Continuum Limit of Lattice Gas Cellular Automaton Model

We have seen from running the program `lgca.cpp` that the 2D lattice gas on a hexagonal lattice approximates the behavior of a fluid.

It is interesting to see how the lattice gas automaton model approximates the equations of fluid dynamics. To do this, we need to

- form statistical averages over a large number of lattice gas systems, and
- examine the limit in which the *microscopic scale* of the model, i.e., the lattice spacing which determines the *mean free path* of the fluid particles, is much smaller than the *macroscopic scale* of variations in fluid density and velocity.

The equations of fluid dynamics

The equations of fluid dynamics follow from conservation of mass and momentum.

Consider a volume V inside the fluid. The mass of fluid in this volume is given by

$$\int \rho \, \mathrm{d}V \, ,$$

where ρ is the fluid density. The rate at which this mass decreases is determined by the rate at which fluid leaves the volume

$$\frac{\mathrm{d}}{\mathrm{d}t} \int \rho \, \mathrm{d}V = - \int \rho \mathbf{u} \cdot \mathrm{d}\mathbf{S} \, ,$$

where $\mathbf{u}$ is the fluid velocity and the integral on the right is taken over the surface of the volume with $\mathrm{d}\mathbf{S}$ being a surface element with direction along the *outward* normal. Using the *divergence theorem*

$$\int \rho \mathbf{u} \cdot \mathrm{d}\mathbf{S} = \int \nabla \cdot \rho \mathbf{u} \, \mathrm{d}V \, ,$$

we obtain the *continuity equation*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \, .$$

Next, consider conservation of momentum

$$\rho \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{F} \ ,$$

which is just Newton's equation of motion for an element of fluid with unit mass. The total derivative on the left has two contributions

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \ ,$$

the first term on the right represents the change in fluid velocity with t at a *fixed* point in space, and the second *advective* term represents the change in fluid velocity due to motion of fluid from neighboring points in space.

The force density $\mathbf{F}$ has three contributions:

- external or *body forces* acting on the fluid, for example the force of gravity

  $$\mathbf{F}_{\mathrm{gravity}} = \rho \mathbf{g} \ ,$$

  where $\mathbf{g}$ is the acceleration due to gravity
- *pressure forces* due to neighboring fluid elements

  $$-\int p \, \mathrm{d}\mathbf{S} = -\int \nabla p \, \mathrm{d}V \ ,$$

  $$\mathbf{F}_{\mathrm{pressure}} = -\nabla p \ ,$$

  where p is the fluid pressure and the integrals are taken over the surface and volume of the element, respectively
- *viscous forces* due to internal friction or shearing stresses in the moving fluid

  $$\mathbf{F}_{\mathrm{viscous}} = \mu \nabla^2 \mathbf{u} + (\mu + \xi)\nabla(\nabla \cdot \mathbf{u}) \ ,$$

  where μ is the *dynamic viscosity coefficient* and ξ is the *bulk viscosity coefficient* of the fluid.

A special case that is interesting for many applications is that of *incompressible flow*

$$\rho = \text{constant} , \qquad \nabla \cdot \mathbf{u} = 0 .$$

Taking these forces into account results in the *Navier-Stokes equations* for incompressible viscous flow:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \mathbf{g} - \frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} ,$$

where $\nu = \mu/\rho$ is the *kinematic viscosity*.

Microscopic lattice gas equations

The lattice gas on a 2D hexagonal lattice can be represented by a vector $\mathbf{n}(\mathbf{x}) = (n_0, n_1, n_2, n_3, n_4, n_5)$ of *Boolean* variables that indicate the presence $(n_i = 1)$ or absence $(n_i = 0)$ of particles at cell $\mathbf{x}$ and moving with velocities

$$\mathbf{c}_i = \left[\cos\left(\frac{\pi i}{3}\right), -\sin\left(\frac{\pi i}{3}\right) \right] , \qquad i = 0, 1, 2, 3, 4, 5,$$

measured in units of lattice spacing per time step.

The synchronous dynamics of the system is described by the equation

$$n_i(\mathbf{x} + \mathbf{c}_i, t + 1) = n_i(\mathbf{x}, t) + \Delta_i[\mathbf{n}(\mathbf{x}, t)] ,$$

where the first term on the right hand side gives the result of free streaming of particle i from cell $\mathbf{x}$ to cell $\mathbf{x} + \mathbf{c}_i$, and Δ_i is the *collision term*. In this equation, $n_i(\mathbf{x}, t)$ is the result of free streaming from time $t - 1$. The collision term then alters the particle velocities according to the collision rules of the model.

To obtain an explicit formula for Δ_i we define the *negation* of n_i to be $\bar{n}_i = 1 - n_i$: if $n_i = 1$ then $\bar{n}_i = 0$ and vice versa. Consider for example a 3-particle collision with zero total momentum for which there are 2 states

`east | southwest | northwest` $\Leftrightarrow$ `southeast | west | northeast`

which get exchanged when the particles collide. It is easy to see that this rule can be written

$$\Delta_i^{(3)} = n_{i+1}n_{i+3}n_{i+5}\bar{n}_i\bar{n}_{i+2}\bar{n}_{i+4} - n_i n_{i+2}n_{i+4}\bar{n}_{i+1}\bar{n}_{i+3}\bar{n}_{i+5} \ ,$$

where the sums in the subscripts are taken modulo 6.

As another example, the cyclic 2-body collision rule

`east | west` $\Rightarrow$ `southwest | northeast` $\Rightarrow$ `northwest | southeast`

is represented by the collision term

$$\Delta_i^{(2)} = n_{i+2}n_{i+5}\bar{n}_i\bar{n}_{i+1}\bar{n}_{i+3}\bar{n}_{i+4} - n_i n_{i+3}\bar{n}_{i+1}\bar{n}_{i+2}\bar{n}_{i+4}\bar{n}_{i+5} \ .$$

Similar expressions can be written for the other 3-particle collisions, and the cyclic 4-particle collisions. Then Δ_i is the *sum* of all of these mutually exclusive collision terms.

Note that each collision term conserves mass and momentum

$$\sum_i \Delta_i(\mathbf{n}) = 0 \ , \qquad \sum_i \mathbf{c}_i \Delta_i(\mathbf{n}) = 0 \ .$$

Using these relations, we can write the lattice analog of the continuity equation as

$$\sum_i n_i(\mathbf{x} + \mathbf{c}_i, t+1) = \sum_i n_i(\mathbf{x}, t) \ ,$$

and the lattice analog of momentum conservation as

$$\sum_i \mathbf{c}_i n_i(\mathbf{x} + \mathbf{c}_i, t+1) = \sum_i \mathbf{c}_i n_i(\mathbf{x}, t) \ .$$

Continuum limit of the lattice gas equations

Frish, Hasslacher, and Pomeau, *Phys. Rev. Lett.* **56**, 1505 (1986) showed that the lattice gas equations reduced to the Navier-Stokes equations in the continuum limit for small enough fluid velocities.

The lattice gas variables are the boolean occupation numbers n_i at each site. Let $N_i = \langle n_i \rangle$ be statistical average values of these variables, i.e., averages over many time steps after the system has come to a steady state. The fluid density ρ and velocity $\mathbf{u}$ are then defined as

$$\rho = \sum_i N_i \ , \qquad \rho \mathbf{u} = \sum_i N_i \mathbf{c}_i \ .$$

By assuming that ρ and $\mathbf{u}$ vary slowly in space (measured in units of the lattice spacing) and time (measured in automaton time steps), and making Taylor series expansions in $\mathbf{u}$, Frish et al., were able to derive the following equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \ ,$$

$$\frac{\partial}{\partial t}(\rho u_\alpha) + \sum_\beta \frac{\partial}{\partial x_\beta} \left[g(\rho) \rho u_\alpha u_\beta + \mathcal{O}(u^4) \right] = -\frac{\partial}{\partial x_\alpha} p + \eta_1(\rho) \nabla^2 u_\alpha + \eta_2(\rho) \frac{\partial}{\partial x_\alpha} \nabla \cdot \mathbf{u} \ ,$$

where $g(\rho) = (\rho - 3)/(\rho - 6)$, $p = (\rho/2)[1 - g(\rho) u^2]$, and $\eta_{1,2}$ are viscosity coefficients which depend on ρ.

Notice that these equations are *rotationally invariant*, i.e., the underlying hexagonal symmetry of the lattice gas has disappeared in the continuum limit! The second equation looks very similar to the Navier-Stokes equation, but there are some differences:

- The factor $g(\rho)$ on the left hand side is not present in the Navier-Stokes equations. This term breaks Galilean invariance, i.e., the equation is not invariant under a transformation to a moving reference frame.
- The pressure p is velocity dependent and does not give the correct value for the speed of sound $c_s = \sqrt{\mathrm{d}p/\mathrm{d}\rho}$ in the fluid.

In addition to these difficulties, it has been found that lattice gas simulations suffer from the following problems:

- The fluctuations in the fluid flow are too large: the flow is too noisy.

- Only low Reynolds numbers, i.e., very viscous fluid flows, can be simulated correctly.
- There are unphysical conserved quantities in addition to the physical conserved quantities (mass, momentum, energy, angular momentum).
- The collision rules become exponentially complex in many models, including the simplest realistic 3-D model.

The last problem is interesting. In the 2-D model, each cell can have up to 6 particles, each with a different velocity. The number of possible states is $2^6 = 64$ because each particle type can either be present or absent. In a collision, each state is transformed to a definite other state. One way of implementing collisions is with a 64×64 lookup table.

In 2-D, Frisch, Hasslacher and Pomeau found that a hexagonal lattice of cells was sufficient to recover isotropy (rotational invariance) in the Navier-Stokes equations: an earlier model with a square lattice did not have this property and did not give realistic results.

In 3-D it can be shown that there there is *no* regular crystal lattice that leads to isotropic Navier-Stokes flows! A clever trick was found to solve this problem: use a 4-D face-centered hyper-cubic lattice. The velocities in 4-D are taken to be $c_1 = [\pm 1, \pm 1, 0, 0]$ and 23 other permutations. These velocities are projected onto a cube in 3-D to give

- 12 velocities to the centers of the 12 cube edges. These velocities have zero fourth-component. A cell in 3-D is allowed to have at most one of these particles.
- 6 velocities to the centers of the 6 cube faces. These velocites have fourth-component ± 1, so the cell in 3-D is allowed to have at most *two* of these particles.

With 24 different velocities possible at each cell, the number of states is of order $2^{24} = 16,777,216$. It is not easy to specify appropriate collision rules for such a huge number of states. Once the rules are specified, it is very difficult to code them. The earliest calculations with this model were done using a 48 MByte lookup table which took about 2 hours of CRAY-2 CPU time to initialize properly!

The Lattice Boltzmann Method

The resolution of these problems led to the introduction of Lattice Boltzmann methods by G. McNamara and G. Zanetti, *Phys. Rev. Lett.* **61**, 2332 (1988), and F. Higuera and J. Jimenez *Europhys. Lett.* **9**, 663 (1989).

The continuum theory of fluids can be viewed at different length scales:

- At the molecular level, the fluid molecules obey deterministic Newtonian equations of motion for the positions $\mathbf{r}_i(t)$ and velocities $\mathbf{v}_i(t)$ of the particles.
- At the kinetic theory level, and for a dilute gas, the individual particles are replaced by a probability distribution function $n(\mathbf{r}, \mathbf{v}, t)$, which is the probability that there is a particle with position $\mathbf{r}_i$ and velocity $\mathbf{v}_i$ at time t. This distribution function obeys the famous Boltzmann equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + \mathbf{F} \cdot \nabla_{\mathbf{v}} n = \left(\frac{dn}{dt} \right)_{\text{coll}} ,$$

  where the collision term is determined by the 2-body scattering cross section

$$\left(\frac{dn}{dt} \right)_{\text{coll}} = \int d^3 v_2 d\Omega \, (n_{1'} n_{2'} - n_1 n_2) v_{\text{rel}} \sigma(v_{\text{rel}}, \Omega) \, .$$

- At the fluid-dynamics level, one averages over small but macroscopic regions of space and over times much longer than the molecular mean free time: the Boltzmann equation then reduces to the Navier-Stokes and continuity equations for fluid flow.

The Lattice Boltzmann model is derived in a similar way:

- The analog of Newtonian dynamics is the Lattice Gas Cellular Automaton with its deterministic dynamics. The fixed number of particles with definite positions an velocities are discretized by populating the cells with a finite number of particles with discrete velocity values.
- A Lattice Boltzmann Model is obtained by replacing the particles with definite velocities at each cell by a *probability distribution* $n_i(\mathbf{r}, t)$ to find a particle with discrete velocity c_i at discrete cell position $\mathbf{r}$ at time t. This distribution function obeys the Lattice Boltzmann Equation

$$n_i(\mathbf{r} + \mathbf{c}_i, t + 1) = n_i(\mathbf{r}, t) + C_i(n) \, ,$$

where C_i is a discrete version of the collision operator. In the approximation of Bhatnagar, Gross and Krook

$$C_i(n) = -\frac{n_i - n_i^{\rm eq}}{\tau} \ .$$

- The fluid-dynamic limit of this model leads to the Navier-Stokes and continuity equations for fluid flow.

Comparing Lattice Gas and Lattice Boltzmann

Lattice Gas Cellular Automaton Model: Velocities c_i are discrete.

- Advantage: integer arithmetic can be used and computations are very fast.
- Disadvantage: the fluid velocity also takes only a finite number of discrete values. This is the origin of the breakdown of Galilean invariance and the anomalous dependence of pressure on the sound velocity.

Lattice Boltzmann Model: The velocites c_i of the fluid particles are discrete, but we average over an *ensemble* of systems to obtain a probabilistic distribution n_i of velocities.

- Disadvantage: n_i are real numbers and we need to use floating point arithmetic. The advantage over finite difference approximations is lost.
- Advantage: the fluid density and velocity

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

are both *continuous*, which makes it possible to satisfy Galilean invariance and to avoid other problems with the Lattice Gas Model.