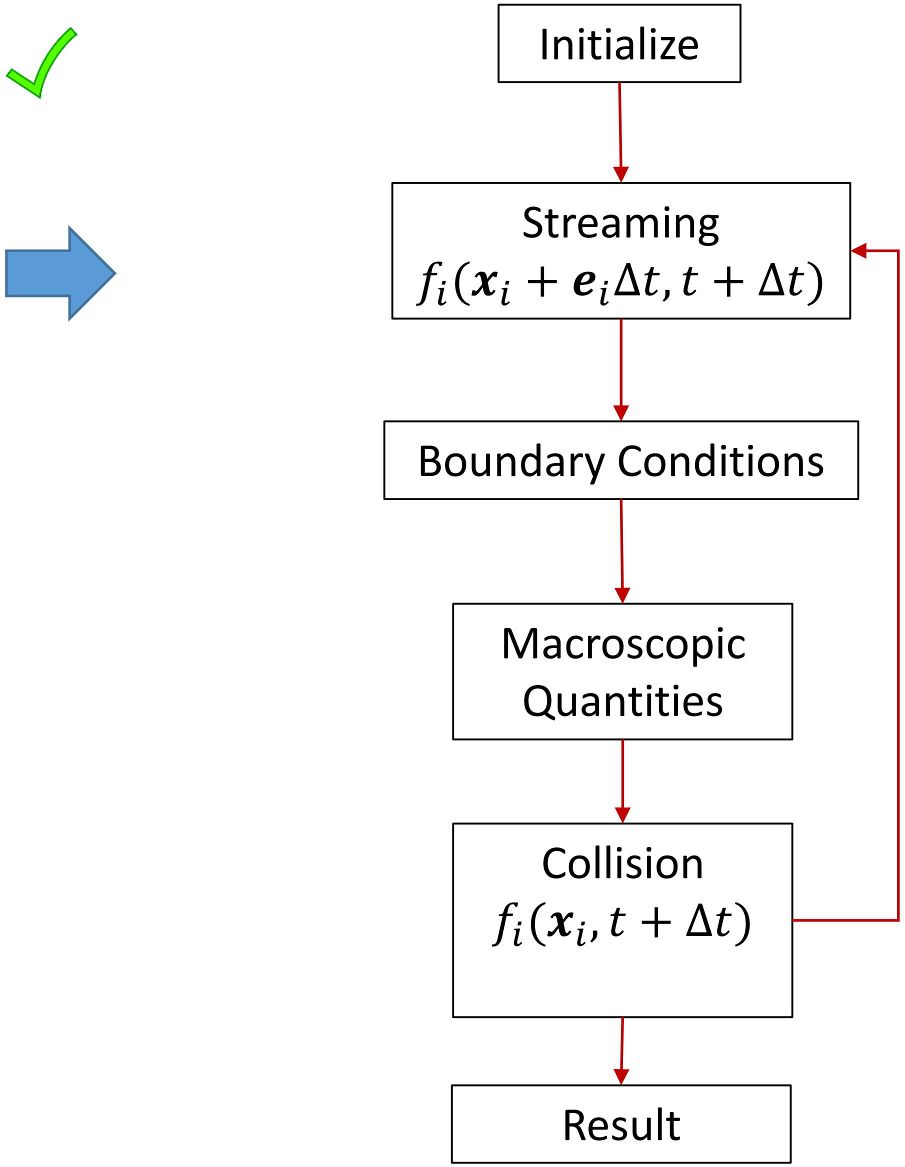
For nodes 4,5,6

$$\begin{cases} f_0 = \frac{4}{9} \\ f_{1-4} = \frac{1}{9} \\ f_{5-8} = \frac{1}{36} \end{cases}$$

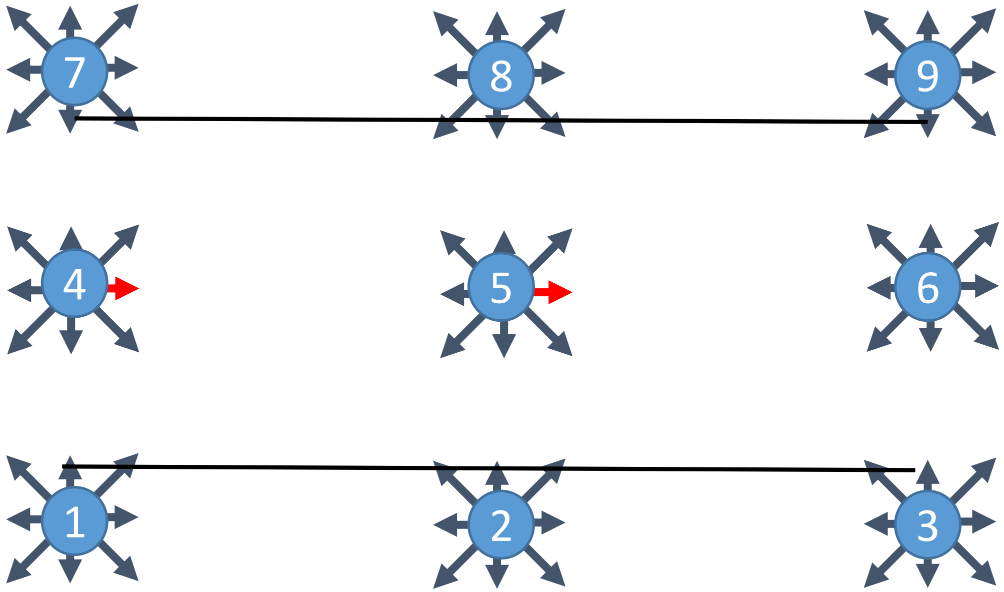
For nodes 1,2,3,7,8,9

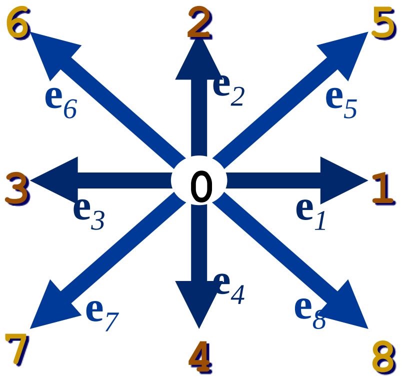
$$\begin{cases} f_0 = 0 \\ f_{1-4} = 0 \\ f_{5-8} = 0 \end{cases}$$

Calculation Example

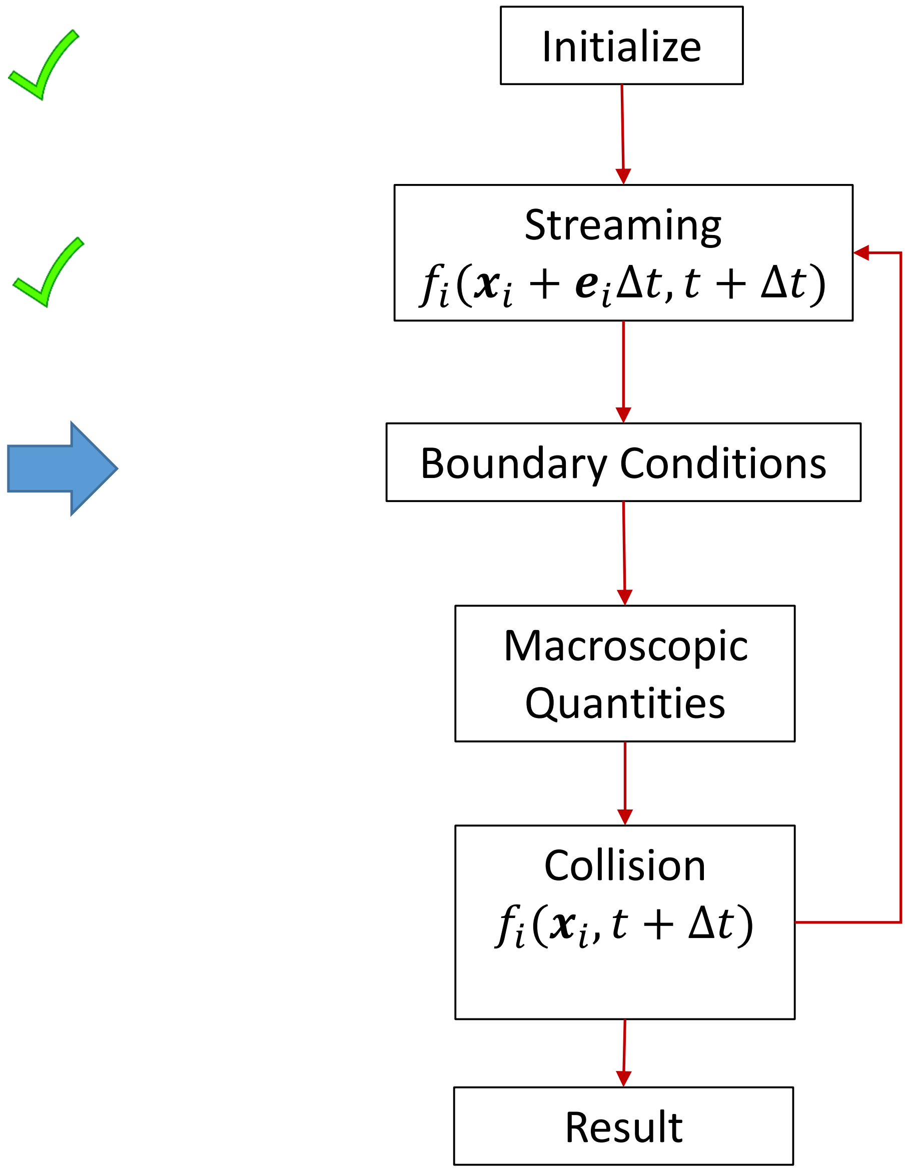


Calculation Example: Streaming

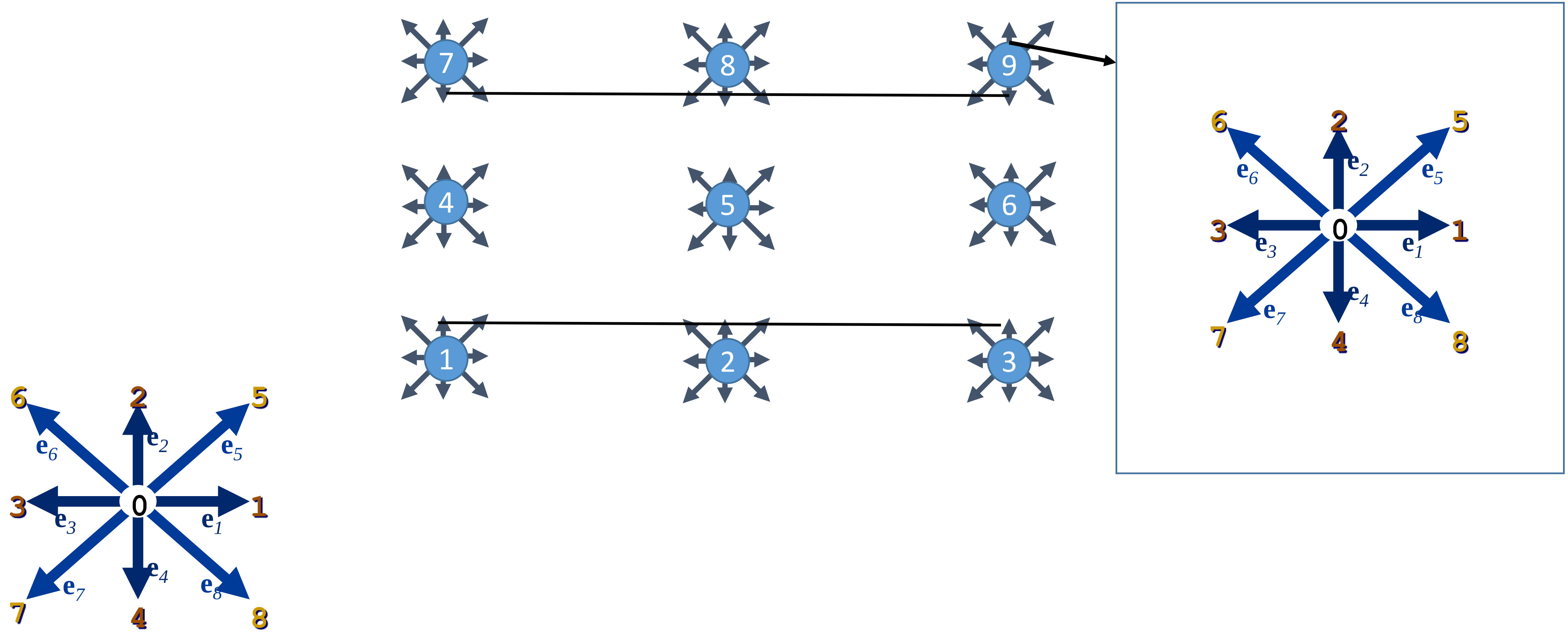




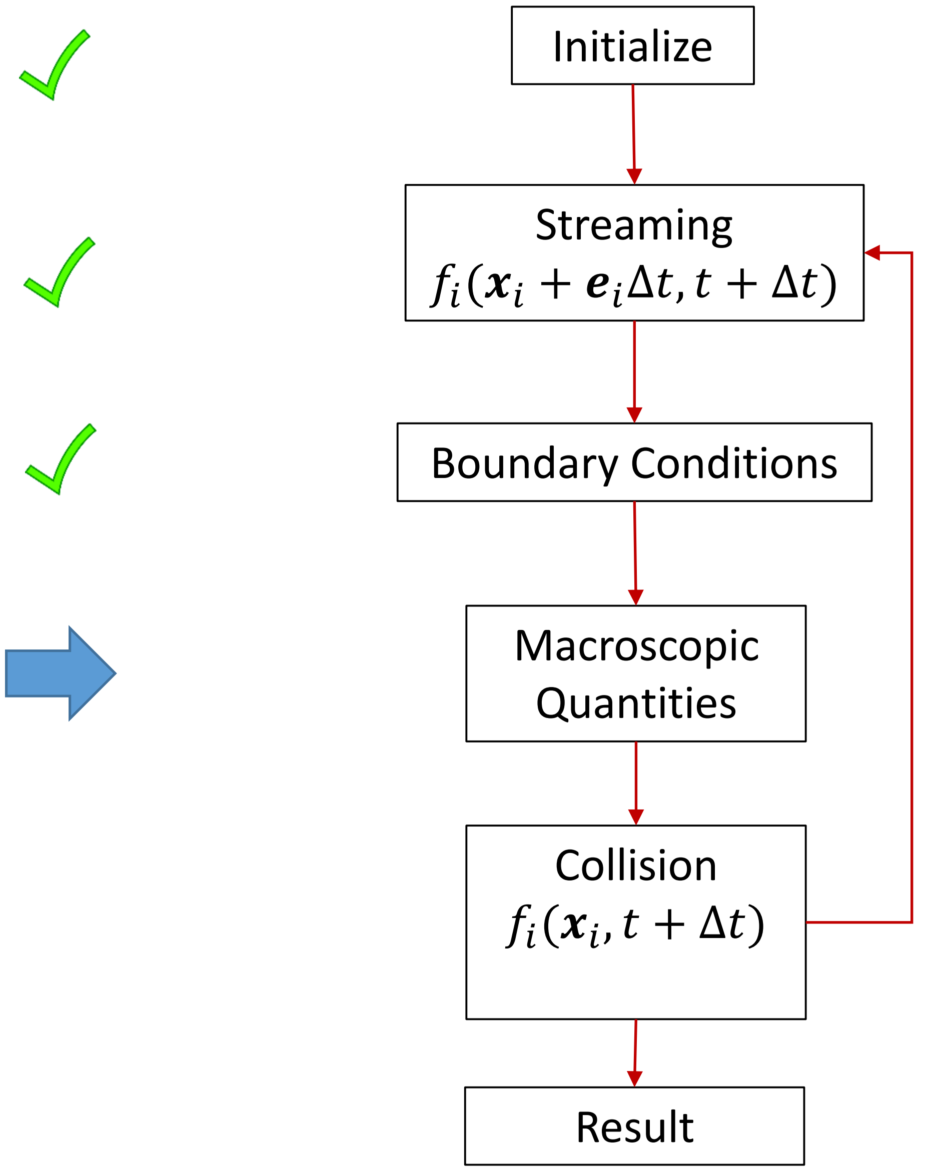
Calculation Example



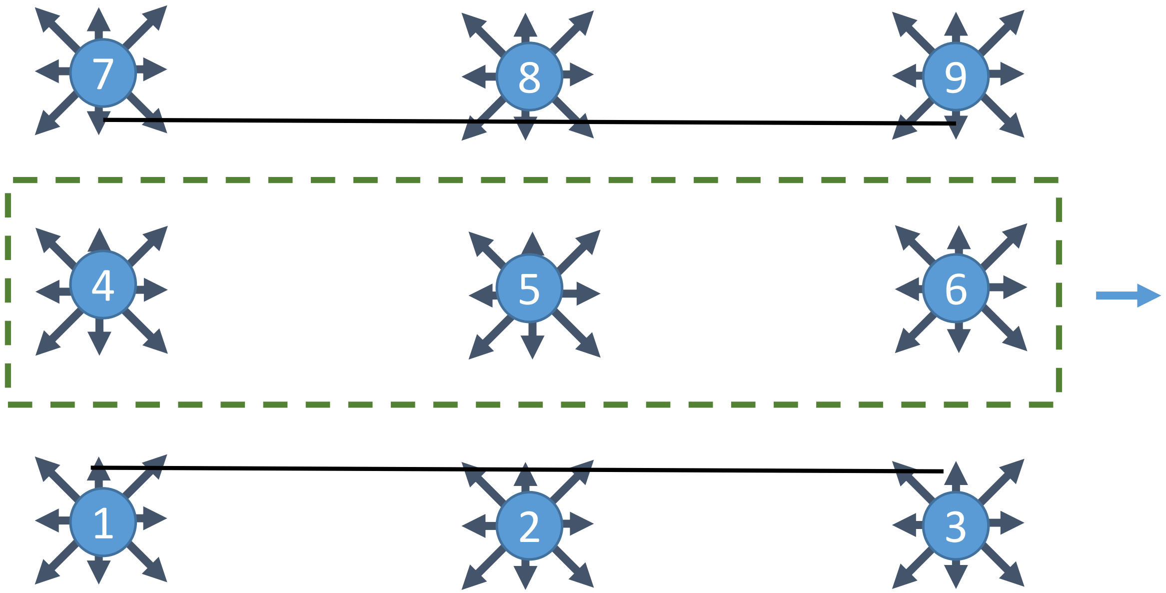
Calculation Example: Boundary conditions



Calculation Example



Calculation Example: Macroscopic Quantities

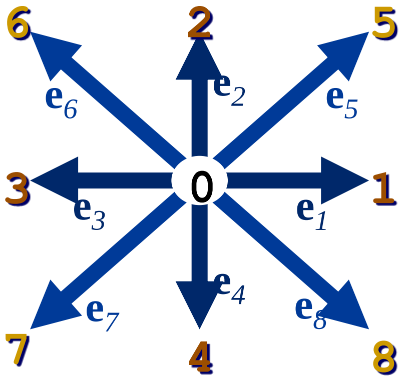


$$\rho = \sum_a f_a \quad \boldsymbol{u} = \frac{1}{\rho}\sum_a e_a f_a$$

$$u_x = \frac{1}{\rho}[(f_1 + f_5 + f_8) - (f_6 + f_3 + f_7)]$$

$$u_y = \frac{1}{\rho}[(f_2 + f_5 + f_6) - (f_4 + f_7 + f_8)]$$

$$\rho = 1, u_x = u_y = 0.0$$

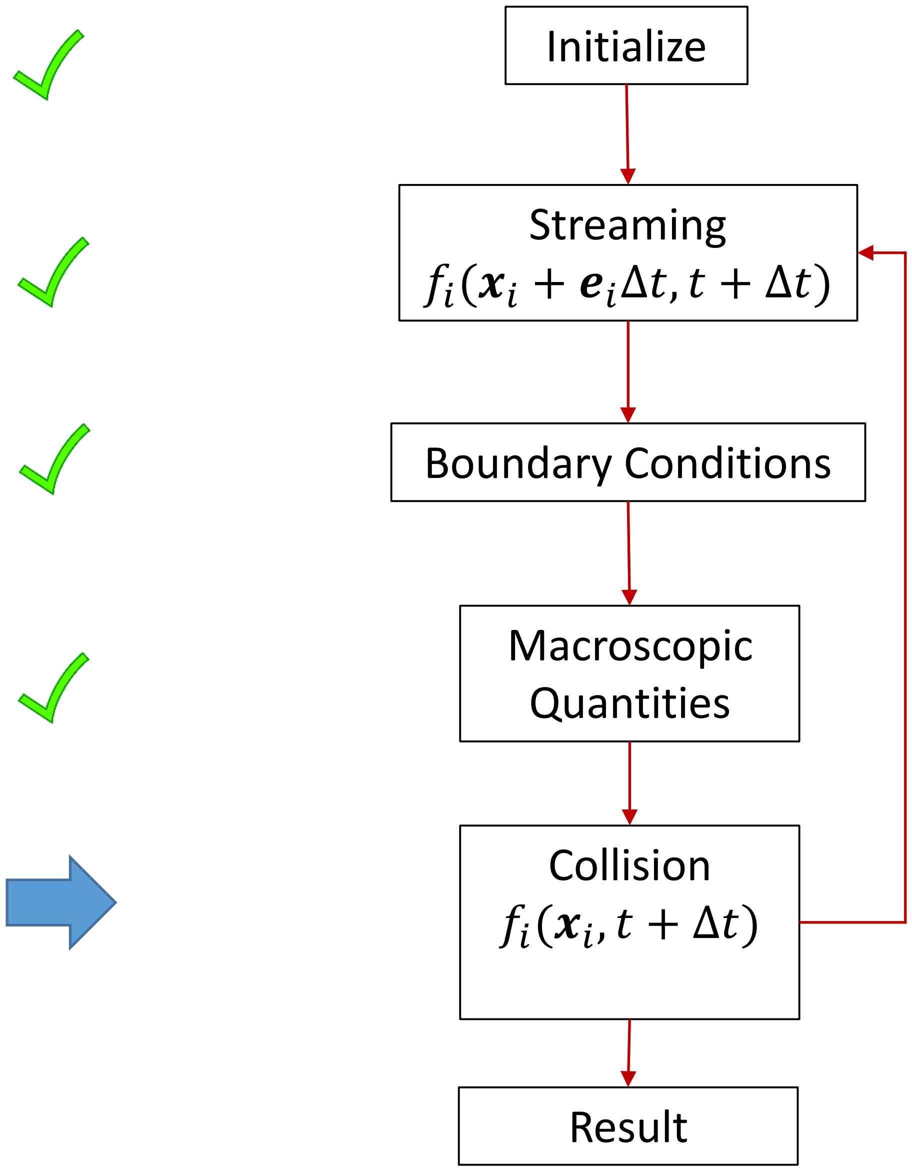


$$u = u + \frac{\tau F}{\rho}$$

$$u_x = u_x + \frac{0.001 \times 1}{1}$$

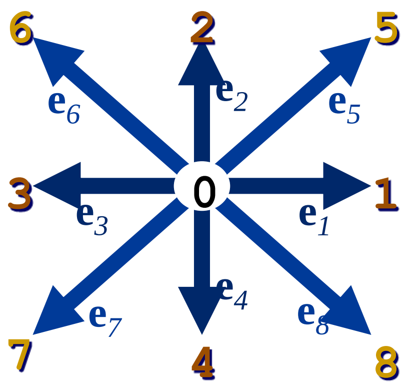
$$u_y = 0.0$$

Calculation Example



Calculation Example: Collision

$$f_a^{eq}(x) = w_a \rho(x)[1 + 3\frac{e_a.\boldsymbol{u}}{c^2} + \frac{9}{2}\frac{(e_a.\boldsymbol{u})^2}{c^4} - \frac{3}{2}\frac{\boldsymbol{u}^2}{c^2}]$$



$$u = \begin{pmatrix} u_x \\ u_y \end{pmatrix} \qquad e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad e_6 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$\boldsymbol{f_1^{eq}(4)}$:

$$u = \begin{pmatrix} 0.001 \\ 0 \end{pmatrix} \qquad w_1 = \frac{1}{9}, \qquad \rho(4) = 1.0$$

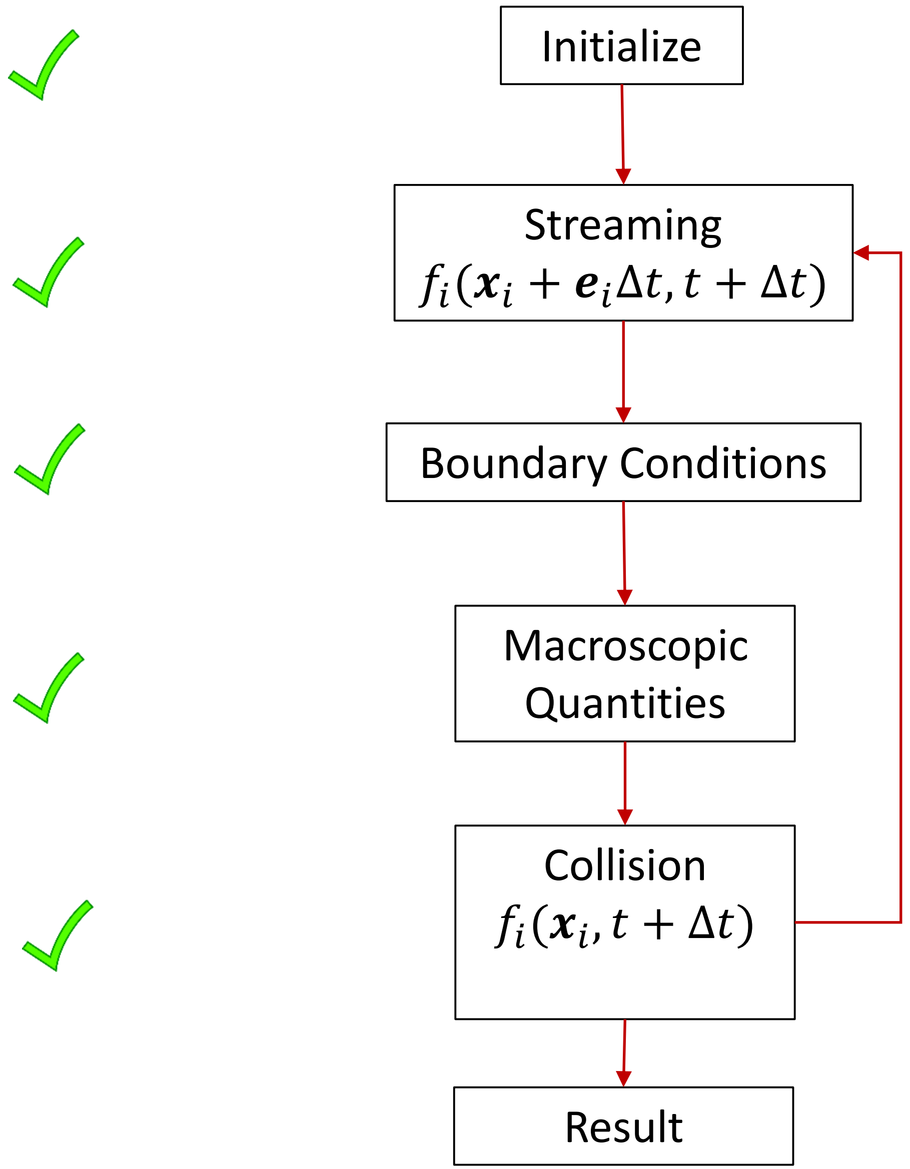
$$e_1.u = 0.001 \longrightarrow f_1^{eq}(4) = 0.111445$$

$$f_a(\boldsymbol{X} + e_a \Delta t, t + \Delta t) = f_a(\boldsymbol{x}, t) - \frac{[f_a(\boldsymbol{x}, t) - f_a^{eq}(\boldsymbol{x}, t)]}{\tau}$$

new ***old***

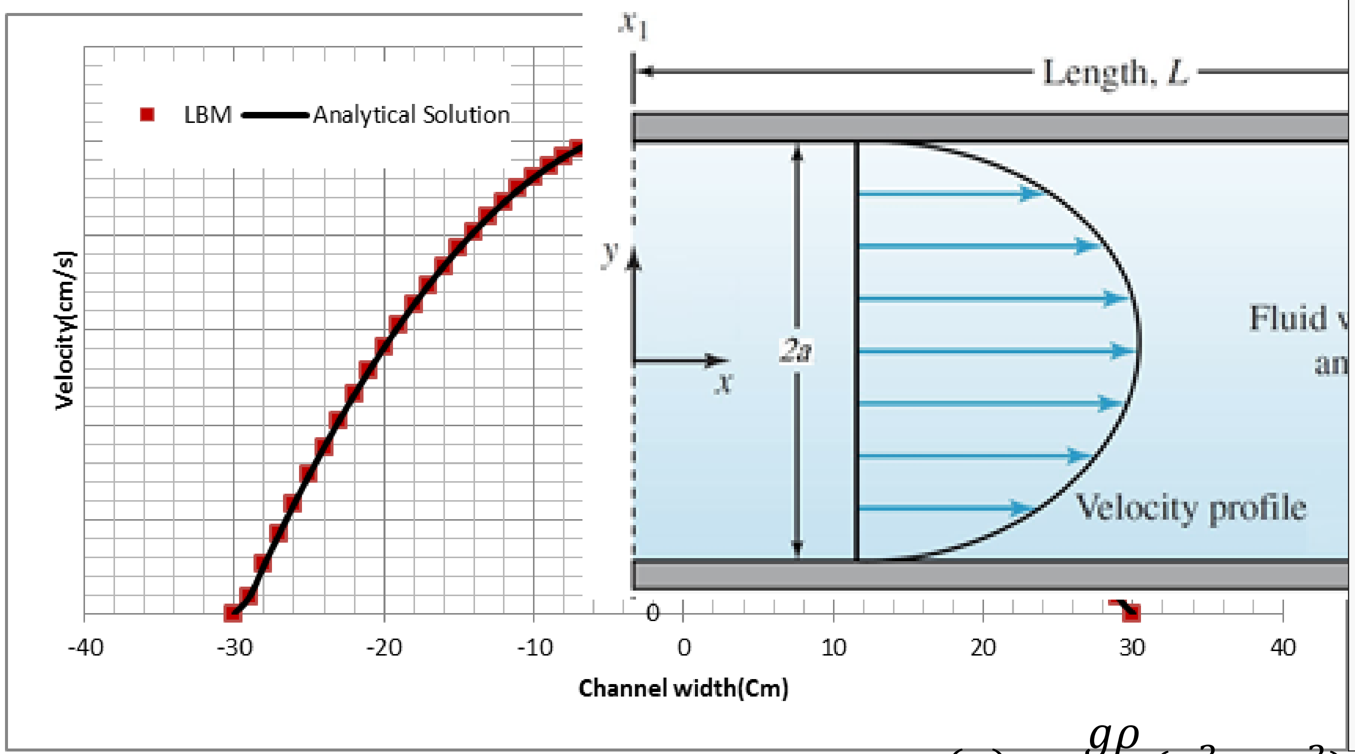
$$f_1(4) = \frac{1}{9} - \frac{\left[\frac{1}{9} - 0.111445\right]}{1.0} = 0.111445$$

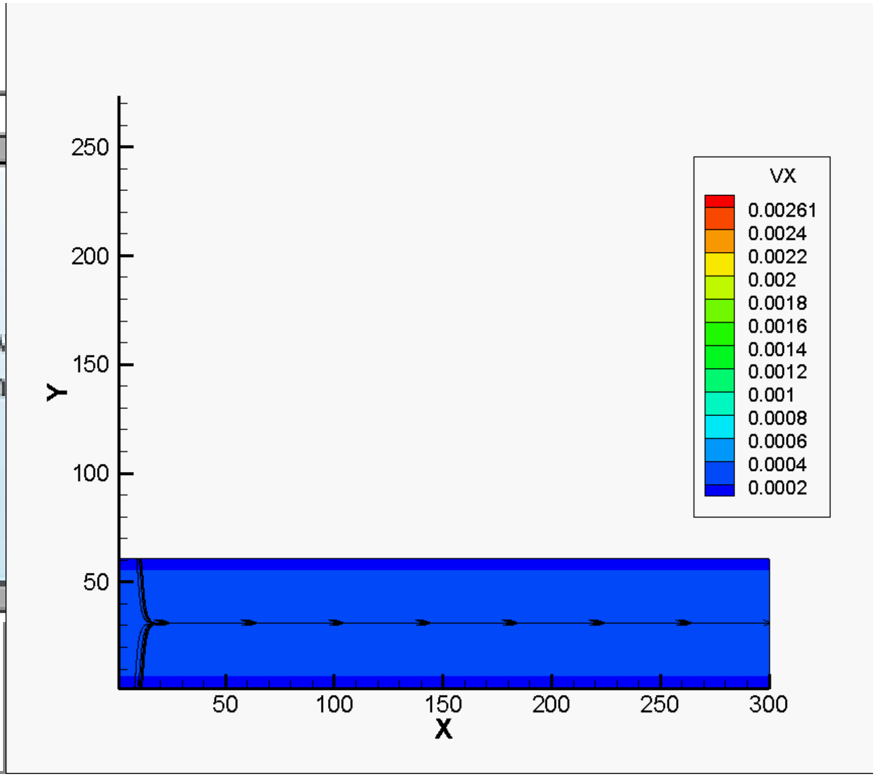
Calculation Example



Numerical Examples

Poiseuille Flow

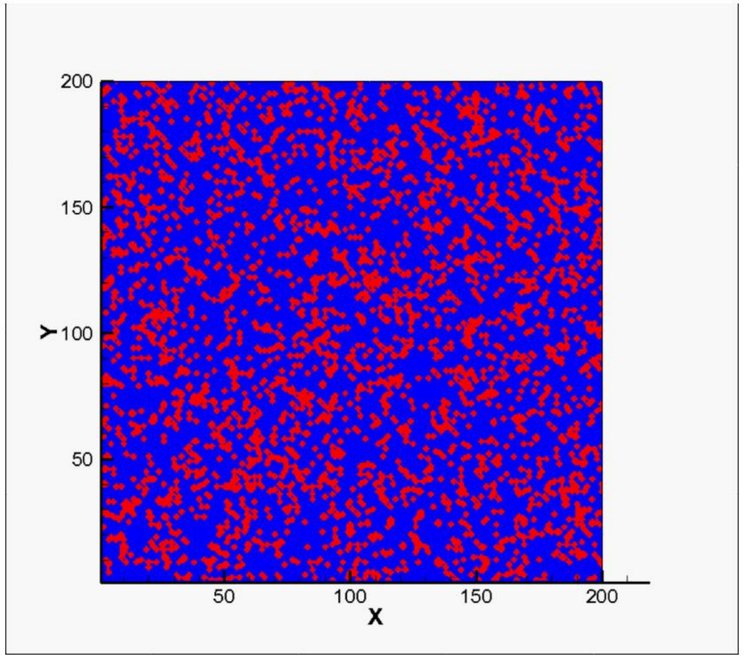




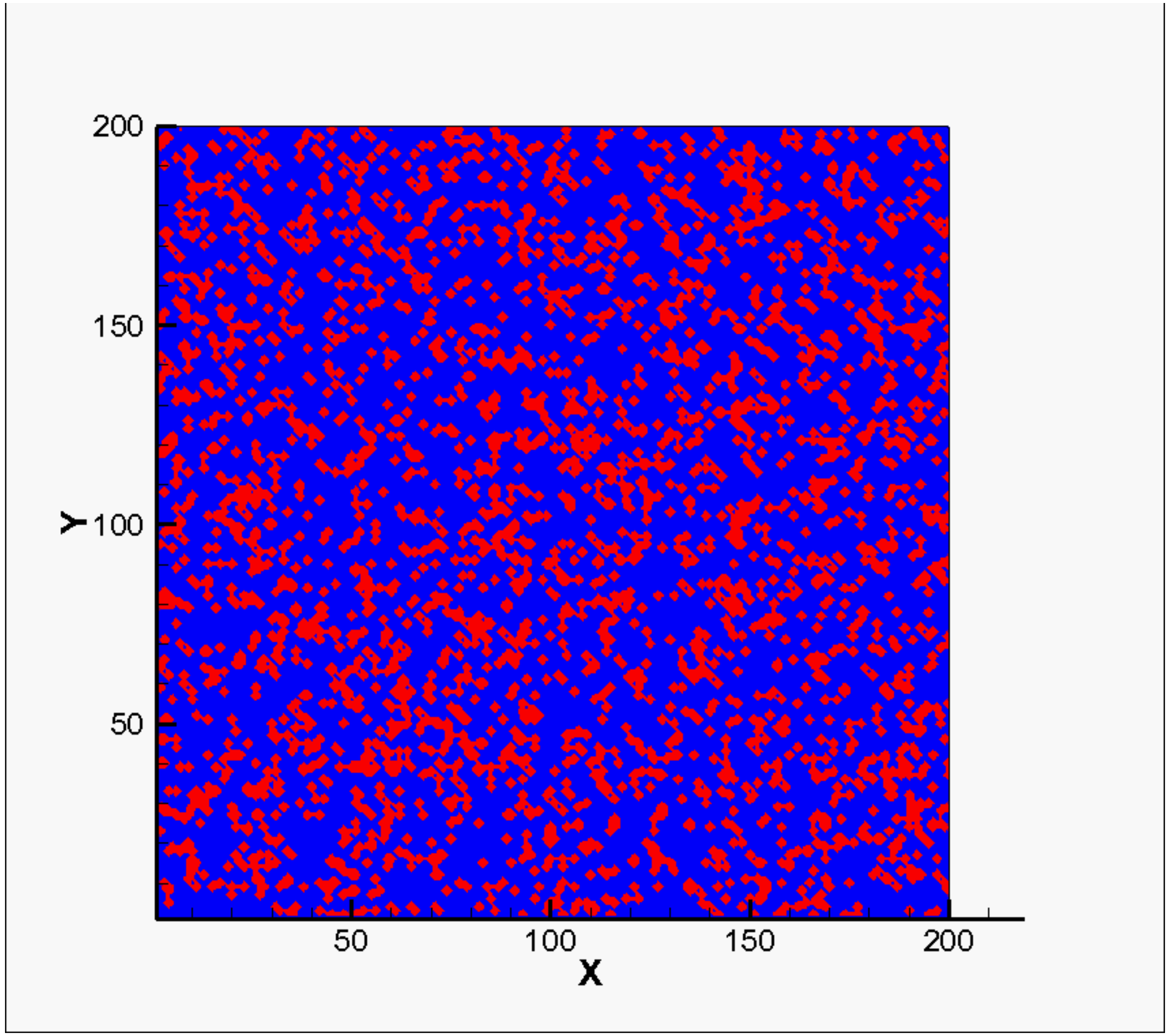
$$u(y) = \frac{g\rho}{2\mu}(a^2 - y^2)$$

Phase Separation and Laplace Law

Laplace Law $\Delta p = \frac{\sigma}{R}$

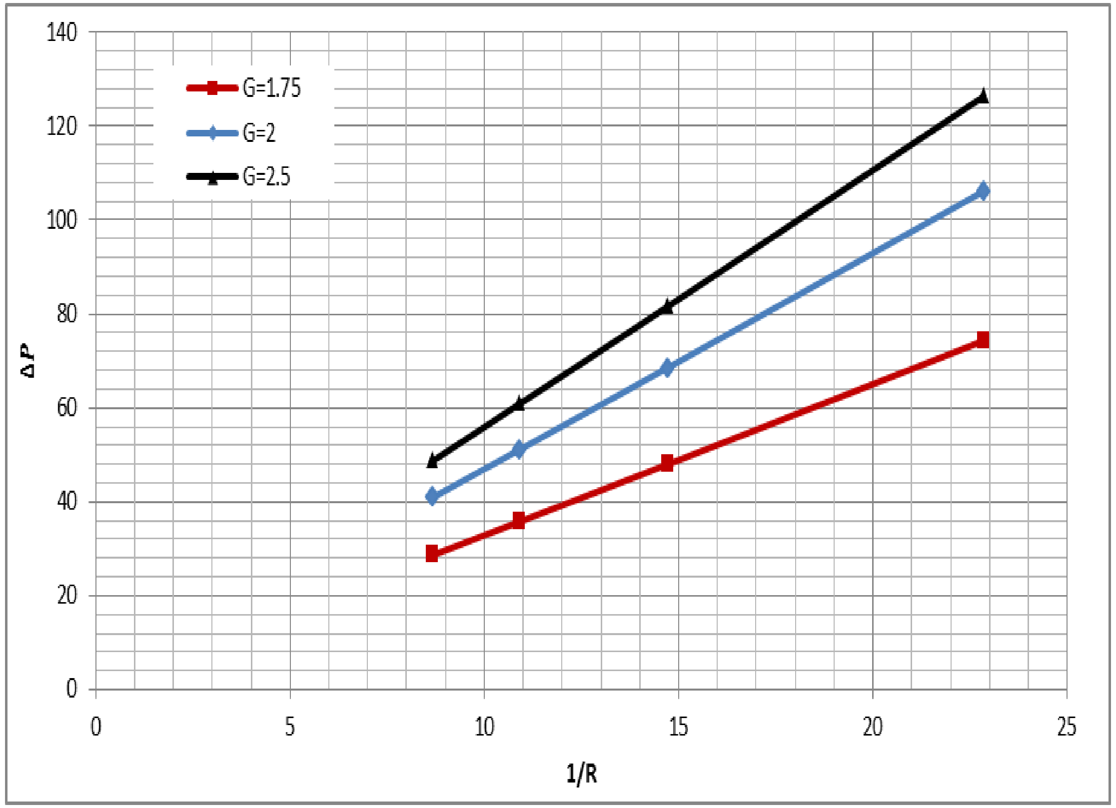


Initial condition



Laplace Law

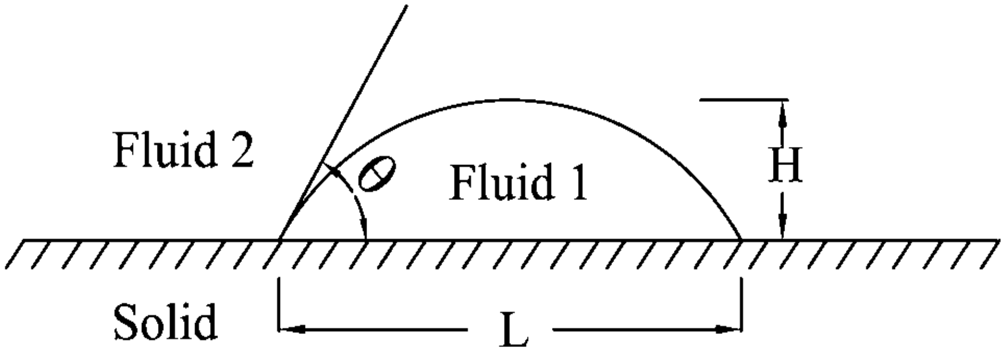
Laplace Law $$\Delta p = \frac{\sigma}{R}$$



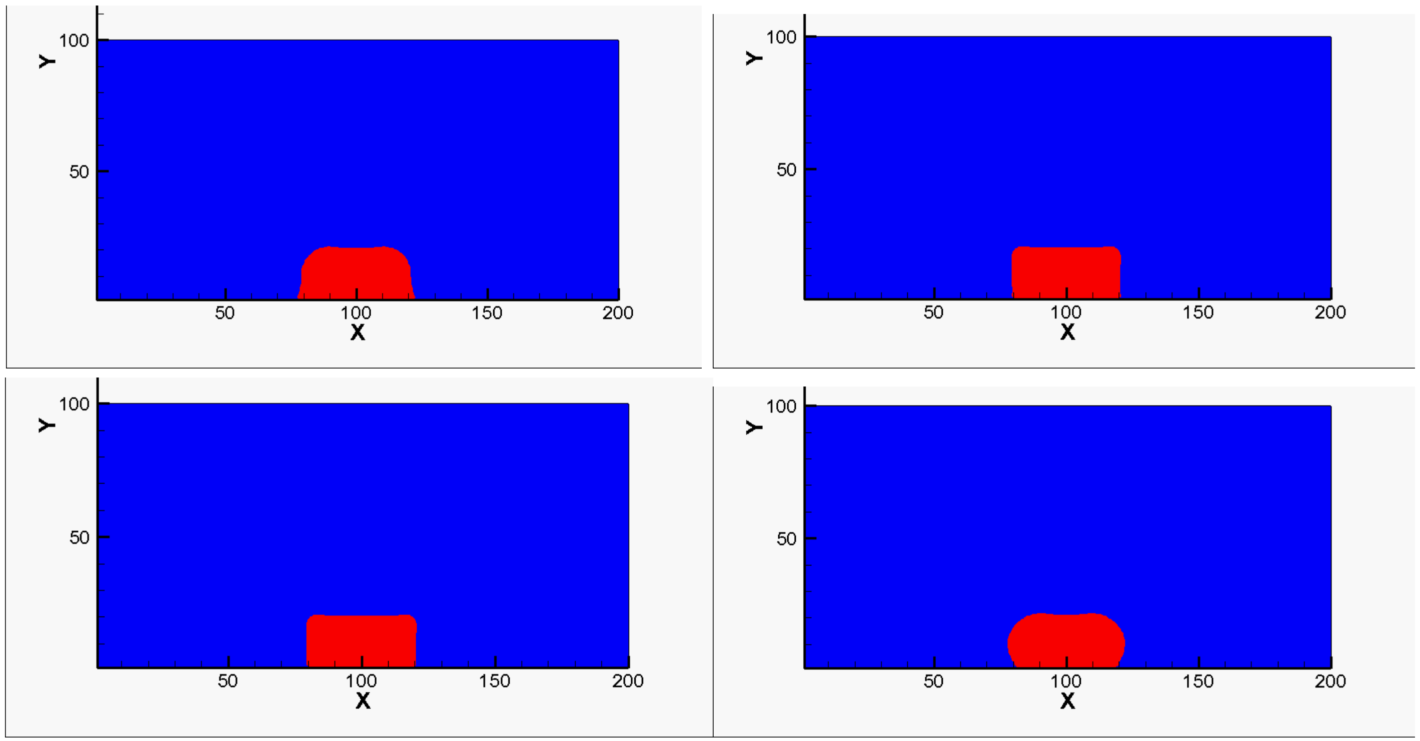
Surface Wettability or Contact Angle

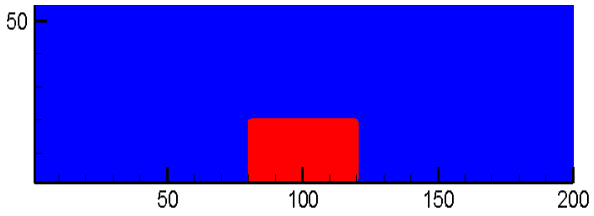
$$R = \frac{(4H^2 + L^2)}{8H}$$

$$tan\theta = \frac{L}{2(R - H)}$$



Dullien, 1992

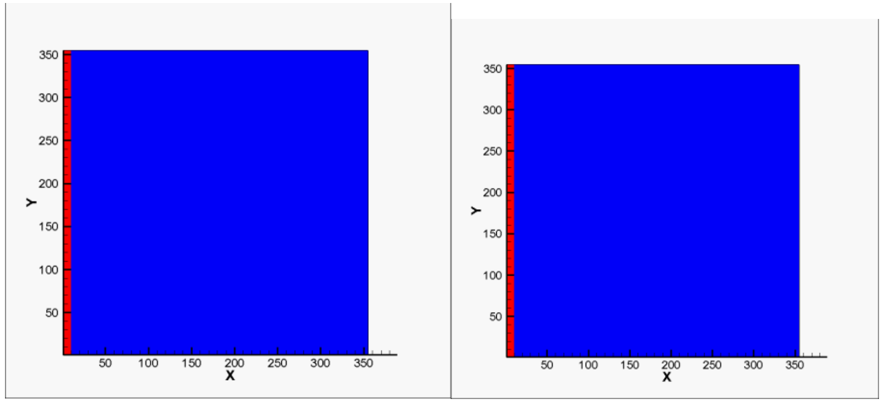




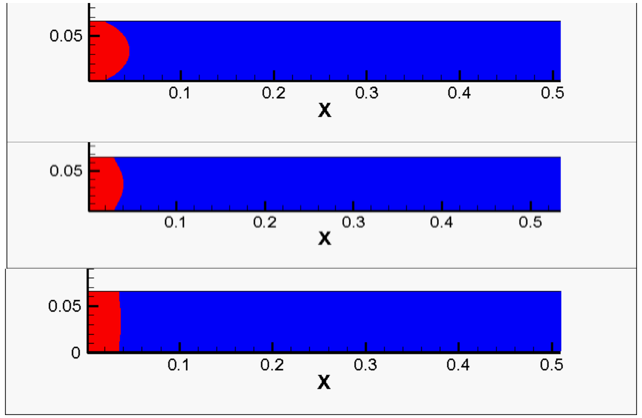
Initial condition

Example Applications

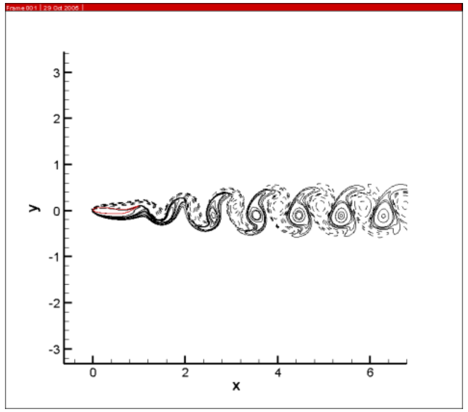
LBM Example Applications



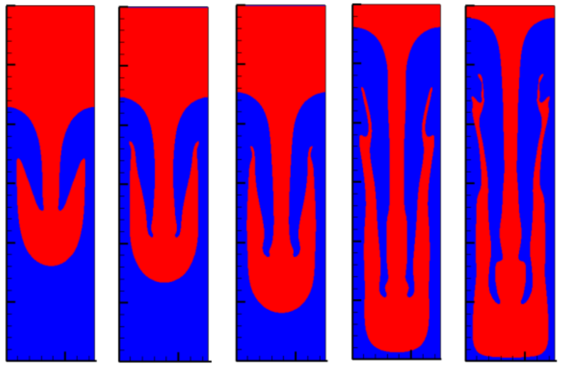
Oil-water displacement in porous media



Fingering phenomenon



Calculating the drag force



Rayleigh-Taylor instability

Absolute Permeability of Porous Media

Proposed equtions:

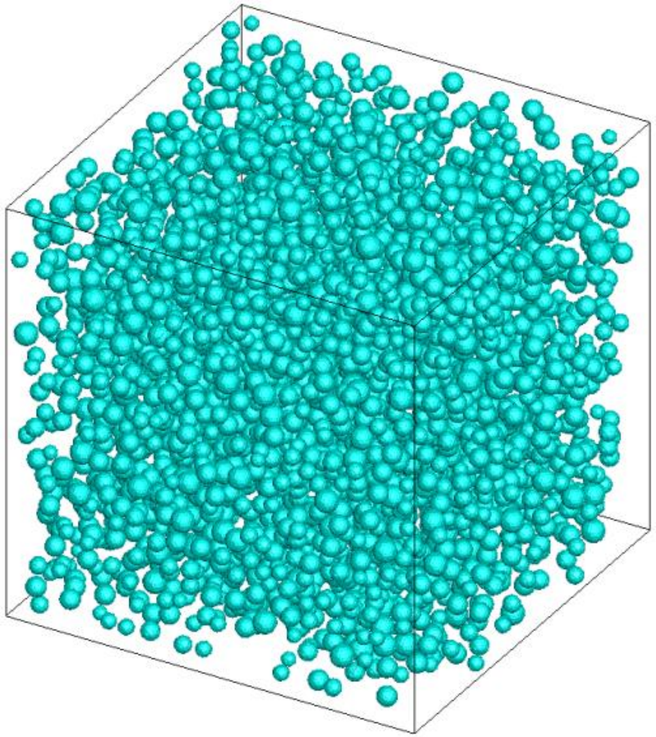
- Kozeny-Carmen, 1956 $$k = \frac{\phi^3}{(1-\phi)^2}\frac{d_p^2}{180}$$

- Bear and Bachmat, 1990 $$k = \frac{1-1.209(1-\phi)^{2/3}}{60\phi}\frac{\phi^3}{(1-\phi)^2}d_p^2$$

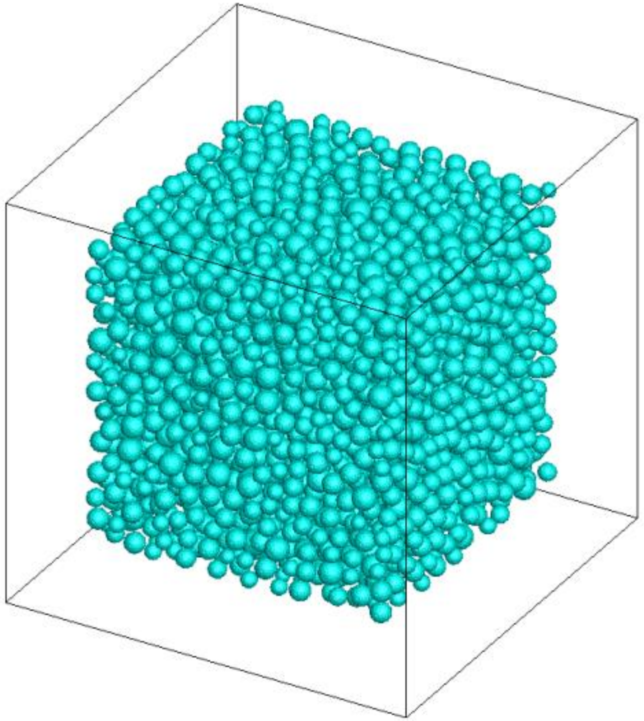
- Ahmadi et al., 2011 $$k = \frac{1-1.209(1-\phi)^{2/3}}{30[1-1.209(1-\phi)^{2/3}+\ 2\phi]}\frac{\phi^3}{(1-\phi)^2}d_p^2$$

Generating Dense Porous Media

Using Discrete Element Method (DEM):

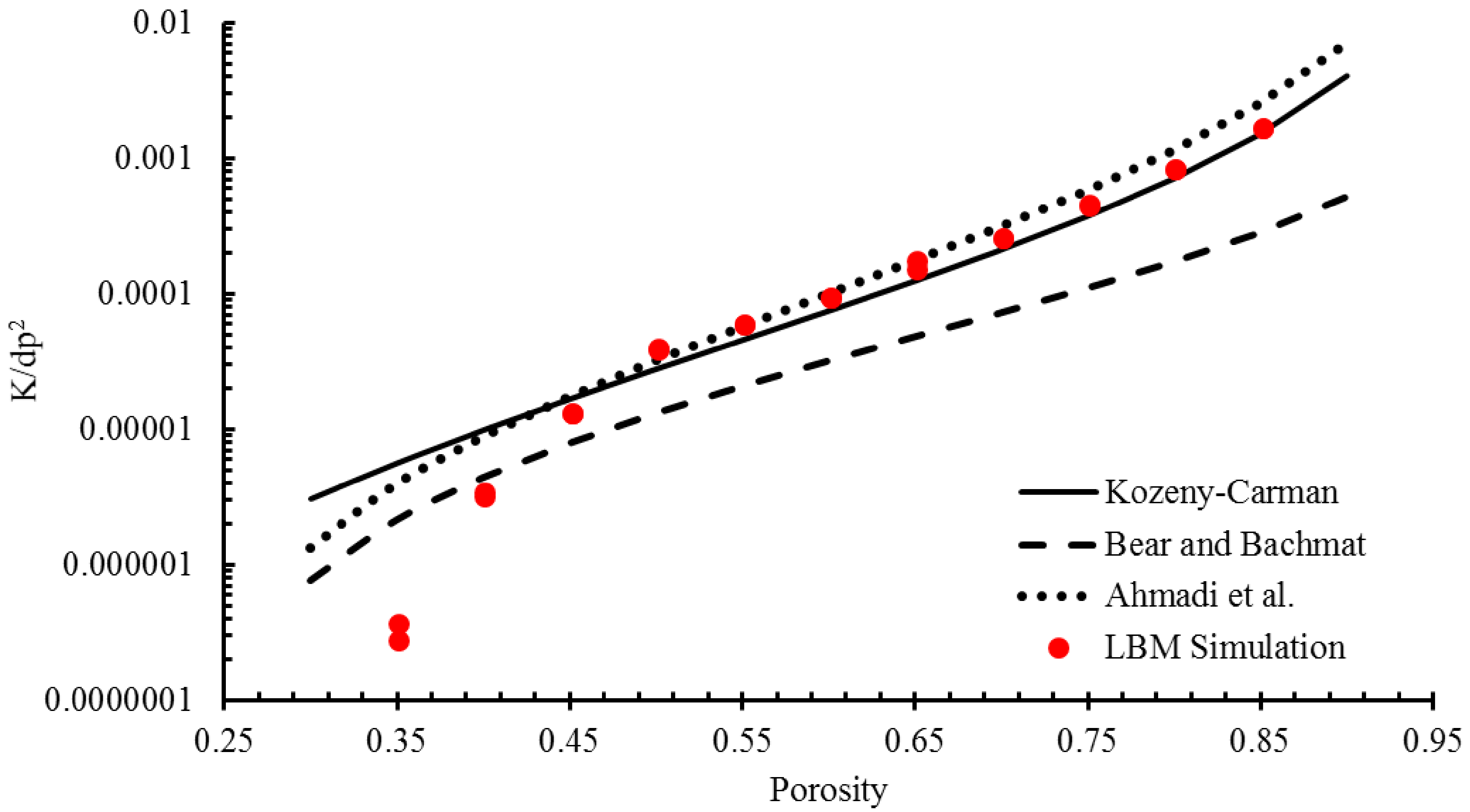


Before isotropic compaction



After isotropic compaction

Absolute Permeability of Porous Media



Thank you!

Additional Applications and Resources

- Books
  - Wolf-Gladrow 2000
  - Sukop and Thorne 2007
  - Wagner 2008
  - A.A. Mohammed 2011
  - Huang and Sukop 2015

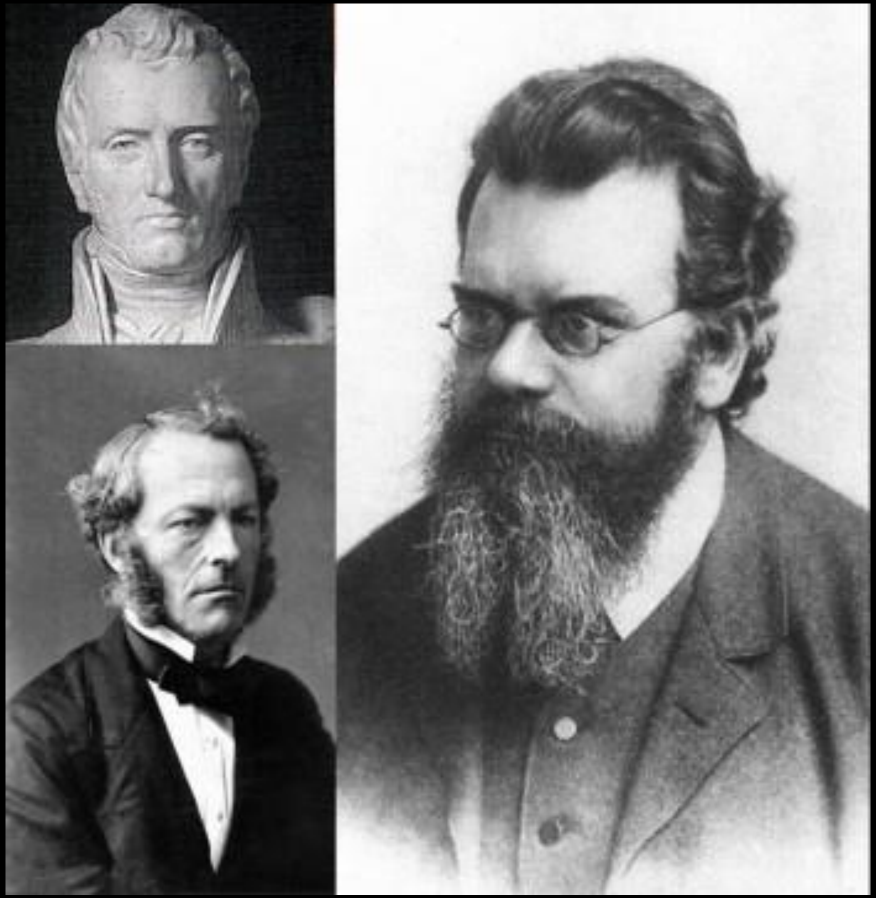
- Software
  - Palabos (Open Source)
  - Exa

- Applications
  - Lattice Boltzmann Simulator Video
  - Blood Flow
  - Free Surface Flows

The Lattice Boltzmann Method

Bahman Sheikh and Nirjhor Chakraborty

Claude-Louis Navier



Sir George Stokes Ludwig Boltzmann

Numerical Microscope for Fluid Mechanics

Microscopic Model

using

Mesoscopic Kinetic Equations

to solve

Macroscopic Fluid Mechanics