Topic 5: Computational Fluid Dynamics – Particle Suspension

The Immersed Boundary Method was invented by Peskin in the 1970's to model the flow of blood in the heart. The flow is regulated by heart valves, which are moving boundaries immersed in the fluid. *J. Computational Physics* **25**, 220 (1977).

Another application of the method was by Fogelson who used it to study blood platelet adhesion and aggregation during blood clotting in narrow blood vessels: his model system consisted of blood plasma treated as an incompressible viscous fluid, and platelets treated as discs-shaped particles using the immersed boundary technique. The platelets themselves and damaged areas of the blood vessel were allowed to secrete a chemical ADP into the blood: this chemical caused platelets to stick to one another and to the damaged wall areas. *J. Computational Physics* **56**, 111 (1984).

Disc Suspensions in 2-D Incompressible Flow

The Immersed Boundary Method allows very efficient solution of the Navier-Stokes equations in 3-D. To illustrate the method we consider the simpler case of 2-D flow and follow Fogelson's treatement of platelets in blood without the complications of ADP secretion and platelet aggregation.

Assuming that the Reynolds number is small, we can neglect the quadrative convective term in the Navier-Stokes equations to obtain the Stokes equations:

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\nabla P + \eta \nabla^2 \mathbf{v} + \mathbf{f} \ .$$

Here $\mathbf{f}(\mathbf{r},\mathbf{t})$ is the sum of all *body forces* which act on unit fluid volume at $\mathbf{r}, t$.

An additional assumption made by Peskin and Fogelson is that *inertial effects* are negligible. This means that the the fluid flow very quickly adjusts to any changes in the body forces. The flow is quasi-steady, which implies that we can neglect the term $\rho\frac{\partial \mathbf{v}}{\partial t}$ on the left hand side to obtain

$$\eta\nabla^2\mathbf{v} = \nabla P - \mathbf{f} \ .$$

Since the flow is incompressible and quasi-steady, we have in addition the continuity equation

$$\nabla \cdot \mathbf{v} = 0 \ ,$$

appropriate to steady flow.

The fluid equations will be solved by introducing a computational grid.

Suspended particles as immersed boundaries

Fogelson treats the platelets as point particles which are essentially swept along with the fluid. Suppose that particle k has position $\mathbf{r}_k(t)$. Since it moves along with the local fluid velocity, its equation of motion is simply

$$\frac{d\mathbf{r}_k}{dt} = \mathbf{v}(\mathbf{r}_k, t) \ ,$$

where the right hand side is the fluid velocity at the position of the particle. If the fluid velocity is known at some particular time in the simulation, the position of each particle can be updated to the next discrete time step by using an Euler type algorithm.

Note that the suspended particles move continuously in space and are not confined to the lattice sites of the computational grid. However, if the fluid equations are solved on the grid, we will need to interpolate the fluid velocity to the current particle positions in order to solve the particle equations.

Suppose that $\mathbf{F}_k$ is the net force on particle k, which can include the force of gravity, and also forces between the particles generated for example by a molecular potential such as Lennard-Jones. The essential logic behind the Immersed Boundary Technique is as follows:

- The particle is a disc immersed in the fluid which moves under the action of the applied force $\mathbf{F}_k$, and the pressure and viscous foces due to the surrounding fluid.
- The particle moves essentially with the local fluid velocity.
- Replace the particle by a region of fluid surrounded by an imaginary disc-shaped boundary, and the replace the force $\mathbf{F}_k$ on the particle by an equivalent body-force acting on the fluid within this boundary.
- If the density of the particle is different from the density of the fluid, this needs to be taken into account. It may also be necessary to change the fluid viscosity in

the immersed region if the friction between fluid layers differs substantially from the friction between the fluid and the particle surface.

Discrete δ-function

Since the fluid velocity $\mathbf{v}$ is defined only on the computational grid points and the particles can move anywhere in space, prescriptions are needed to

- compute the fluid velocity at the positions of the particles, and
- from the positions of the particles to compute the body force per unit volume on the fluid at the grid points.

Peskin introduced a *discrete δ-function*

$$D_{ij}(x,y) = d(x-ih)d(y-jh) \ ,$$

where

$$d(r) = \begin{cases} \frac{1}{4h}\left[1+\cos\left(\frac{\pi r}{2h}\right)\right] , & \text{for } |r| \leq 2h \\ 0, & \text{for } |r| \geq 2h \end{cases}$$

where the grid spacing is assumed to be h in both x and y directions, and i,j are grid indices in the x and y directions. This function has the essential property

$$\sum_i hd(x-ih) = \int_{-\infty}^{\infty} d(x)\, dx = 1 \ ,$$

that is appropriate to a delta function, and it approached the Dirac $\delta(x)$ function in the limit $h \to 0$. The function $d(r)$ is essentially one cycle of the cosine function with a constant added to make it positive. Since $d(\pm 2h) = 0$, the function D has support on a square whose side is 4 grid spacings h.

The Immersed Boundary Method uses Peskin's D function (or a similar function) to interpolate from the particle continuum to the fluid grid and *vice versa*.

Fluid velocity at particle positions: This is approximated using the prescription

$$\mathbf{v}(\mathbf{r}_k) = h^2 \sum_{i,j} \mathbf{v}_{ij} D_{ij}(\mathbf{x}_k) \ ,$$

where the sum runs over all grid points. This gives a weighted average of the fluid velocities at all grid that are within two grid spacings of the particle position.

Body force at grid points: This is approximated using the prescription

$$\mathbf{f}_{ij} = \sum_{k} \mathbf{F}_k(\mathbf{r}_1, \ldots \mathbf{r}_N) D_{ij}(\mathbf{x}_k) \ ,$$

where the sum runs over all particles $1 \ldots N$. Note that the force on particle k depends on the positions of all of the other particles. If these forces are short-ranged, then the body force $\mathbf{f}$ at lattice site ij is determined essentially by the forces acting on particles within a distance $2h$ in x or y from the grid point. Note that D has dimensions $[\mathrm{L}]^{-2}$ so $\mathbf{f}$ is a force density.

Numerical algorithm

The fluid is assumed to be contained in a 2-D rectangular region with appropriate fluid boundary conditions at the 4 fixed boundaries. In Fogelson's application, the upper and lower boundaries represent the wall of a blood vessel, and the blood flows in at the left boundary and out at the right. Particles can be injected into the system at the the inlet, or they can be placed in the fluid volume initially and their subsequent motion studied.

A discrete time step Δt is chosen to study the evolution of the system in time $t = 0, \Delta t, \ldots n\Delta t, \ldots$. To advance the system by one time step, the following computations are performed:

- The forces $\mathbf{F}_k$ acting on the particles are computed using an *approximately implicit scheme* to avoid numerical instabilities in the motion of the particles which obey *stiff* differential equations.

- The force values $\mathbf{F}_k$ are used to compute the body force densities at the grid points.

- The Stokes equations are solved to find the fluid velocities at the grid points. In 2-D this time-independent problem can be solved by introducing a stream function ψ and vorticity ζ. In 3-D the pressure P also needs to be taken into account.

- The fluid velocities at the particle positions are computed, and the particles are moved to their new positions using a simple Euler prescription.