CASA Seminar
Boundary conditions for the Lattice Boltzmann equation

Oleg Matveichuk

4 March 2009

Outline

1. Lattice Boltzmann equation
2. General formulation of boundary conditions
3. Elementary types of boundary conditions
   - Periodic, No-slip, Free-slip, Frictional slip, Sliding walls, Open inlet/outlets
4. Complex types of boundary conditions
   - Staircasing, Extrapolation
5. References

Lattice Boltzmann equation

- Boltzmann equation for continuous media

$$\left[\partial_t + \frac{\vec{p}}{m} \cdot \partial_{\vec{r}} + \vec{F} \cdot \partial_{\vec{p}}\right] f\left(\vec{r}, \vec{p}, t\right) = C_{12}$$

$f\left(\vec{r}, \vec{p}, t\right)$ - probability density to find the particle in the the point $\left(\vec{r}, \vec{p}\right)$ at the moment t

C_{12} - collision operator

- Lattice Boltzmann Equation

$$\left[f_i\left(\vec{x} + \vec{c}_i, t + 1\right) - f_i\left(\vec{x}, t\right)\right] = \sum_j A_{ij}\left(f_j - f_j^{eq}\right)$$

i - enumerates different allowed velocities

$f_i\left(\vec{x}, t\right)$ - probability to find a particle in the state $\left(\vec{x}, \vec{c}_i\right)$ at the moment time t

A_{ij} - the matrix of collisions

f_j^{eq} - Mach-expanded equilibrium distribution function

General formulation of boundary conditions

Notations:

$\vec{n}$ - outward normal to the surface of the boundary

f_i^{out} - the outgoing population, if i satisfies condition $(\vec{c}_i \cdot \vec{n}) > 0$

f_i^{in} - the incoming population, if i satisfies condition $(\vec{c}_i \cdot \vec{n}) < 0$

The main question to solve on the boundary is to find the relation between incoming and outgoing flux. Assumption that, the relation between f_i^{in} and f_i^{out} is linear gives:

$$f_i^{in}(\vec{x}) = \sum_{\vec{y}} \sum_{j} B_{ij}(\vec{x} - \vec{y}) f_j^{out}(\vec{y})$$

$B_{ij}(\vec{x} - \vec{y})$ - boundary operator
$\vec{x}$ - point on the boundary
$\vec{y}$ - finite amount of points near the boundary

Various boundary conditions

- *Elementary;*
  - *Periodic;*
  - *No-slip;*
  - *Free-slip;*
  - *Frictional-slip;*
  - *Sliding-walls;*
  - *Open inlet/outlets.*
- *Complex.*
  - *Staircasing;*
  - *Extrapolation;*

Periodic boundary conditions

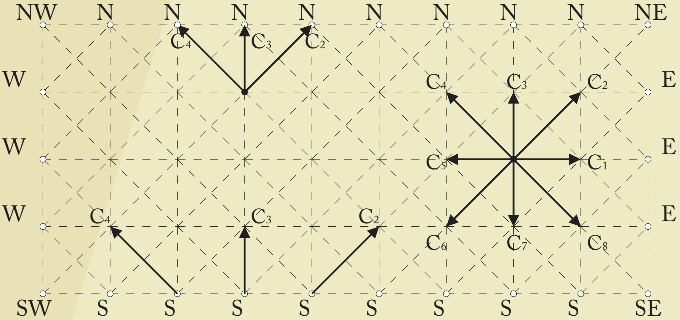

Figure 1: Illustration to periodic boundary conditions

Typical code sequence:

1. Set boundary;
2. Streams;
3. Collide.

Periodic boundary conditions

Used to model bulk phenomena, when boundary plays small role.
Consider a rectangular box, consisting of $N \times M$ lattice sites;
Fluid is represented by 9 matrices $f_i(l, m)$,
$l = 1, ..., N$,$m = 1, ...M$, $i = 0, ..., 8$

Let's introduce four extra layers of nodes $\mathbf{N}, \mathbf{S}, \mathbf{W}, \mathbf{E}$:

$\mathbf{N} = [l = 0, ..., N + 1; m = M + 1]$
$\mathbf{S} = [l = 0, ..., N + 1; m = 0]$
$\mathbf{W} = [l = 0; m = 0, ..., M + 1]$
$\mathbf{E} = [l = N + 1; m = 0, ..., M + 1]$

$f_{in,\mathbf{W}} = f_{out,\mathbf{E}}$
$f_{in,\mathbf{E}} = f_{out,\mathbf{W}}$
$f_{in,\mathbf{N}} = f_{out,\mathbf{S}}$
$f_{in,\mathbf{S}} = f_{out,\mathbf{N}}$

Four corners require special treatment.

No-slip boundary conditions

Used, when fluid velocity is zero at the given solid surface.

$f_{in,\mathbf{N}} = f_{out,\mathbf{N}}$, $f_{in,\mathbf{S}} = f_{out,\mathbf{S}}$
Types of implementation

- On-grid;
  In terms of the boundary kernel (on the top wall):
  $$\begin{pmatrix} f_6(x,y) \\ f_7(x,y) \\ f_8(x,y) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} f_2(x,y) \\ f_3(x,y) \\ f_4(x,y) \end{pmatrix}$$
- Mid-grid.
  on the top wall:
  $$\begin{pmatrix} f_6(x,y) \\ f_7(x,y) \\ f_8(x,y) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} f_2(x-1,y-1) \\ f_3(x,y-1) \\ f_4(x+1,y-1) \end{pmatrix}$$

No-slip boundary conditions

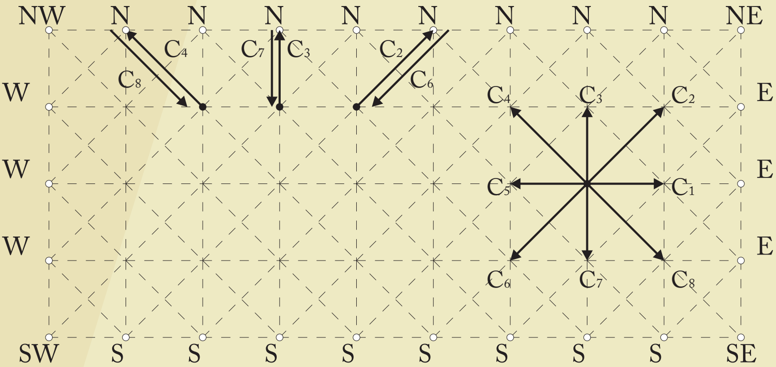

Figure 2: Picture of collisions for no-slip boundary conditions

Free-slip boundary conditions

The case of smooth boundaries with negligible friction exerted on the flowing gas or liquid.

$fin(\mathbf{N}) = fout(\mathbf{N})$

On-grid case: $\begin{pmatrix} f_6(x,y) \\ f_7(x,y) \\ f_8(x,y) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} f_2(x,y) \\ f_3(x,y) \\ f_4(x,y) \end{pmatrix}$

Mid-grid case:

$$\begin{pmatrix} f_6(x,y) \\ f_7(x,y) \\ f_8(x,y) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} f_2(x-1,y-1) \\ f_3(x,y-1) \\ f_4(x+1,y-1) \end{pmatrix}$$

This condition implies no momentum transfer to the wall.

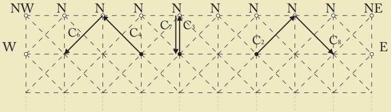

Figure 3: Picture of collisions for free-slip boundary conditions

Frictional slip

The case, when between liquid and the solid boundary acts frictional force (but it is not strong enough to consider this case as no-slip case).

For simple on-grid implementation:

$$\begin{pmatrix} f_6(x,y) \\ f_7(x,y) \\ f_8(x,y) \end{pmatrix} = \begin{pmatrix} p & 0 & q \\ 0 & 1 & 0 \\ q & 0 & p \end{pmatrix} \begin{pmatrix} f_2(x,y) \\ f_3(x,y) \\ f_4(x,y) \end{pmatrix}$$

where

p - part of bounce-back reflections;

q - part of slipping reflections (absolutely elastic reflections);

Obvious, that $p + q = 1$.

Momentum transfer to the wall $\delta J_x = -2p(f_2 - f_4)$.

For any positive value of p results in a δJ_x are opposite to J_x, thus the flow near the walls relaxes.

Sliding walls

Used if the walls have a given tangential velocity $u(walls) = u_w$

Method to handle sliding walls consists again in using adjustable reflection coefficients p and q.

On the upper wall:

$$\begin{pmatrix} f_6(x,y) \\ f_7(x,y) \\ f_8(x,y) \end{pmatrix} = \begin{pmatrix} p & 0 & q \\ 0 & 1 & 0 \\ q & 0 & p \end{pmatrix} \begin{pmatrix} f_2(x,y) \\ f_3(x,y) \\ f_4(x,y) \end{pmatrix}$$

Calculation of normal and tangent currents yields:

$$J_y = f_2+f_3+f_4-f_6-f_7-f_8 = (f_2+f_4)(1-p-q) = 0 \Longrightarrow p+q = 1$$

$$J_x = 2(1-p)(f_2 - f_4) = \rho_w u_w \Longrightarrow q = \frac{\rho_w u_w}{2(f_2 - f_4)} \sim \frac{u_w}{2u}$$

where u - tangent velocity of the fluid

$\rho_w = \frac{\rho}{6}$, since only states f_2, f_4, f_6, f_8 are involved.

Open boundaries

This case is appropriate, if the system has open boundaries, such as fluid inlets and outlets.

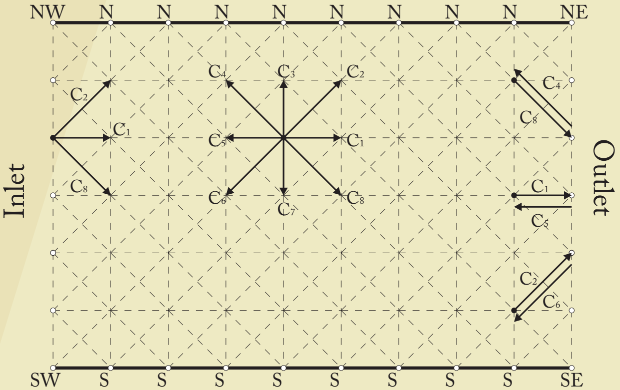

Figure 4: Two-dimensional pipe with additional layers, one inlet and one outlet

Open boundaries

Inlet flow is implemented by constantly refilling the buffer with equilibrium population, corresponding to the desired density and flow speed

$$f_{in}(\vec{y}) = (f^e)\left[\rho^e, u_{in}\right]$$

On the outlets, so-called 'porous plug' boundary condition is applied.
The idea - not all particles, reaching the outlet leave the domain. They they are reflected back with probability r, which is adjusted to ensure mass conservation. This yields

$$r = 1 + 4\frac{u - u_{in}}{1 - 2u} + O(u^2)$$

Staircased boundaries

The quickest approach to a complex boundary is to ’staircase’ the cutting boundary by replacing it with zig-zagging contour, lying entirely on the grid.

This method introduces artificial errors of order L^{-1}, where L - typical linear size of the obstacle in lattice units.

Staircased boundaries are relevant to flows in porous media.

Extrapolation schemes

Places the wall on boundary nodes and lets them undergo the same collision step as the fluid nodes. The only difference, that $f_i(onwalls)$ is explicitly tuned on the desired wall speed u_w.

Boundary nodes import information from solid nodes lying inside the solid wall.

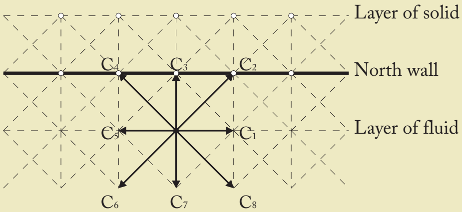

Figure 5: F - fluid, N - north wall, S - solid.

$$f_{2,3,4}(N) = f_{2,3,4}(S) - f_{2,3,4}(F)$$

Summary

- Various boundary conditions can be well transformed to the language of the Lattice Boltzmann method. Physical properties assigned to the layer strongly influence on the behavior of the liquid in the bulk.
- Lattice Boltzmann model deals with physical interactions on the kinetic level, where it is much simpler accounted, than on the hydrodynamic level.
- Several types of boundary conditions are adjusted to maintain second-order accuracy.
- Relatively easy to realize boundary conditions for complex geometry.

References

1. Sauro Succi, ”The Lattice Boltzmann Equation for fluid Dynamics and Beyond”
2. Shiyi Chen and Gary D.Doolen, ”Lattice Boltzmann method for fluid flows”, *Fluid Mech.* 1998. 30:329-64