

# Chemical Engineering 374

## *Fluid Mechanics*

### Computational Fluid Dynamics II (CFD II)



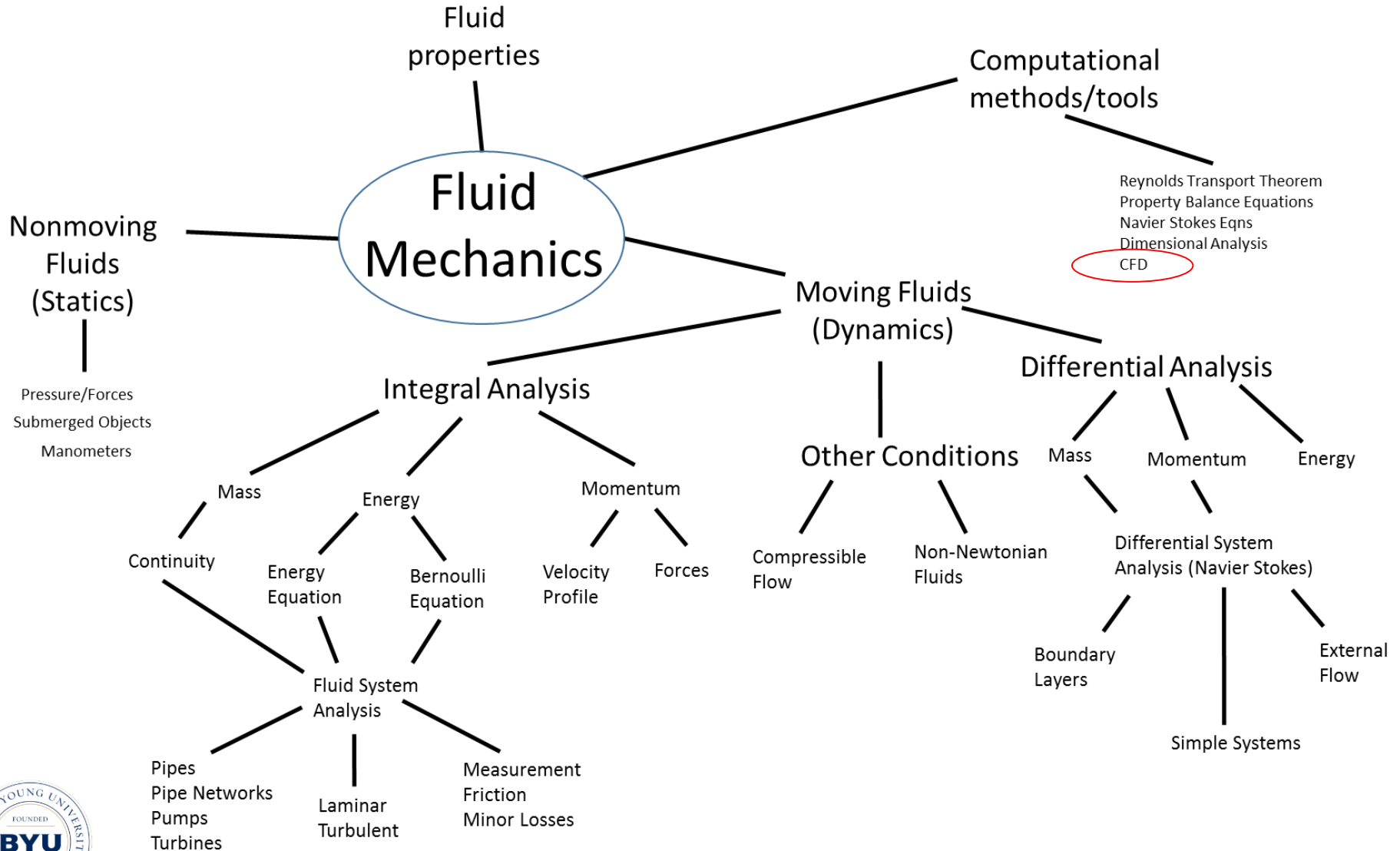
# Spiritual Thought

“Let me repeat and emphasize that point—*you will lead the Church in 20 to 30 years from now*. Some of you will serve as bishops; stake presidents; mission presidents; Primary, Young Women, and Relief Society presidents; and temple presidents and matrons. Yes, within the reach of my voice tonight are those who will most likely become leaders in communities and nations of the world. There will be those who will be members of the general women’s presidencies or even a General Authority Seventy or perhaps a member of the Quorum of the Twelve Apostles.”

Elder M. Russell Ballard



# Fluids Roadmap



# Last time

- 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 2<sup>nd</sup> 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  $\longrightarrow$  N-2 ODE's (coupled)



# Solve ODE's

- Use your favorite ODE solver
- Or, use Explicit Euler:

- $\frac{\partial u}{\partial t} = f(u) = \left( \frac{u^{n+1} - u^n}{\Delta t} \right) = f(u^n)$

- $u^{n+1} = u^n + \Delta t * f(u^n)$

- Therefore:

- $u^{n+1} = u_i^n + \frac{\Delta t \mu}{\rho \Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) - \frac{1}{\rho} \frac{\partial P}{\partial x}$

– See Excel Solution

- 2D is similar:

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

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



# Laminar Jet

- 2-D unsteady Laminar Jet
- 3 eqns, 3 unknowns:  $u$ ,  $v$ ,  $P$

– Cont:  $\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 = \nabla \cdot \vec{v}$

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

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

– P equation?

- Derive by taking  $\nabla \cdot$  mom, and inserting continuity

- $\nabla \cdot \nabla P = \frac{1}{\rho} \nabla \cdot (\vec{v} \cdot \nabla \vec{v})$



# Laminar Jet

- Boundary Conditions
  - Walls:  $u=v=0$
  - Inlet:  $u=u_{in}, v=v^{in}$
  - Outlet:  $\frac{\partial u}{\partial x_n} = 0, \frac{\partial v}{\partial x_n} = 0$
- See MatLab Code Solution online



# Other Issues

- If incompressible:
  - Need small timesteps, capture  $c$
  - Need energy equation as well
  - $\rho = \frac{MP}{RT}$ ,  $u, v, P, e, \rho$  – 5 eqns. 5 unknowns
- Reacting Flows:
  - Solve for  $Y^i$
- Turbulent flow (2 options):
  - “Resolve” turbulence – EXPENSIVE
  - Model turbulence





- Grid Quality
  - Structured
  - Unstructured
    - easier for complex geometries
- Staggered Grid
- Numerical Diffusion
- Etc.
- More detail in ChEn54



# Turbulence

- 3D, Unsteady, Chaotic, many timescales
- Large difference in lengths & time scales
- To get enough grid points to resolve is expensive computationally
  - Cost scales as  $Re^3$ , so doubling domain size ( $2xRe$ ) is 8x the cost!!
- Resolving all scales of turbulence in CFD is called DNS: Direct Numerical Simulations – Only used in RESEARCH!



# Practical CFD

- All Practical CFD codes model turbulence
  - Only resolve large eddies, no small ones
    - LES = Large Eddy Simulation
    - Cheaper than DNS, but still expensive
    - Mostly research applications
  - Solve for average flows – RANS
    - Reynolds Average Navier Stokes
- Average Flow Equations:  $\bar{\phi} = \frac{1}{T} \int_0^T \phi dt$ 
  - Where  $\phi$  is some quantity and T is a long time



# Decompose $v$

- 2 eqns, 2 unknowns  $\bar{v}$ ,  $\bar{P}$
- We don't know  $\overline{v'v'}$  - have to model it
  - This is primary challenge of CFD: Finding good models for these terms
  - $\overline{v'v'}$  is Reynolds Stress
    - Units of stress
    - Usually modeled as  $\overline{v'v'} = \nu_t \nabla \cdot \bar{v}$
    - Where  $\nu_t$  is some modeled turbulent kinematic viscosity
    - Standard Model is k- $\epsilon$  model

