CFD - lecture 5

- Molecular story (handwavy \rightarrow just for intuition)
- Internal energy
- Continuum hypotheses
- Euler equations
- Resume OpenFOAM tutorial
Euler's Equations -> Continuum Hypothesis

- What do we need to describe a fluid?
  - Consider air w/ ideal gas (explain in picture)
  
  At the microscopic level, a good model is billiard balls bouncing around. For details, take a thermo course, but for us this is fine to get intuition.

  \[ \mathcal{S}_\varepsilon = \left\{ \text{unit cube scaled by } \varepsilon \right\} \]
  \[ N = \text{number of particles in box} \]

  We will make the assumption that there are many, many particles within our box so that we can characterize state of fluid with average quantities

  \[ \rho := \frac{\left( \sum_{i=1}^N m_i \right)}{\text{vol}(\mathcal{S}_\varepsilon)} \]
  \[ \rho \mathbf{U} := \frac{\sum_{i=1}^N m_i \mathbf{U}_i}{\text{vol}(\mathcal{S}_\varepsilon)} \]

  *Density
  *Momentum

  Internal Energy how much energy is associated with the "internal state" of a fluid

  - For ideal gas example, this can loosely be thought of as the kinetic energy of the particles (not quite right, but fine for getting a rough picture)

  \[ e_e := \frac{\sum_{i} m_i u_i^2}{\text{vol}(\mathcal{S}_\varepsilon)} \]

  \[ \rightarrow \text{more on this later} \]
- From thermodynamics, in the case where we have sufficiently large $N$ such that these averages converge, these three quantities completely determine the state of the system.

- We'll make additional assumption that we have a continuous fluid ("continuum hypothesis").

- This lets us go from a discrete system of particles (with many, many DOF) to something we can do calculus on.

$\rightarrow$ Make a priori assumption that these average quantities converge to a smoothly varying field $\bar{\rho}(x)$, $\bar{u}(x)$, $\bar{e}(x) \rightarrow \mathbb{R}$

Let's think back to our derivation of conservation of mass...

\[- \frac{d}{dt} \int_D \rho e \, dx + \oint_{\partial D} \rho \bar{e} \cdot n \, dA = 0 \]

- Take $\bar{\rho} \equiv 0$

\[- \frac{d}{dt} \int_D \rho \bar{e} \, dx + \oint_{\partial D} \rho \bar{e} \cdot n \, dA = 0 \]

Physically, we can't take $\bar{\rho} \equiv 0$, since reality is discrete, and for a small enough $\Delta x$ our continuum hypothesis will break down.
Knudsen number

\[ Kn = \frac{\lambda}{\xi} \]

\[ \text{mean free path} \]

For \( Kn \ll 1 \), the continuum hypothesis is appropriate.

What sort of applications would this break down for?

Back to equations of motion...

We've assumed that we can characterize fluid with:

\[ \rho \rightarrow \text{continuity equation} \]

\[ \rho u \rightarrow \text{momentum equation} \]

\[ \rho e \rightarrow \text{energy equation} \]

Pressure (informally, technical details are more complicated)

Looking back to the molecular picture, two types of interactions in ideal gas model:

- if particle bounces, there must be an equal and opposite reaction force
- Define pressure as the average force density acting on each face:

\[ p = -\frac{\sum_{i=1}^{\text{number of collisions}} F_i}{\text{vol}(S_i)} \]

- Together w/ continuum hypothesis, this lets us define the force acting on any volume so that:

\[
\frac{\partial}{\partial t} \int_{S} \rho u \, dA + \int_{S} \rho u (u \cdot n) \, dA = \sum F
\]

\[
= -\int_{S} \rho v \cdot n \, dA
\]

\[
= -\int_{\Omega} \nabla p \, dx
\]

\[
\Rightarrow \quad \partial_t (\rho u) + \nabla (\rho u^2) = -\nabla p
\]

Back to the energy equation

- Some basic thermo:

\[ \Delta \text{Energy} = \text{SQ} - \text{SW} \]

\[ \uparrow \quad \uparrow \]

heat work

- In our ideal gas model, there are no friction forces to account for:

no friction \(\Rightarrow\) no dissipation \(\Rightarrow\) no heat
Back to our usual framework

\[ \frac{d}{dt} \int \text{energy} + \int \text{flux of energy} = \int \text{internal change of energy} + \text{rate of work done on fluid in } S \]

\[ \frac{d}{dt} \int_{S^2} e \, dx + \int_{S^2} e \, \hat{u} \cdot \hat{n} \, da = - \int \text{rate of work done on fluid in } S \]

Think back to Physics 101

\[ \text{work} = \int_{x^1}^{x^2} F \cdot ds \]

with units \([FL]\)

We will define (without a technical derivation)

\[ (\text{work}) = \int_{S^2} p \, \hat{n} \cdot \hat{u} \, da \]

with units \([\frac{FL}{A} \rightarrow \text{work}}{\text{time}}\]

\[ 2\epsilon (\epsilon e) + \nabla \cdot (\epsilon e u) = -\nabla \cdot (p u) \]
Equation of state

- Provided we can compute the pressure we're good to go.

- For ideal gas, pressure is related to density and energy

\[ e = c T \]

\[ \rho = e R T \]

- Where does this come from? Assuming pressure comes from wall collisions only, and noting that collision frequency scales with number of particles in box \((e)\) and kinetic energy of particles \((T \sim e \sim \frac{1}{2}mv^2)\)

We can write the whole system compactly as

\[ \frac{\partial}{\partial t} \vec{y} + \nabla \cdot \vec{F}(\vec{y}) = 0 \]

where

\[ \vec{y} = \begin{pmatrix} e \\ \rho u \\ \rho e \end{pmatrix} \]

\[ \vec{F} = \begin{pmatrix} e u \\ \rho u^2 + p I \\ \rho u \vec{e} + (\rho + p) \vec{u} \end{pmatrix} \]