Brief course outline

- **Introduction**
  - reactor systems applications
  - two-phase flow regimes
- **Direct numerical simulation (DNS)**
  - Navier-Stokes equations
  - Conservation of mass, momentum, energy
  - incompressible flows
  - Turbulence resolution requirements
- **Interface tracking methods (ITM)**
  - Overview of modeling approaches at various scales
  - One-fluid approach: incompressible N.S. incorporating interface treatment
  - Surface tension
  - Dimensionless groups
- **Numerical considerations:**
  - Overview of ITM methods
  - Time integration (explicit and implicit methods)
  - Spatial discretization
  - Boundary conditions
  - One-fluid approach:
    - Volume of Fluid method
    - Front-tracking method
    - Level-Set method
- **Computational Multiphase Fluid Dynamics (CMFD)**
  - Reynolds-averaged Navier-Stokes equations (RANS)
  - Turbulence modeling:
    - Gradient-diffusion and turbulent viscosity hypothesis
    - Shear stress and turbulent shear stress
    - law of the wall
    - turbulence models
  - two-phase modeling approach
  - interfacial forces
  - interfacial area density evolution
  - subcooled boiling modeling
  - critical heat flux

Direct numerical simulation (DNS)

1. **Introduction**
2. **Direct numerical simulation (DNS)**
   - Conservation of mass, momentum, energy
   - Navier-Stokes equations
   - incompressible flows
   - Turbulence resolution requirements
3. **Interface tracking methods (ITM)**
4. **Numerical considerations**
5. **Computational Multiphase Fluid Dynamics (CMFD)**

Comments on Governing Equations (1)

- broadly referred to as Navier-Stokes Equations (N.-S.)
- for inviscid flows called "Euler" equations
- can be presented in cylindrical, spherical, general curvilinear coordinates
- work for single-phase, non-reacting flows
- there is no general closed-form analytical solution to these equations which has been found today – the **main reason** for CFD existence !
- it is important that a CFD problem is well-posed, e.g.:
  - the solution to the equations exist and unique
  - the solution depend continuously upon the initial and boundary conditions
- Boundary conditions are of crucial importance to DNS/LES; initial conditions are of secondary importance (why ?)

Comments on Governing Equations (2)

- it is important to classify if the governing equations are hyperbolic, parabolic or elliptic
  - elliptic equations must be solved simultaneously over the whole domain
  - parabolic and hyperbolic are propagated from one location to another
- it can be shown that unsteady N.-S. equations have mixed behavior:
  - elliptic in space
  - parabolic in time
- the fundamental equations apply to both laminar and turbulent flows:
  - numerical solution to a “satisfactory degree” of accuracy will give the answers. For practical problems, the computing resource is the major restriction
- turbulence has a broad range of time and length scales which lead to high computing costs of direct solution

Comments on Governing Equations (3)

- traditional CFD avoids it by focusing on mean flow, in which Reynolds- or ensemble-averaged equations are solved
  - this leads to the necessity of closure models for unknown correlations:
    - $\overline{\rho u_i' u_j'}$ - Reynolds stresses
    - $\overline{\rho c_v u_i' T'}$ - turbulent heat fluxes
  - determination of these closures is the subject of turbulence modeling
- while the governing equations are the same, the solutions can be widely different
  - boundary conditions play a big role

Turbulence

Characteristics of turbulent flows:

- 3D, unsteady and involve 3D fluctuations
- Mixing of mass, momentum and heat is more effective compared to molecular diffusion in laminar flows
- Turbulence has been viewed as stochastic (random) phenomenon, however it is now established that there is some degree of structure and order in it
- Turbulence maybe viewed as a vortical flow with a wide spectrum of eddy sizes and fluctuating frequencies; it involves wide spectrum of length and time scales
- Large eddies correspond to low frequencies and small eddies to high frequencies. Larger eddies break into smaller ones in a chain process which is referred to as energy cascade. The supply of energy to maintain the turbulence is extracted from the main flow.

Turbulence (2)

Characteristics of turbulent flows (2):

- Turbulence is a continuum process: smallest eddies are much greater in size than molecular interactions.
- Large eddy dynamics is determined by the boundary conditions and influenced by the mean flow
- The largest eddies are anisotropic and responsible for most of the turbulent mixing
- The smallest eddies do not contribute much to turbulent mixing and contain a small fraction of the turbulent kinetic energy (TKE). They are nearly isotropic.

Incompressible Flows

- For liquid flows and gas flows at low speeds ($M < 0.3$) where density is almost constant compressibility effects are negligible
- For such flows the incompressible form of the governing equations is always used
- There are SEVERE problems if a compressible code is used for incompressible flows:
  - As the Mach number becomes smaller, typical compressible flow solvers suffer severe deficiencies in both efficiency and accuracy (they are density-based, and pressure is computed from density and temperature)
  - Incompressible solvers are pressure based (Poisson equation for pressure is solved)

Notes on Gov. Eq. (Incompressible Flows)

Unsteady
3D
Incompressible
Viscous flow

- We formulate the Incompressible NS for
- Continuity:

$$\nabla \cdot \vec{u} = 0 \qquad (8)$$

- Momentum:

$$\rho \frac{Du_i}{Dt} = -p_{,i} + \mu \nabla^2 u_i + \rho f_i \qquad (9)$$

- Energy:

$$\rho \frac{De}{Dt} = \rho \dot{q} + \left(kT_{,i}\right)_{,i} + \rho \Phi + \rho \vec{f} \cdot \vec{u} \qquad (10)$$

where the Laplacian is defined as:

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \blacksquare_{,ii}$$

and μ is assumed to be constant.

Notes on Gov. Eq. (2)

- Energy equation used the following assumptions:
  - Kinetic energy per unit mass $\frac{u^2}{2} = (u_1^2 + u_2^2 + u_3^2)/2$ is much smaller than the internal energy
  - Work done by pressure in negligible
  - The energy equation is decoupled from continuity and momentum equations

Note: the last point is not valid for two-phase boiling flows!

  - The rate of dissipation per unit mass is the work done by viscous stresses:

$$\Phi = \nu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad (11)$$

Notes on Gov. Eq. (3)

- For incompressible flows, the fundamental governing equations lack an independent equation for pressure. The continuity equation cannot be used directly.
- Taking the divergence of the momentum equations and them simplifying using the continuity equation, the Poisson's equation for pressure can be obtained as:

$$\nabla^2 p = -\rho\left[\left(u_i u_j\right)_{,j}\right]_{,i} \qquad (12)$$

- Note: Eq. (12) is an elliptic problem: pressure values on boundaries MUST be known to compute the whole flow field.

Notes on Gov. Eq. (4)

- In fluid dynamics the Boussinesq (1903) approximation is used in buoyancy-driven flows and low-speed reacting flows:
  - Density differences are neglected
  - Only implemented as body forces (such as gravity multiplied by a variable density)

- Example 1.1: Laminar flow in a channel
  - <whiteboard>

Direct Numerical Simulation (1)

- Directly solves all the relevant scales of turbulent motion.
- No model (simplification or approximation) is needed
- Extremely expensive for most engineering problems
- The cost of meshing requirements for DNS are estimated using the smallest turbulence scales

<whiteboard: on the Kolmogorov's scales and mesh size estimate procedure>

Direct Numerical Simulation (2)

- DNS can be superior to experimental measurements in permitting full access to all the instantaneous flow variables, so that turbulent structures and transport mechanisms can be extensively analyzed.
- Experimental measurement techniques can be tested and evaluated against detailed and accurate DNS results
- DNS can provide precise and detailed turbulence statistics, which is useful in evaluating and developing turbulence models
- Effects of important parameters characterizing the flow and scalar fields, such as Reynolds number, Prandtl number, and Schmidt number, can be systematically varied and examined
- DNS can offer an opportunity to accurately study a virtual flow field that would not occur in reality