Topic 6: Cellular Automaton Methods – Continued

We need to discuss some additional features of the Lattice Boltzmann Equation and its numerical implementation.

Boundary Conditions

Various types of boundary conditions are possible:

- Periodic boundary conditions are useful for modeling bulk systems because they tend to minimize finite size edge effects.
- No-slip boundary conditions are appropriate for most fluids in contact with a wall.
- Frictional slip (or the limiting case of free-slip) boundary conditions may be appropriate for smooth boundaries with small (or negligible) friction exerted on the flowing gas or liquid.
- Open inlets and outlets.

Periodic Boundary Conditions

Boundary conditions are straightforward to derive once the model is specified. Consider the D2Q9 model with a rectangular region. The discrete velocities are numbered as follows:

```
6   2   5

3   0   1

7   4   8
```

The boundary values at the West end of the region $(x = 0, y)$ are implemented by transfering the densities with positive x component of velocity from the East boundary $(x = n_x, y)$:

```
/* East */
for (y = 1; y <= n_y; y++) {
     n[XYI(0,y,1)] = n[XYI(n_x,y,1)];
     n[XYI(0,y,5)] = n[XYI(n_x,y,5)];
     n[XYI(0,y,8)] = n[XYI(n_x,y,8)];
}
```

Note that it is only necessary to transfer three of the 9 densities that will then flow into the region.

No-slip Boundary Conditions

Let's consider the North wall with lattice sites $(x, y = n_y + 1)$. The appropriate boundary conditions, which will ensure that the fluid velocity at the wall is zero, are implemented as follows:

```
    /* North */
    for (x = 1; x <= n_x; x++) {
         n[XYI(x,n_y+1,4)] = n[XYI(x,n_y,2)];
         n[XYI(x,n_y+1,8)] = n[XYI(x,n_y,6)];
         n[XYI(x,n_y+1,7)] = n[XYI(x,n_y,5)];
    }
```

We only need to set the densities with negative y component of velocity, namely (4,7,8). The boundary conditions are implemented by simply reversing these velocities. This fluid velocity normal to the wall is proportional to

$$(n_6 + n_2 + n_5) - (n_7 + n_4 + n_8) = 0 \ .$$

The tangential fluid velocity component is proportional to

$$(n_5 + n_1 + n_8) - (n_6 + n_3 + n_7) = n_1 - n_3 \ .$$

Since the components $n_{1,3}$ parallel to the wall do not change during the simulation, we can set $n_1 = n_3$ at the wall initially so the parallel velocity component will remain zero.

Obstacle

Succi's program also allows for a thin vertical obstacle with no-slip boundary conditions centered at $(x = n_x/4, y = n_y/2)$.

Poiseuille Flow Problem

This is viscous flow through a channel under the action of a pressure gradient. With no-slip boundary conditions at the wall of the channel the flow develops a parabolic velocity profile which is stable up to Reynolds numbers of about 2000.

There is a problem with simulating Poiseuille flow using the Lattice Boltzmann Equation because the system behaves like an ideal gas with equation of state

$$P = \rho c_s^2 ,$$

where c_s is the speed of sound. For the D2Q9 model $c_s^2 = 1/3$. In addition, the flow is incompressible with constant ρ. Thus in equilibrium, the pressure P is constant and there cannot be a pressure gradient to drive the flow!

In a real incompressible fluid, the speed of sound is very large compared with the fluid velocity, and small pressures gradients are consistent with almost constant density. But in the lattice model, the speed of sound is comparable to the fluid velocity! A trick to simulate a constant pressure gradient is to introduce a *body force* which transfers the same momentum to the fluid to overcome viscosity as would a pressure gradient. This is done in the program as follows:

```
cs2 = 1 / 3.0;               /* speed of sound squared */
nu = (tau - 0.5) * cs2;      /* kinematic viscosity */
f = 8.0 * nu * u_f / (n_x * n_y);
f *= rho / 6;
for (x = 1; x <= n_x; x++) {
```

```
        for (y = 1; y <= n_y; y++) {
             n[XYI(x,y,1)] += f;
             n[XYI(x,y,5)] += f;
             n[XYI(x,y,8)] += f;

             n[XYI(x,y,3)] -= f;
             n[XYI(x,y,6)] -= f;
             n[XYI(x,y,7)] -= f;
        }
   }
```

Here ν is the kinematic viscosity, and u_f is the desired final fluid velocity in the $+x$ direction. Note that if $u_f > 0$ then the densities $n_{1,5,8}$ of particles moving in the $+x$ direction are increased by a constant amount at each lattice site, and the densities $n_{3,6,7}$ in the opposite direction are decreased correspondingly: thus momentum in continually injected into the fluid which preserving constant density.