UNIVERSITY OF PORTSMOUTH

Introduction to Lattice Boltzmann models

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Fluid Dynamics Recap

In a previous lecture, we introduced *Lattice Gas Model (LGM) t*o simulate fluid flows.

We discussed various CA-based approaches to simulates the kinetics of particles in gases and liquids:

1. HPP model
2. FHP model

Lattice Boltzmann Models

Another possible approach is *Lattice Boltzmann Models (LBMs).*

LBM originated from the Lattice Gas Cellular Automata method

This approach is based on *statistical mechanics* of molecules – i.e. their probability distributions.

Probability Distributions

In the Navier-Stokes Equation we had density (ρ) and flow ($\boldsymbol{u}$) fields that were functions of position and also varied with time – e.g. in 2 dimensions: $\rho(x, y, t)$.

In the 1870s, Boltzmann considered instead a *single* function, f, representing the *probability* or distribution of *individual molecules* having a *particular position and a particular velocity* – $f(x, y, v_x, v_y, t)$.

Note that this is a function of *two* vectors – position *and* velocity.

At any given time, for every possible position, it characterizes the probability that molecules may be in any possible velocity state.

This complicated probability distribution is captured by the function, f.

The Boltzmann Equation

Boltzmann showed the continuum function f would obey a partial differential equation like this:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} f + \boldsymbol{g} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = \Omega(f)$$

where:

- $\boldsymbol{\nabla} f$ is the vector $\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)$,
- $\frac{\partial f}{\partial \boldsymbol{v}}$ is the vector $(\frac{\partial f}{\partial v_x}, \frac{\partial f}{\partial v_y})$,
- $\boldsymbol{g}$ is the acceleration due to gravity or other external field, and, importantly,
- $\Omega(f)$ is the *collision operator*.

Lattice Gas Reminder

The mathematical formulation here is probably confusing. To make it more concrete, think back to the *lattice gases* we considered in earlier weeks.

There, for any given site, there were a finite number of velocity states particles could be in.

In that case the rule was that only *one or zero* particles could be in any given velocity state at any given position (lattice site).

Think of the population of lattice gas particles as a function of (discrete) position and (discrete) velocity. For every combination of position and velocity there is a certain value, 0 or 1.

The function f is similar, but its range is continuous – not just 0 or 1.

(Domain – space and velocity, also happens to be continuous!)

From Lattice Gas to LBM

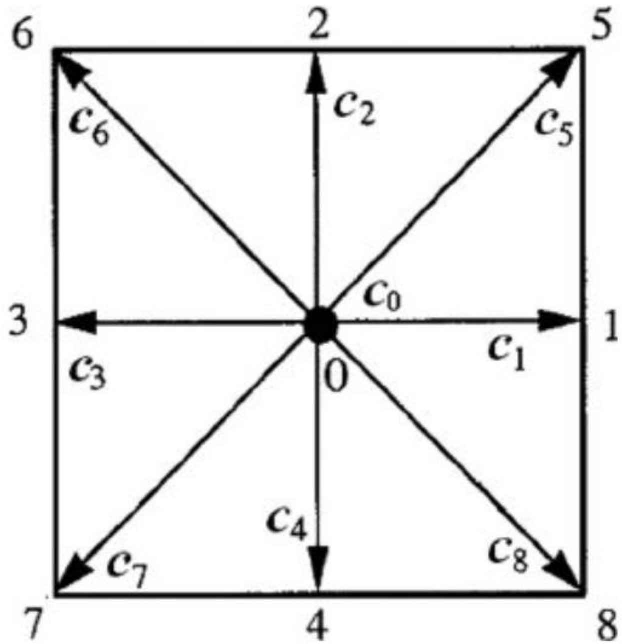
Following on from the theoretical discussion on the previous slides, the main steps going from a Lattice Gas model to a Lattice Boltzmann Model are:

1. Generalize the “population function” for the discrete velocity states from simply taking values 0 or 1 (occupied or unoccupied) at each site, to taking a *floating point value* representing either a probability or expected number of “molecules” in that state.

2. Modify the collision step based on the probability function f.

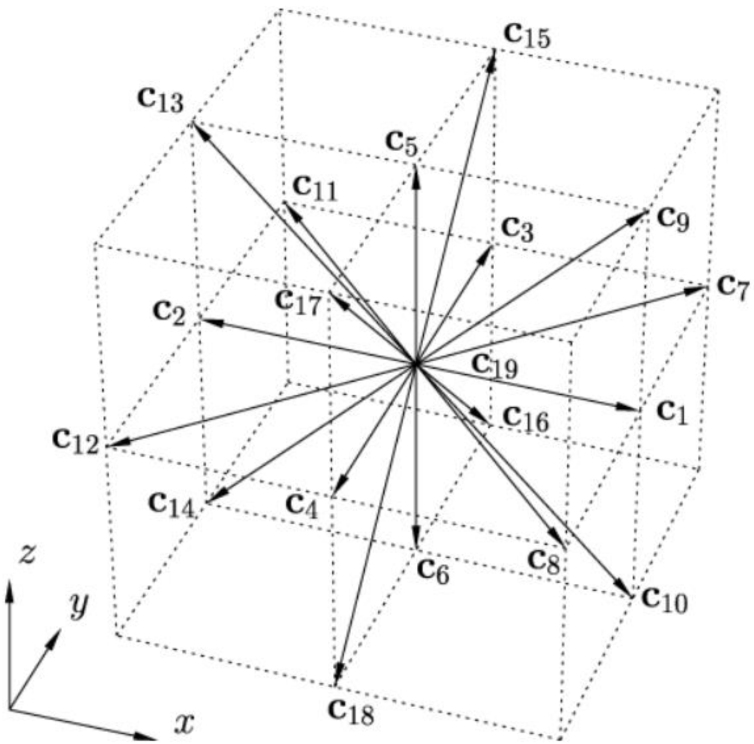
Cell state in LBM

In *D2Q9 lattice model*, a gas substance is modelled using a two dimensional square grid populated by a set of particles with 9 different velocities or states.



†Image from *Numerical Illustrations of the Coupling Between the Lattice Boltzmann Method and Finite-Type Macro-Numerical Methods*, Huan-Bo Luan et al, 2010

D3Q19 Velocity States†



†Image from *Implementation of on-site velocity boundary conditions for D3Q19 lattice Boltzmann simulations*, Martin Hecht and Jens Harting, 2010

Velocity State Notation

We see that in general the velocity states can be represented by a set of Q vectors.

Commonly these Q vectors are referred to as $\boldsymbol{c}_i$, where $i = 0, \ldots, Q - 1$.

Note each of these vectors is itself D dimensional, where $D = 2$ or 3 in our examples (so the set of velocity states is characterized by $D \cdot Q$ numbers in total).

Discretized Distribution

Boltzmann's distribution function f can now be given in its discrete form.

For instance, a cell state array in D2Q9 model:

	f_0	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8
F									

The elements of the array are now *real* (double or float), rather than Boolean.

Macroscopic Quantities

Based on the proposed desilication, we can approximate the local density (ρ) and local fluid flow velocity ($\boldsymbol{u}$), that appear in equations like Navier-Stokes.

In LBM, the local density is just the sum of the expected number of particles in all local (velocity) states:

$$\rho(x, y) = \sum_{i=0}^{Q-1} f_i(x, y)$$

Local velocity is a weighted average of discrete flow velocities:

$$\boldsymbol{u}(x, y) = \frac{1}{\rho(x, y)} \sum_{i=0}^{Q-1} \boldsymbol{c}_i f_i(x, y)$$

Update Rule in LBMs

As usually presented, an individual time step in a LBM has exactly the same form as we have seen previously in a Lattice Gas.

Recall that there are these two steps:

1. *Collision step*
2. *Streaming step*

And in fact the streaming step is again essentially identical to that in a Lattice Gas model. To recap:

A distribution component $f_i(x, y)$ with velocity *in a particular direction* at a particular site, is copied one place to the *next site in that direction*:

Steps may now be diagonal, and the zero velocity components are unaffected by streaming. Otherwise, not much has changed.

Collision Step Update

The collision step update is:

$$f_i^{out}(x,y) = f_i^{in}(x,y) - \frac{f_i^{in}(x,y) - f_i^{eq}(x,y)}{\tau}$$

Where:

$f_i^{in}(x,y)$ is distribution before the collision step

$f_i^{out}(x,y)$ is the distribution after the collision step

τ is a constant parameter related to the desired *viscosity* of the simulated fluid.

LBM Equilibrium Distribution

$f_i^{eq}(x, y)$ is the baseline equilibrium distribution defined as:

$$f_i^{eq}(x, y) = w_i \rho \left(1 + \frac{\boldsymbol{u} \cdot \boldsymbol{c}_i}{c_s^2} + \frac{(\boldsymbol{u} \cdot \boldsymbol{c}_i)^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2} \right)$$

(recall ρ and $\boldsymbol{u}$ are also functions of x and y.)

Here w_i and c_s are constants that depend on the velocity states.

Lab 7

You now have enough information to simulate realistic LBM flow of a two dimensional fluid.

We will do this in the lab, but we haven't yet discussed the vital matters of choosing initial conditions, boundary conditions, or other free parameters – we return to these next week.