Chemical Engineering 374

Fluid Mechanics

Computational Fluid Dynamics
(CFD)

Spiritual Thought

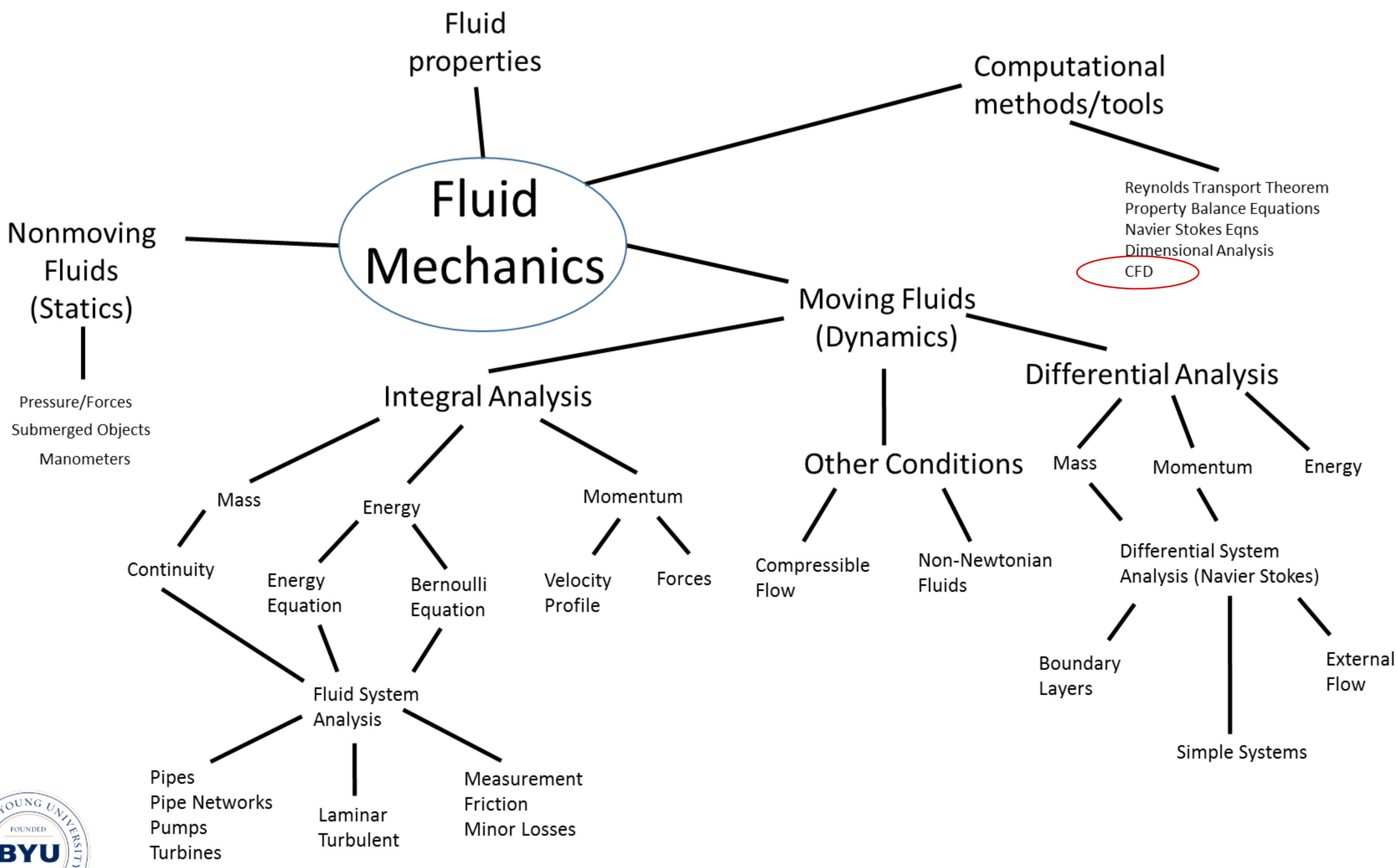
“*When He answers* yes, *it is to give us confidence.*

When He answers no, *it is to prevent error.*

When he withholds an answer, *it is to have us grow through faith in Him, obedience to His commandments, and a willingness to act on truth.*”

Elder Richard G. Scott

Fluids Roadmap



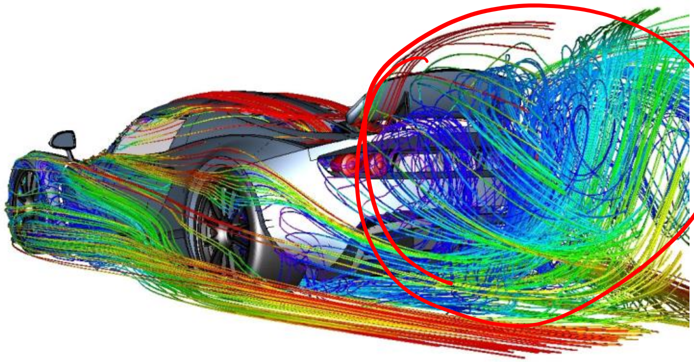
ABET

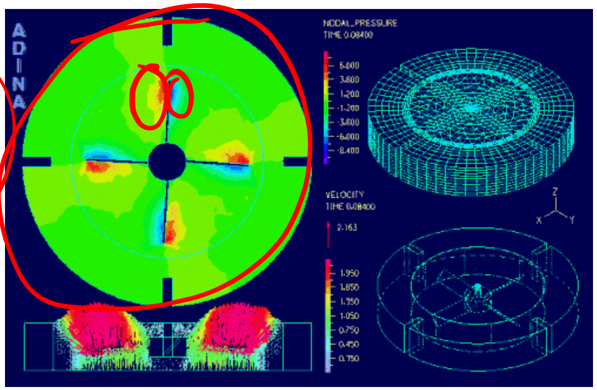
- Please fill out the survey
- Located at: https://goo.gl/forms/3S09A5RWynLLRdTx1
- 2nd to last quiz (due Friday) will be asking whether or not you filled out ABET questionnaire
- Please also fill out student evaluations for course and instructor!!!

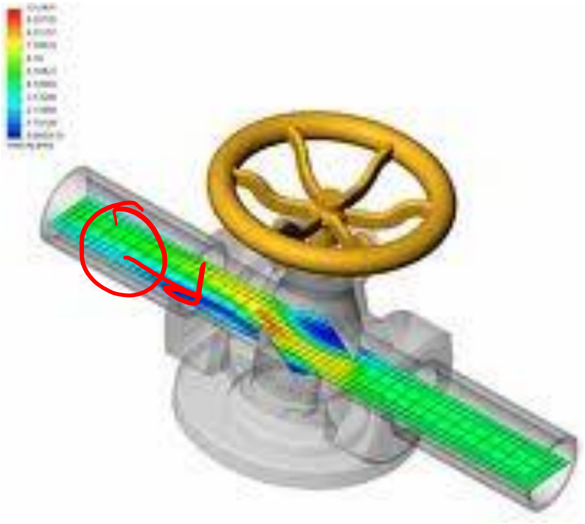
So far…

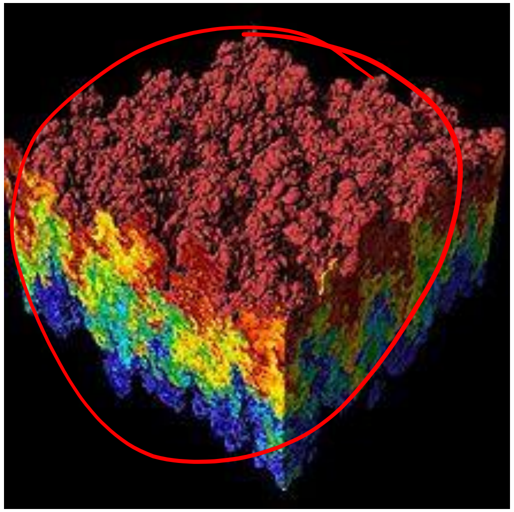
- Fluid statics (no flow)
- Basic flows: Bernoulli Equation
- Integral Balances: Control volume → mass, momentum, energy
- Differential Balances → momentum and mass (Navier Stokes)
- All of this was for
  - Simple configurations that we could directly solve analytically
  - 0-D, or 1-D
  - Steady State
  - Incompressible
- 2D or 3D flow in complex geometry, or turbulent, or compressible, are too complex for analytic solution
  - → Solve with computers
- Big Subject → give a basic introduction

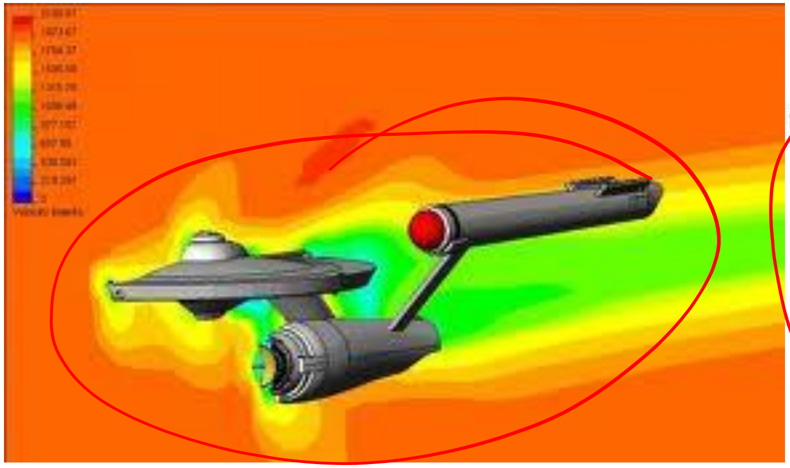
Examples

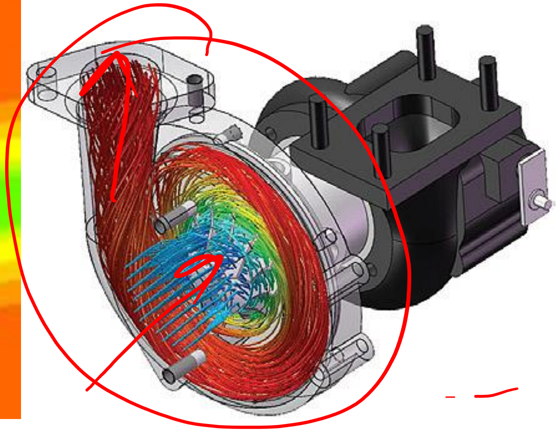












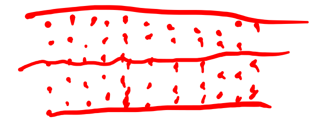
Key Aspects

- Governing equations
- Mathmatical description
- Grid generation
- Numerical algorithm
- Turbulence modeling
- Convergence
- Stability
- Verification
- Validation

Software

- Commercial
  - Ansys Fluent
  - CD-Adapco—Star CD
- Free
  - OpenFOAM
  - Free CFD
- In-house codes
  - (everyone's got one)
- Many others
  - www.cfd-online.com

Nuts and Bolts



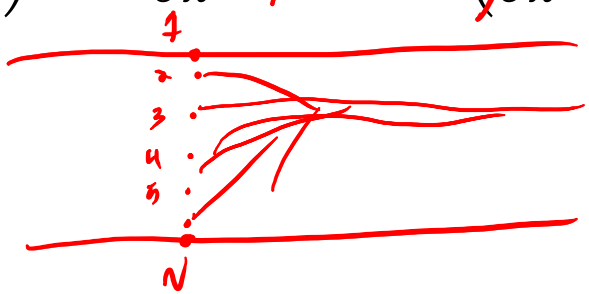
- Most of CFD boils down to the following
- Create a spatial grid for the solution
  - Finite difference → grid of points
  - Finite volume → grid of connected 0-D control volumes
- Here we will focus on finite difference
  - Approximate the derivatives using the grid points.
    - 1 PDE → many coupled ODE's, one for each point.
    - Solve the system of ODE's at each grid point.

Example 1

- Unsteady, fully developed, laminar duct flow, 1-D
  - Start with Navier-Stokes equations – x momentum

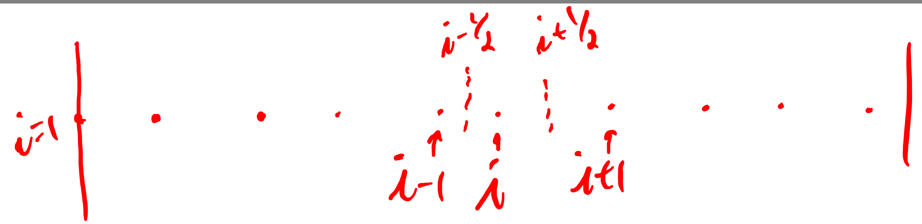
$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial P}{\partial x}+\rho g_x+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)$$

$$\frac{\partial u}{\partial t}=\frac{\mu}{\rho}\frac{\partial^2 u}{\partial y^2}-\frac{1}{\rho}\frac{\partial P}{\partial x}$$



  - Then make a grid of points across D of duct
    - And recognize that $-\frac{1}{\rho}\frac{\partial P}{\partial x}$ is a constant
    - $\Delta y = D/(N-1)$

Numerical Derivative



- $\frac{\partial^2 u}{\partial y^2} = \frac{\partial u}{\partial y}\left(\frac{\partial u}{\partial y}\right)$
- $\left(\frac{\partial u}{\partial y}\right)_{i+1/2} \approx \frac{u_{i+1} - u_i}{\Delta y}$
- $\left(\frac{\partial u}{\partial y}\right)_{i-1/2} \approx \frac{u_i - u_{i-1}}{\Delta y}$
- $\frac{\partial^2 u}{\partial y^2} \approx \frac{\left(\frac{\partial u}{\partial y}\right)_{i+1/2} - \left(\frac{\partial u}{\partial y}\right)_{i-1/2}}{\Delta y}$
- $\approx \frac{\frac{u_{i+1} - u_i}{\Delta y} - \frac{u_i - u_{i-1}}{\Delta y}}{\Delta y} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta y^2}$

Numerical Equation

- $\frac{\partial u}{\partial t} = \frac{\mu}{\rho}\frac{\partial^2 u}{\partial y^2} - \frac{1}{\rho}\frac{\partial P}{\partial x} \approx \frac{\partial u}{\partial t} = \frac{\mu}{\rho}\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta y^2}\right) - \frac{1}{\rho}\frac{\partial P}{\partial x}$
  - Works only for interior nodes
    - Why?
  - For edge nodes, need BC
  - $u_1 = 0$
  - $u_N = 0$
- This transforms PDE (difficult to solve)
  - N-2 ODE's
  - coupled

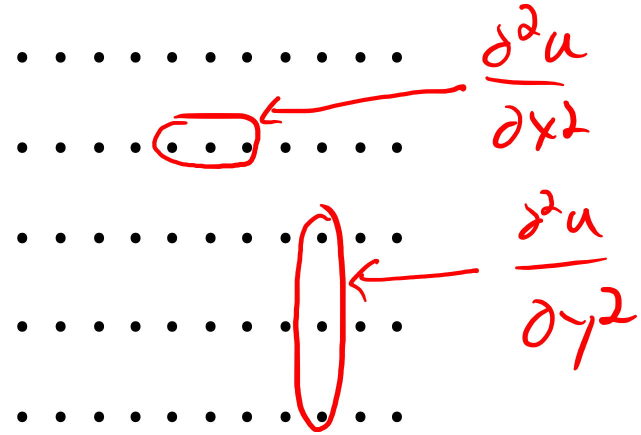
Solve ODE's

- Can use any ODE solver
  - Example using explicit Euler
  - $\frac{du}{dt} = f(u) \rightarrow \frac{u^{n+1} - u^n}{\Delta t} = f(u^n)$

    $\rightarrow u^{n+1} = u^n + \Delta t \cdot f(u^n)$
  - Thus:
  - $u^{n+1} = u^n + \Delta t \frac{\mu}{\rho \Delta y^2} \cdot \left[\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta y^2} \right) - \frac{1}{\rho} \frac{\partial P}{\partial x} \right] \Delta t$
- Solve in excel or python

2D Problem

- Very similar to 1D, but have more derivatives
- Grid:



$$\frac{\partial u_i}{\partial t} = f(u, v, P \text{ on grid})$$

$$\frac{\partial v_i}{\partial t} = f(u, v, P \text{ on grid})$$

Solve w/ ODE solver

Summary

- 1D laminar, unsteady, pipe flow:
  - $\frac{\partial u}{\partial t} = \frac{\mu}{\rho}\frac{\partial^2 u}{\partial y^2} - \frac{1}{\rho}\frac{\partial P}{\partial x}$
- Grid of points across pipe diameter
- Approximated 2nd derivative numerically:
  - $\left(\frac{\partial^2 u}{\partial x^2}\right)_i \cong \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$
- $\frac{\partial u_i}{\partial t} = \frac{\mu}{\rho}\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}\right) - \frac{1}{\rho}\frac{\partial P}{\partial x}$
- BC's: $u_1 = 0, u_N = 0$
  - PDE → N-2 ODE's (coupled)
- Solve