Chemical Engineering 374

Fluid Mechanics
Fall 2011

Computational Fluid Dynamics
(CFD)

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So far…

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- 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

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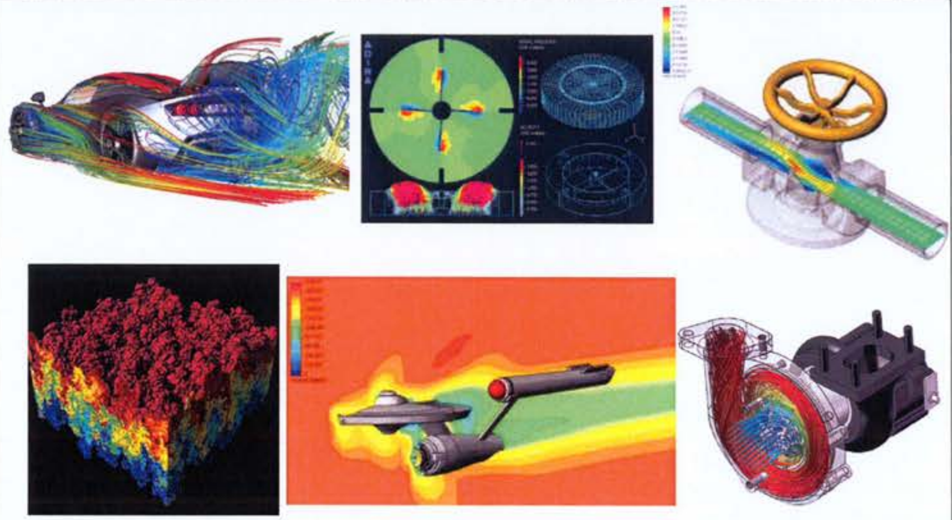
Examples



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Key Aspects

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

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Software

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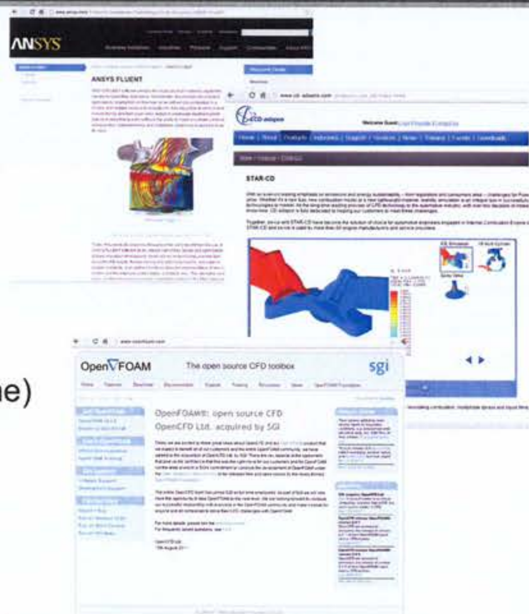
- Commercial
  - Ansys Fluent
  - CD-Adapco—Star CD
- Free
  - OpenFOAM
  - Free CFD
- In-house codes
  - (everyone's got one)
- Many others
  - www.cfd-online.com



Nuts and Bolts

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- 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 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

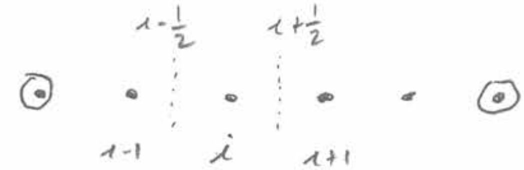
Unsteady, Laminar pipe flow, 1-D

X-momentum

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

- $\dfrac{\partial u}{\partial t} = \dfrac{\mu}{\rho}\dfrac{\partial^2 u}{\partial x^2} - \dfrac{1}{\rho}\dfrac{\partial P}{\partial x}$
- Grid of points across D

  $\Delta x = \dfrac{D}{N-1}$



- $\left(-\dfrac{1}{\rho}\dfrac{\partial P}{\partial x}\right)$ is a constant.
- Approximate $\dfrac{\partial^2 u}{\partial x^2}$ at each point i

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

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

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

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

- $\dfrac{\partial u_i}{\partial t} = \dfrac{\mu}{\rho}\left(\dfrac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}\right) - \dfrac{1}{\rho}\dfrac{\partial P}{\partial x}$ for interior $i = 2, N-1$
  - $u_1 = 0$, $u_N = 0$ are B.C.
  - PDE $\longrightarrow$ N-2 ODE's (coupled)

Now Solve These ODE's.

- Use your favorite ODE Solver.
- Or use Explicit Euler:

$$\frac{du}{dt} = f(u) \longrightarrow \frac{u^{n+1} - u^n}{\Delta t} = f(u^n)$$

$$\longrightarrow u^{n+1} = u^n + \Delta t \cdot f(u^n)$$

So, for us:

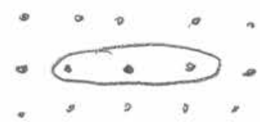
$$u_i^{n+1} = u_i^n + \frac{\Delta t \mu}{\rho \Delta x^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) - \frac{1}{\rho}\frac{\partial P}{\partial x} \cdot \Delta t$$

Solve in Excel. See Attached

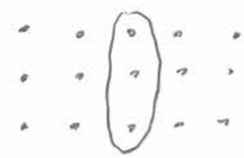
Now, in 2-D its very similar,

Grid

$$\frac{\partial^2 u}{\partial x^2} \longrightarrow$$



$$\frac{\partial^2 u}{\partial y^2} \longrightarrow$$



Have $\dfrac{\partial u_i}{\partial t} = f(u, v, P \text{ on the Grid})$

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

Solve with ODE Solver.

Example 2

2-D unsteady Laminar Jet

3 eqns in 3 unknowns u, v, P

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

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

- x-mom is the u eqn
- y-mom is the v eqn
- but where is the P eqn? Continuity?

Get a P eqn by taking $\nabla \cdot$ mom eqn, and inserting continuity

$\rightarrow \nabla \cdot \nabla p = -\frac{1}{\rho} \nabla \cdot (\vec{u} \cdot \nabla \vec{v})$

- Discretize in space, Solve in Time.

Boundary conditions.

- Walls: $u = v = 0$ (or $u = v = V_{wall}$)
- Inlet: $u = u_{in}$, $v = v_{in}$
- Outlet: $\frac{\partial u}{\partial x_n} = 0$; $\frac{\partial v}{\partial x_n} = 0$

  - Recirculation at outlets is a problem! $\rightarrow$ locate Down stream

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See jet Code

Other Issues.

- Last examples were incompressible.
- When Compressible.
  - Capture Sound Speed → Small timesteps.
  - Solve an Energy equation two
  - $\rho = \dfrac{MP}{RT} \rightarrow u, v, P, \rho, e$ 5 eqns / unknowns
- When Reacting.
  - Solve eqns for Y_i
- When turbulent
  - Have to resolve the turbulence → expensive.

    or model it (next time)
- Grid Quality

  | . . . . . | vs |. . . . .|
- Staggered Grid
- Numerical Diffusion
- etc.
- Many issues Discussed in Detail in CHEn 541.

Turbulent Flows.

Turbulence is 3D
Unsteady
Chaotic
Has a range of Length & time Scales.

To get enough Grid points to <u>resolve</u> the Structure is Expensive Computationally.

Cost Scales as Re^3, So Doubling the Domain Size ($2\times Re$) $\rightarrow$ 8 × The cost (and a bigger Domain needs a longer run time)

Resolving Turbulence in CFD is called DNS : Direct Numerical Simulations — Only used in research!

All practical CFD codes <u>model</u> the turbulence.

- Solve for The <u>average</u> Flow → RANS (Reynold Average Navier Stokes)
- Only resolve The Large eddies, but not the Small ones (LES = Large Eddy Simulation) (LES is expensive → mostly research, but <u>way</u> less expensive than DNS)

Average the Flow equations : $\overline{\phi} = \frac{1}{T}\int_0^T \phi \, dt$ where ϕ is Some quantity, Like V, and T is a long time, Decompose v into $\bar{v} + v'$ where $\bar{v}$ is avg, v' is fluctuation. We Discussed this before with turbulent pipe flow.

$\nabla \cdot v = 0$

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

- $\frac{\partial v}{\partial t} \rightarrow \frac{\partial(\bar{v}+v')}{\partial t} \xrightarrow{\text{average}} \frac{\partial}{\partial t}\overline{(\bar{v}+v')}$

$$= \frac{\partial}{\partial t}(\underbrace{\cancel{\bar{\bar{v}}}}_{\bar{v}} + \overset{0}{\cancel{\overline{v'}}})$$

$\rightarrow \frac{\partial \bar{v}}{\partial t}$.

- $\nabla^2 v \rightarrow \nabla^2 \bar{v}$ likewise.

- $\nabla \cdot (vv) \xrightarrow{\text{avg}} \nabla \cdot \overline{\left((\bar{v}+v')(\bar{v}+v')\right)} \rightarrow$

$$= \nabla \cdot \overline{(\bar{v}\bar{v} + 2\bar{v}v' + v'v')}$$

$$= \nabla \cdot (\overline{\bar{v}\bar{v}} + \cancel{\overline{2\bar{v}v'}} + \overline{v'v'})$$

$$= \nabla \cdot (\bar{v}\bar{v}) + \boxed{\nabla \cdot \overline{v'v'}} \rightsquigarrow \text{new term.}$$

$\nabla \cdot \bar{v}$

$$\frac{\partial \bar{v}}{\partial t} + \nabla \cdot (\bar{v}\bar{v}) = -\frac{1}{\rho}\nabla \bar{P} + g + \nu \nabla^2 \bar{v} + \boxed{\nabla \cdot (\overline{v'v'})}$$

- we have 2 eqns in 2 unknowns: $\bar{v}$, $\bar{P}$
- but we Don't know $\overline{v'v'}$ $\rightarrow$ have to model it.

  This is The challenge of CFD: Finding Good models for These Terms.
- $\overline{v'v'}$ is The Reynolds Stress, has units of Stress and is usually modeled as $\overline{v'v'} = \nu_t \nabla \cdot \bar{v}$

  where μ_t is some modeled turbulent kinematic viscosity.
- The Standard model is $\boxed{k - \epsilon}$: The "kay-epsilon model"