Topic 5: Computational Fluid Dynamics – Particle Suspension

Computational Fluid Dynamics (CFD) is a very important topic in computational science and engineering with applications in many areas such as

- designing mechanical devices and components for fluids flowing through and around them,
- designing automobiles, aerospace and marine vehicles with fluids flowing around them,
- modeling the flow of biofluids, for example blood in the circulatory system,
- modeling the motion of particles in the cytosol or cytoplasm of biological cells,
- modeling the dynamics of fluids of charged particles (plasmas) in fusion reactors and astronomical systems, and
- modeling the evolution of the universe as a relativistic fluid.

Equations of Fluid Dynamics

The equations of fluid dynamics are based on a *continuum* approximation: the fluid consists of such a large number of particles (molecules) that observables such as the fluid velocity $\mathbf{v}(\mathbf{r}, t)$, the pressure $P(\mathbf{r}, t)$, and density $\rho(\mathbf{r}, t)$, can be considered to be continuous differentiable functions of position $\mathbf{r}$ in space and of time t.

The equations are derived from fundamental physical principles

1. The conservation of mass. In non-relativistic theories, the number of atoms in the fluid does not change.

2. Newton's second law of motion: $\mathbf{F} = m\mathbf{a}$.

3. The conservation of energy.

Conservation of mass

Conservation of mass implies a continuity equation

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

One way of interpreting this equation is to imagine a small volume fixed in space. The continuity equation ensures that

$$\frac{d}{dt} \int_{\mathcal{V}} \rho \, dV = - \int_{\mathcal{S}} \mathbf{v} \cdot \mathbf{n} \, dS \ ,$$

where $\mathbf{n}$ is the outward normal. This says that the increase in mass of fluid inside the volume $\mathcal{V}$ is due to the inflow of fluid thorugh the surface $\mathcal{S}$.

A very important and useful approximation is that of an *incompressible* fluid, i.e., one in which $\rho =$ constant. This implies that the fluid velocity is divergence free:

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

Generally speaking, a fluid behaves more or less incompressibly if the magnitude of the fluid velocity is much smaller than the speed of sound in the fluid.

Newton's second law of motion

The motion of the fluid is governed by forces of various types:

- A pressure gradient in the fluid will cause it to flow

  $$\mathbf{f}^{\text{pressure}} = -\nabla P \ .$$

  Here f is the force per unit volume of the fluid. Recall that pressure is force per unit area.

- An external force (body force) like gravity can cause the fluid to move.

  $$\mathbf{f}^{\text{gravity}} = -\rho\mathbf{g}; \ .$$

  Here $\mathbf{g}$ is the vector acceleration of gravity. A charged fluid might also be subjected to electric and magnetic forces.

- Viscous forces tend to damp fluid motion. If the velocity gradients in the fluid are not too large, the viscous force on unit volume of fluid can be approximated by

$$f_i^{\text{viscous}} = \frac{\partial}{\partial x_j}\left[\eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + \lambda\delta_{ij}\nabla\cdot\mathbf{v}\right] ,$$

  where η is the *dynamic viscosity* coefficient (essentially the ratio of shear stress to shear strain), and λ is the *bulk viscosity* coefficient (essentially the ratio of compressional stress to compressional strain).

Appling Newton's second law of motion to a unit volume of fluid

$$\rho\frac{d\mathbf{v}}{dt} = \mathbf{f}^{\text{pressure}} + \mathbf{f}^{\text{gravity}} + \mathbf{f}^{\text{viscous}} ,$$

we obtain the *Navier-Stokes* equations

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

The left hand side of this equation is the *convective derivative*: the velocity of a fluid element changes with time ($\partial/\partial t$) and also because the element moves to a different location is space where the velocity has a different value ($\mathbf{v}\cdot\nabla$). If the fluid is incompressible, the equations can be written

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

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

Conservation of energy

The equation of continuity and the three components of the Navier-Stokes equations relate five functions, namely the density ρ, and pressure P and the three components of fluid velocity $\mathbf{v}$. The fifth equation required to solve this system is provided by conservation of energy. In general, conservation of energy involves

- work done by the gravity, pressure, and viscous forces,
- thermal conduction in the fluid if there are temperature gradients, and
- volumetric heating if there are sources or sinks of thermal energy in the fluid.

The equations taking all of these effects into account straightforward to derive using the laws of thermodynamics, but they are somewhat complicated. If the fluid can be treated as an ideal gas at constant absolute temperature T, we can use the ideal gas equation of state

$$P = \rho R T \ ,$$

where R is the gas constant, to relate the pressure and density. In general, one must use the equation of state for the fluid. If the temperature of the fluid is not constant one needs an additional equation provided by the laws of thermodynamics.

The Reynolds Number

In the absence of body forces, the incompressible Navier-Stokes equations can be re-written in dimensionless form which reveals a very important dimensionless quantity called the *Reynolds number*. Let L be a typical linear dimension of the system and U be a typical velocity magnitude. Define

$$\mathbf{r}' \equiv \frac{\mathbf{r}}{L} , \qquad \mathbf{v}' \equiv \frac{\mathbf{v}}{U} .$$

By dimensional analysis, we can define dimensionless

$$t' \equiv \frac{tU}{L} , \qquad P' \equiv \frac{P}{\rho U^2} .$$

The Navier-Stokes equations for an incompressible fluid can be written in dimensionless form

$$\frac{\partial \mathbf{v}'}{\partial t'} + \mathbf{v}' \cdot \nabla' \mathbf{v}' = -\nabla' P' + \frac{1}{\mathrm{Re}} \nabla'^2 \mathbf{v}' ,$$

where the dimensionless Reynolds number is

$$\mathrm{Re} \equiv \frac{L\rho U}{\eta} = \frac{LU}{\nu} .$$

The Reynolds number measures the relative importance of pressure and viscous forces

$$\mathrm{Re} \sim \frac{\mathbf{f}^{\mathrm{pressure}}}{\mathbf{f}^{\mathrm{viscous}}} .$$

At low Reynolds number, a flow is dominated by viscosity, and at high Reynolds number by pressure forces. The Reynolds number is also critical in determining whether a flow is regular or turbulent: in fact, it was introduced in 1883 by Osborne Reynolds in a paper on laminar and turbulent flow in pipes.

Incompressible Steady Flow in 2-D

The full set of coupled equations for fluid flow can be quite complicated to solve in general. The equations are nonlinear, and appropriate initial and boundary conditions must be supplied to obtain an unique solution. In fact, proving the existence and smoothness of solutions in general is listed as one of the Millenium Prize Problems by the Clay Mathematics Institute.

However, there are numerous simplified situations in which the Navier-Stokes equations can be solved quite readily. We start by studying steady incompressible flow in 2-D which can be solved using techinques very similar to Poisson's equation!