Lattice Boltzmann simulations of matrix diffusion

Jukka Toivanen*, Pekka Kekäläinen, Timo Riikilä,
Keijo Mattila, Jari Hyväluoma, Jussi Timonen

University of Jyväskylä

Outline

Lattice Boltzmann method

- Discretization of the Boltzmann equation
- Popular especially in simulations of flow through porous media
  - Triangulation of geometry not neccessary
  - Straightforward to construct the lattice from e.g. images
- System of fictitious mesoscopic particles evolves on a lattice
- During one time step, the particles move from their lattice nodes to neighbouring nodes according to their velocities (streaming)
- Particles arriving at the same lattice node collide with each other and change their velocities
- The average motion of the particles describes the macroscopic behaviour of the system

Distribution functions

- Distribution functions $f_i(\vec{r}, t)$ denote the probability of finding a particle at site $\vec{r}$ at time t travelling with velocity $\vec{c}_i$ (discrete set of velocities)
- Mass density and momentum density are obtained as

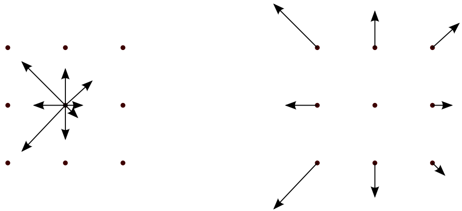
$$\rho(\vec{r}, t) = \sum_i f_i(\vec{r}, t), \qquad \rho(\vec{r}, t)\vec{v}(\vec{r}, t) = \sum_i \vec{c}_i f_i(\vec{r}, t)$$

- Many different grid models have been developed (denoted by DnQm, n = dimension, m = number of velocities)

Streaming and collision

- Distribution functions are updated as

$$f_i(\vec{r} + \Delta t c_i, t + \Delta t) = f_i(\vec{r}, t) - \underbrace{\frac{1}{\tau}\left(f_i(\vec{r}, t) - f_i^{eq}(\vec{r}, t)\right)}_{collision}$$



- Distribution function is driven towards a local equilibrium

$$f_i^{eq} = \rho(\vec{r}, t) w_i \left(1 + \frac{\vec{c}_i \cdot \vec{v}}{c_s^2} + \frac{(\vec{c}_i \cdot \vec{v})^2}{2c_s^4} - \frac{||\vec{v}||^2}{2c_s^2}\right)$$

Implementation

- Lattice Boltzmann flow solver (D3Q19)
- Swap algorithm overcomes the difficulties related to two-step and two-lattice implementations
- Semi-direct addressing (distribution values are not stored for solid nodes)
- Parallelized using MPI (domain decomposition)
- Point-like tracer particles are included
- Tracer particles move in a continuous space (positions not restricted to lattice nodes)
- Several particle time steps inside one time step of LBM

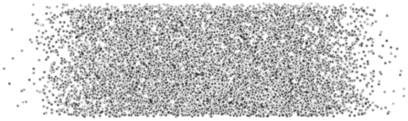
Tracer particle update

$$\vec{X}(t+\Delta t) = \vec{X}(t) + \vec{v}(\vec{X}(t))\Delta t + \sqrt{2D}\Delta \vec{W}(t) + \frac{\vec{F}(t)}{\xi}\Delta t$$

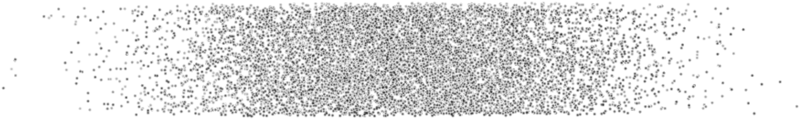
- $\vec{X}$ is the position of the particle
- $\vec{v}$ is the velocity of the flow
- D is the molecular diffusion coefficient
- $\Delta \vec{W}(t)$ is a Gaussian random variable modeling the Brownian motion
- $\vec{F}$ represents all other forces
- ξ is the drag coefficient

Validation of the diffusion modelling

- To validate implementation of diffusion, LB particle simulation is compared to solution of 1D diffusion equation
- Initial particle distribution is created in a narrow channel



- Concentration as a function of x is denoted by $C_0(x)$
- After 1000 LB steps with given diffusion coefficient D and $v = 0$, the final distribution $C_{1000}(x)$ is recorded

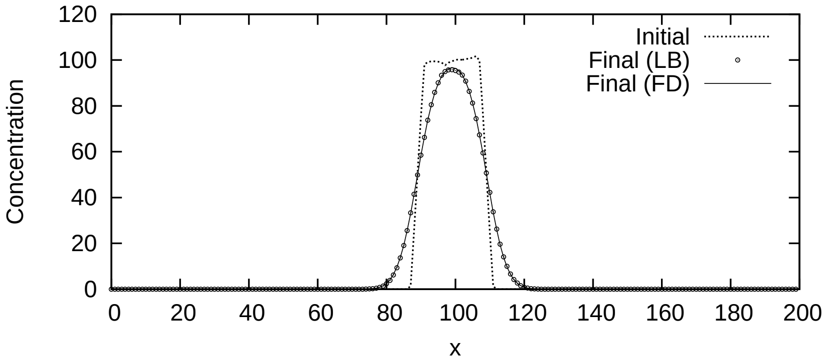


Validation results

- 1D diffusion equation

$$\frac{\partial \mathcal{C}(t)}{\partial t} = D\frac{\partial^2 \mathcal{C}(t)^2}{\partial x^2}$$

  is solved using the finite difference method
- Initial values $C_0(x)$, same amount of time steps



Matrix diffusion

- LB seems to be suitable for matrix diffusion simulations
- Approach is currently being tested and validated
- Test case is chosen so that the related mathematical model can be solved semi-analytically
- Model solutions have been validated against measurements

Mathematical model

$$\frac{\partial C_f}{\partial t}(x,t) + v\frac{\partial C_f}{\partial x}(x,t) - D_f\frac{\partial^2 C_f}{\partial x^2}(x,t) = \frac{\epsilon D}{b}\frac{\partial C_m}{\partial z}(x,0,t)$$
$$\frac{\partial C_m}{\partial t}(x,z,t) - D\frac{\partial^2 C_m}{\partial z^2}(x,z,t) = 0$$

$$C_m(x,z,0) = 0, \quad C_f(x,0) = 0, \quad C_f(0,t) = \frac{M_0}{2wbv}\delta(t)$$
$$C_m(x,0,t) = C_f(x,t), \quad \frac{\partial C_m}{\partial z}(x,L_z,t) = 0$$

Where

- C_f and C_m are concentrations of the tracer (channel/matrix)
- D_f and D are diffusion coefficients
- ϵ is the porosity of the matrix

Dimensionless parameters

The problem is governed by three dimensionless parameters

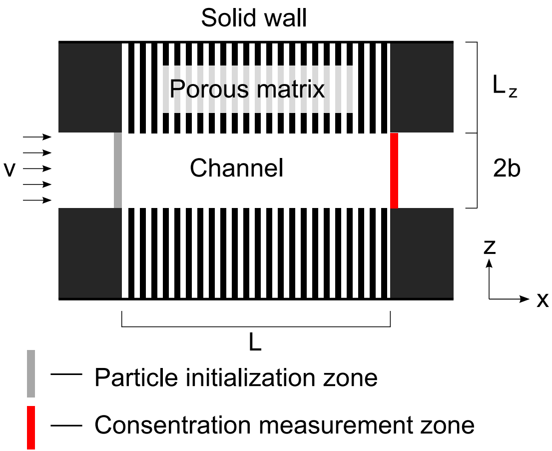
$$\lambda = \epsilon \frac{L}{b} \sqrt{\frac{D}{Lv}}$$

$$\kappa = \frac{L_z}{L} \sqrt{\frac{Lv}{D}}$$

$$\mu = \sqrt{\frac{D_f}{Lv}}$$

where D_f is the effective diffusion coefficient in the channel

Simulation geometry



- Periodic boundary conditions along y-axis
- Matrix idealized for 1D diffusion (perpendicular to the channel)

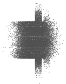
Matrix diffusion simulations

- Performed on a server equipped with 8 Intel Xeon processors, each having 8 cores running at 2.67 GHz
- Typical
  - lattice size 540x9x90
  - simulation time 48 hours (using 9 processes)
  - number of particles 20 000

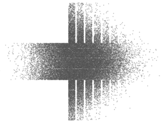
Simulation snapshots

t = 0

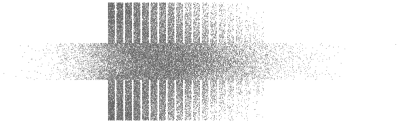
t = 1000



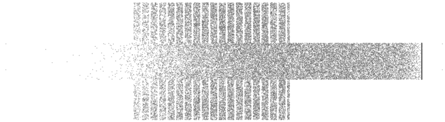
t = 7500



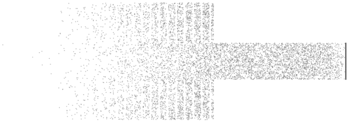
t = 40 000



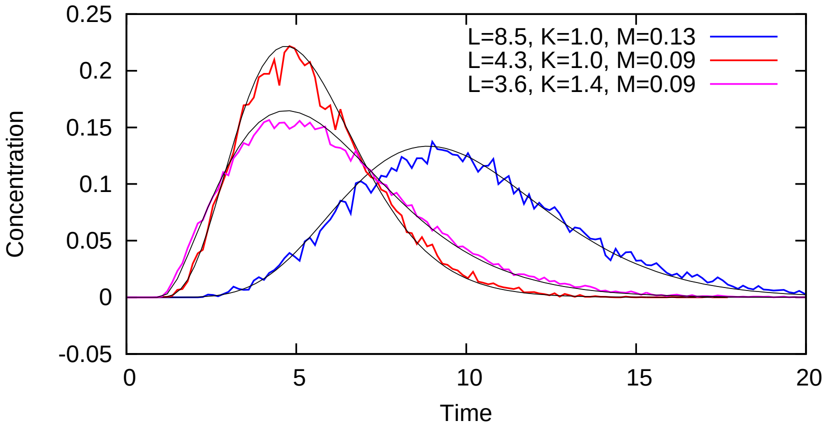
t = 161 000



t = 384 000



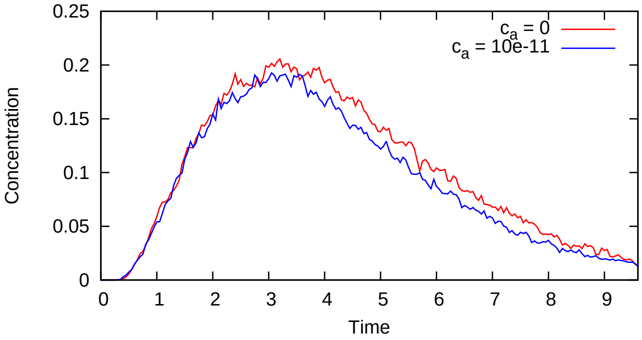
Comparison with analytical solution



Chemical interactions

- Each particle can attach to wall at any time
- Attachment probability is related to the distance from nearest wall *d*

$$P \sim e^{-d/c_a}$$



Future studies

- longitudinal diffusion inside the matrix
- inhomogeneous porosity
- flow channel with complicated shape
- anion exclusion