CFD - lecture 5

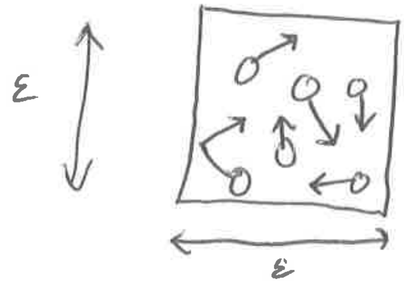
- Molecular story (handwavy → just for intuition)
- Internal energy
- Continuum hypothesis
- Euler equations
- Resume OpenFOAM tutorial

Euler's Equations → Continuum Hypothesis

- What do we need to describe a fluid?

- Consider <u>air</u> 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.



$\Omega_\varepsilon = \{$ unit cube scaled by $\varepsilon \}$

$N =$ 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

$$\rho := \frac{\left(\sum_{i=1}^{N} m_i\right)}{vol(\Omega_\varepsilon)} \qquad \rho \vec{u} := \frac{\sum_{i=1}^{N} m_i \vec{u}_i}{vol(\Omega_\varepsilon)}$$

<u>Density</u> <u>Momentum</u>

<u>Internal Energy</u> 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)

$$\rho e := \frac{\sum_i m_i u_i^2}{vol(\Omega_\varepsilon)} \rightarrow \text{more on this later}$$

- 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

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

Lets think back to our derivation of conservation of mass ...

- $\frac{d}{dt}\int_{\Omega_\varepsilon} \rho \, dx + \oint_{\partial\Omega_\varepsilon} \rho u \cdot n \, dA = 0$

- Take $\varepsilon \searrow 0$

- $\partial_t \rho + \nabla \cdot \rho \vec{u} = 0$

Physically, we <u>can't</u> take $\varepsilon \searrow 0$, since reality is discrete, and for a small enough Ω_ε our continuum hypothesis will break down.

- Knudsen number

$$Kn = \frac{\lambda}{\varepsilon} \leftarrow \text{mean free path}$$

For $Kn << 1$, 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

$\rho \longrightarrow$ continuity equation

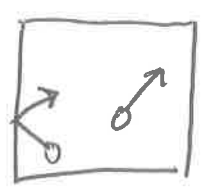
$\rho u \longrightarrow$ momentum equation $\swarrow$ need to figure this out

$$\partial_t \rho u + \nabla \cdot \rho u^2 = F$$

$\rho e \longrightarrow$ energy equation $\leftarrow$ need to define this

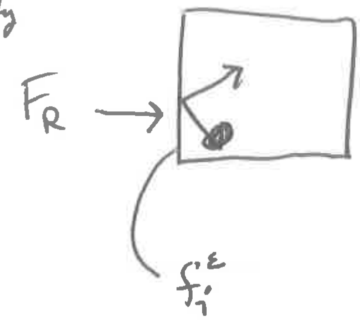
Pressure (informally, technical details are more complicated)

- 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



$$p := \frac{-\sum_{i=1}^{\text{number collisions}} F_i}{\text{vol}(f_i^{\varepsilon})}$$

$\&\ \partial\Omega_{\varepsilon} = \cup f_i^{\varepsilon}$

- together w/ continuum hypothesis, this lets us define the force acting on <u>any</u> volume, so that

$$\frac{d}{dt}\int_{\Omega} \varrho u \, dx + \oint_{\partial\Omega} \varrho u (u\cdot n)\, dA = \sum F$$

$$= -\oint_{\partial\Omega} p \, dA = -\oint_{\partial\Omega} p(I\cdot\hat{n})\, dA$$

$$= -\int_{\Omega} \nabla p \, dx$$

$$\Rightarrow \boxed{\partial_t(\varrho u) + \nabla\cdot(\varrho u^2) = -\nabla p}$$

Back to the energy equation

- Some basic thermo:

$$\Delta \text{Energy} = \underset{\substack{\uparrow \\ \text{heat}}}{\delta Q} - \underset{\substack{\uparrow \\ \text{work}}}{\delta W}$$

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

no friction $\Rightarrow$ no dissipation $\Rightarrow$ no heat

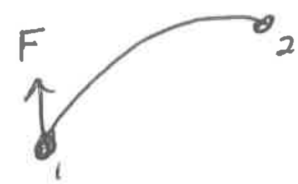
Back to our usual framework

$$\frac{d}{dt}\left(\text{energy}\right) + \left(\text{flux of energy}\right) = \left(\begin{matrix}\cancel{\text{rate of}}\ \text{rate of}\\ \text{internal change}\\ \text{of energy}\end{matrix}\right)$$

$$\frac{d}{dt}\int_{\Omega} \rho e \, dx + \int_{\partial\Omega} \rho e \, \vec{u}\cdot\hat{n} \, dA = -\left(\begin{matrix}\text{rate of}\\ \text{work done on}\\ \text{fluid in } \Omega\end{matrix}\right)$$

Think back to Physics 101

$$\text{work} = \int_{x_1}^{x_2} F \cdot ds$$



with units $[F L]$

We will define (without a technical derivation)

$$\left(\text{work}\right) = \oint_{\partial\Omega} p \, \vec{u}\cdot\hat{n} \, dA$$

with units $\left[\frac{F}{A}\frac{L}{T} A\right] \rightarrow \frac{\text{work}}{\text{time}}$ ✓

$$\boxed{\partial_t(\rho e) + \nabla\cdot(\rho e u) = -\nabla\cdot(p u)}$$

Equation of state

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

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

$$\rightarrow \quad e = cT$$

$$\boxed{p = \rho R T}$$

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

We can write the whole system compactly as

$$\partial_t \vec{y} + \nabla \cdot \vec{F}(y) = 0$$

where

$$\vec{y} = \begin{pmatrix} \rho \\ \rho\vec{u} \\ \rho e \end{pmatrix} \qquad \vec{F} = \begin{pmatrix} \rho\vec{u} \\ \rho u^2 + pI \\ (\rho e + p)\vec{u} \end{pmatrix}$$