Topic 5: Computational Fluid Dynamics – Lattice Boltzmann Technique

We have seen that the Navier-Stokes equations

$$\rho\frac{\partial \mathbf{v}}{\partial t} + \rho\mathbf{v}\cdot\nabla\mathbf{v} = -\nabla P + \eta\nabla^2\mathbf{v} + (\eta+\lambda)\nabla(\nabla\cdot\mathbf{v}) \ ,$$

and the continuity equation

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

can be solved by discretization on a computational grid. Various simplifying approximations are possible in special situations.

Lattice Boltzmann Technique

This is an alternative method for solving fluid dynamics problems which uses a discrete model approximation to the Navier-Stokes equations and continuity equation. Since the non-linear Navier-Stokes equations are complicated to solve, we look for a simpler system obeying simpler equations whose solution approximates the behavior of a real fluid.

The Lattice Boltzmann technique is based on approximating the fluid by a *dilute gas* of particles. In a real fluid, the particles interact strongly and continuously. In a dilute gas, the molecules move as free particles most of the time except for *two-body* collisions. Such a dilute gas can be described by the famous *Boltzmann Equation* which was first derived by Ludwig Boltzmann in 1872. The Navier-Stokes equations can be derived from the Boltzmann Equation in a certain limit. The Lattice Boltzmann technique makes use of particular features of the Boltzmann Equation which lead to the Navier-Stokes equations.

The Boltzmann Equation

This is an equation for the *particle distribution function* $n(\mathbf{r}, \mathbf{v}, t)$ in *phase space*, which is the probability of finding a particle with position $\mathbf{r}$ and velocity $\mathbf{v}$ at time t. This distribution obeys the *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 left hand side accounts for the changes in n due to motion of the particles and the external forces $\mathbf{F}$ acting on them, and the right hand side accounts for the changes in n due to collisions between the particles.

We consider the gas of particles of mass $m = 1$ as a fluid with density

$$\rho(\mathbf{r}, t) = \int d^3v \; n(\mathbf{r}, \mathbf{v}, t) \ ,$$

and average velocity

$$\mathbf{u}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \int d^3v \; \mathbf{v} n(\mathbf{r}, \mathbf{v}, t) \ .$$

The average velocity is determined by the *current* or *particle flux*

$$\mathbf{j}(\mathbf{r},t) = \int d^3v\; \mathbf{v}n(\mathbf{r},\mathbf{v},t)\ .$$

This is the *first moment* in the velocity of the distribution. The *second moment* determines the *momentum flux* tensor

$$\Pi_{ij}(\mathbf{r},t) = \int d^3v\; v_i v_j n(\mathbf{r},\mathbf{v},t)\ .$$

Equilibrium Distribution

If the gas is in thermal equilibrium at temperature T, the distribution is given by the *Maxwell-Boltzmann* distribution

$$n^{\text{eq}}(\mathbf{r},\mathbf{v},t) = \mathcal{N}\rho(\mathbf{r})e^{-\frac{(\mathbf{v}-\mathbf{u})^2}{2k_BT}}\ ,$$

where k_B is Boltzmann's constant, and $\mathcal{N}$ is a normalization constant.

It can be shown that the first moment of the equilibrium distribution leads to the Euler equations for the average velocity $\mathbf{u}$, i.e., the Navier-Stokes equations without viscosity.

The full Navier-Stokes equations can be derived by writing the particle distribution

$$n(\mathbf{r},\mathbf{v},t) = n^{\text{eq}}(\mathbf{r},\mathbf{v},t) + n^{\text{neq}}(\mathbf{r},\mathbf{v},t)\ ,$$

where n^{neq} is a non-equilibrium correction to the equilibrium distribution.

The correction n^{neq} is taken to have zero first moment

$$\int d^3v\ n^{\text{neq}}(\mathbf{r},\mathbf{v},t) = 0\ ,$$

which ensures the conservation of mass, and zero second moment

$$\int d^3v\ \mathbf{v}n^{\text{neq}}(\mathbf{r},\mathbf{v},t) = 0\ ,$$

which ensures conservation of momentum.

The full Navier-Stokes equations with viscosity can be derived by examining the second moment of the the non-equilibrium distribution.

Single relaxation time (BGK) Ansatz

If the system is not in equilibrium, it will *relax* towards equilibrium. In general, this relaxation can be very complicated. Relaxation is effected by the collision term in the Boltzmann equation, which can be written schematically

$$\left(\frac{dn}{dt}\right)_{\text{coll}} = \int d^3v_2 d\Omega\ (n_{1'}n_{2'} - n_1n_2)v_{\text{rel}}\sigma(v_{\text{rel}},\Omega)$$

where σ is the differential scattering cross section for the two-particle collision

$$\mathbf{v}_1 + \mathbf{v}_2 \longrightarrow \mathbf{v}_{1'} + \mathbf{v}_{2'}\ ,$$

and $\mathbf{v}_{\text{rel}} = \mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity and $\Omega = (\theta, \phi)$ is the scattering direction in the center of mass system.

Viscous effects arise from collisions between particles which transform the energy of fluid motion to internal particle motion in the fluid.

A simple approximation for the collision term was introduced by Bhatnagar, Gross and Krook in *Phys. Rev.* **94**, 511 (1954)

$$\left(\frac{dn}{dt}\right)_{\text{coll}} = -\frac{n - n^{\text{eq}}}{\tau} ,$$

where τ is a *relaxation time* constant. This approximation implies that the distribution relaxes exponentially to equilibrium with a time constant τ.

Lattice Boltzmann Equation

The Boltzmann Equation with the BGK approximation for the collision term can be solved numerically on a spatial lattice or grid.

Let's consider a 2-D system with a square grid. The distribution function

$$n(\mathbf{r}, \mathbf{v}, t)$$

is defined on the finite set of grid points. However, it depends on velocity $\mathbf{v}$ in addition to position $\mathbf{r}$. Since we have made space discrete, it is not unreasonable to allow the particles to have only a discrete set of velocity values $\mathbf{c}_i, i = 1, 2, \ldots$. However, instead of setting up a grid in velocity space, the Lattice Boltzmann technique makes the very drastic assumption that the velocity of a particle can have only a very limited number of values!

A minimal number of velocity values in 2-D which leads to reasonable fluid-like behavior is 9: the velocity can be zero, or it can have a constant non-zero magnitude c in any of eight different compass directions on the 2-D lattice, namely N, S, E, W, NE, SE, NW, SW. In this approximation, the distribution function is completely described by 9 real numbers stored at each site of the spatial grid.

Time is also made discrete $t = 0, \delta t, 2\delta t, \ldots$, and the system is evolved one step δt at a time.

If there are no collisions, i.e., if the system is in equilibrium, the appropriate rule to use to advance the system by one time step is

$$n_i(\mathbf{r} + \mathbf{c}_i \delta t, t + \delta t) = n_i(\mathbf{r}, t) \ ,$$

i.e., the particles move according to their velocities which ensures that mass is conserved and the continuity equation is obeyed. For convenience, we choose units so that $\delta t = 1$.

If the system is not in equilibrium, the the time evolution algorithm becomes

$$n_i(\mathbf{r} + \mathbf{c}_i, t + 1) = n_i(\mathbf{r}, t) - \frac{n_i - n_i^{\mathrm{eq}}}{\tau} \ .$$

Since this involves the equilibrium distribution n^{eq} which is not known *a priori*, the following approximation is used

$$n_i = w_i \rho \left[1 + A(\mathbf{c}_i \cdot \mathbf{u}) + B(\mathbf{c}_i \cdot \mathbf{u})^2 + C u^2 \right] \; .$$

The constants in this approximation can be determined by examining the moments of the distribution. It can be shown that

$$w_i = \begin{cases} \frac{4}{9} & \text{for zero velocity} \\ \frac{1}{9} & \text{for N, S, E, W} \\ \frac{1}{36} & \text{for NE, NW, SE, SW} \end{cases}$$

and

$$A = 3 \, , \qquad B = \frac{9}{2} \, , \qquad C = -\frac{3}{2} \, .$$

One must also specifiy suitable boundary conditions.