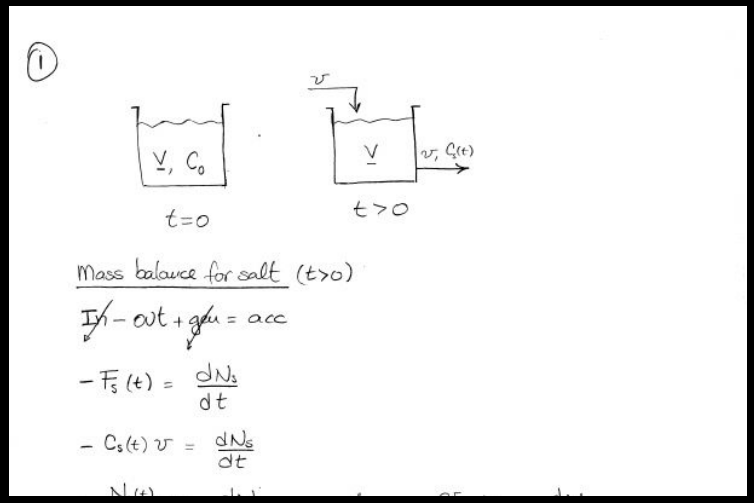
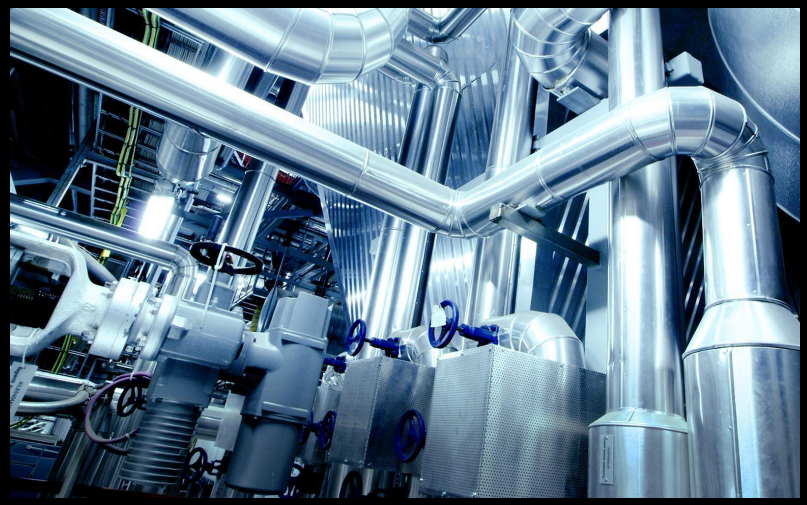
The Cooper Union for the Advancement of Science and Art





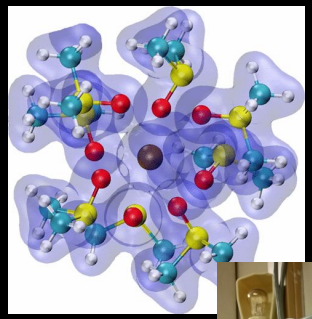
ChE352
Numerical Techniques for Chemical Engineers
Professor Stevenson

Lecture 1

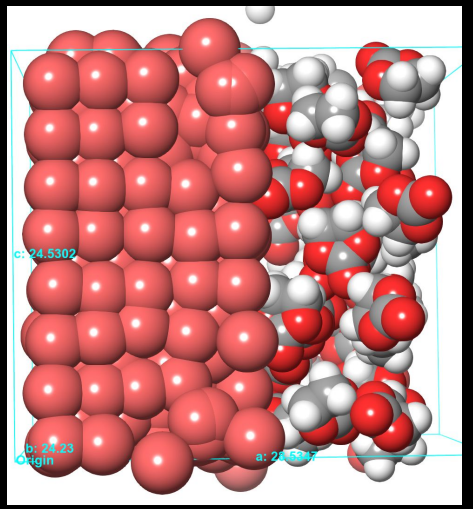
The Cooper Union for the Advancement of Science and Art

Professor Stevenson

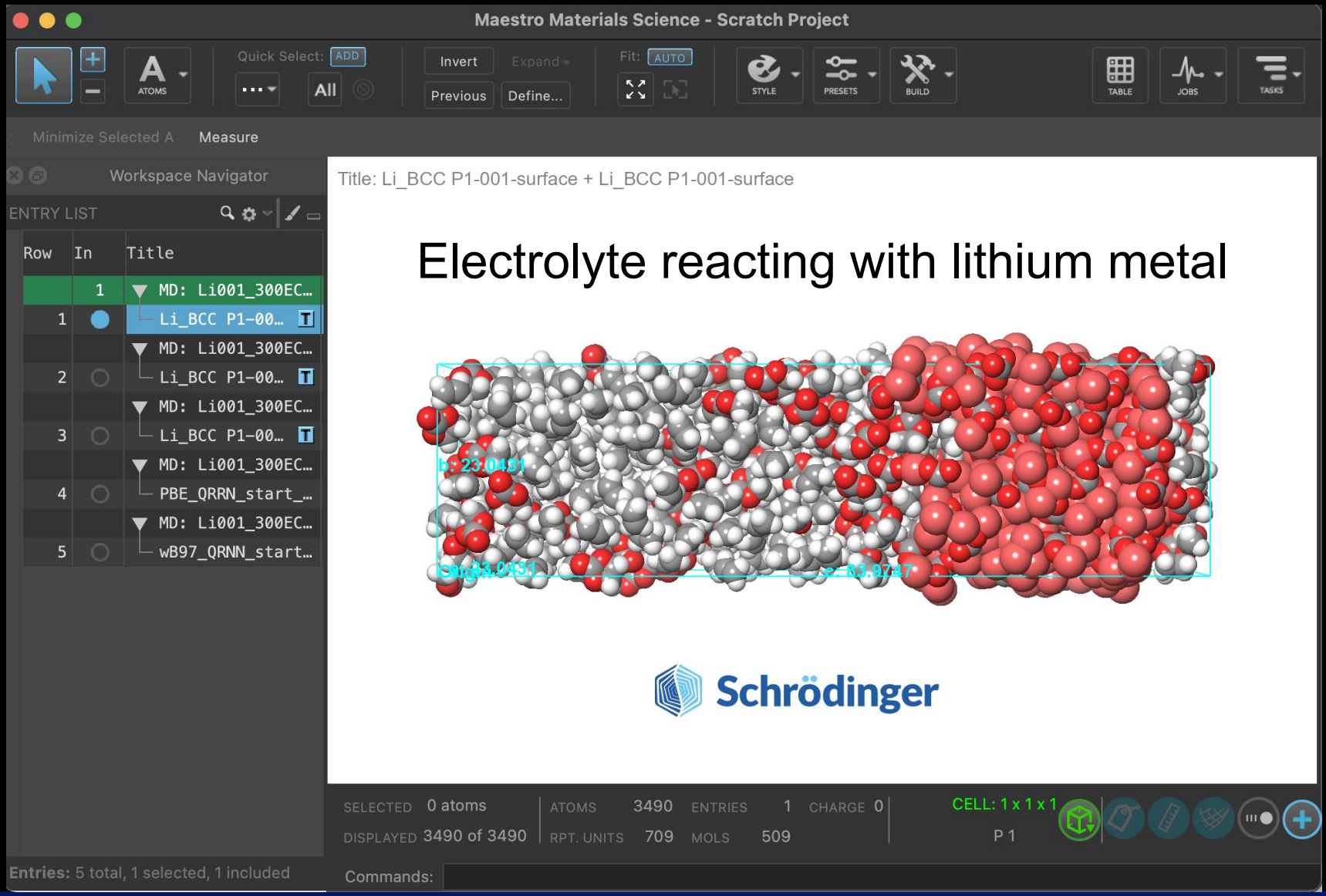
Cooper Union 2011



Cornell 2016

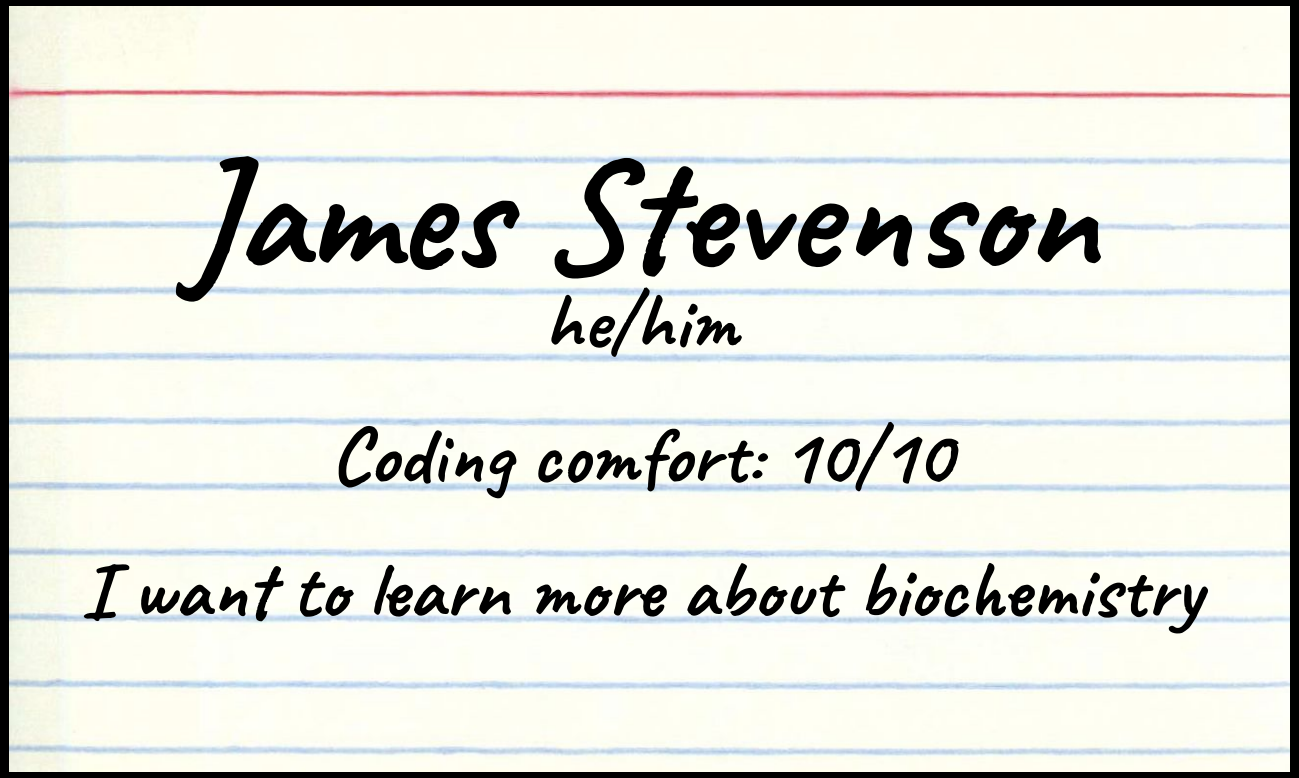


My day job: Schrödinger, Inc



Make a card to introduce yourself

- What is your name?
- What are your pronouns?
- Rate your comfort with coding (1-10)
- Topic you haven't learned yet as an engineer, but want to?



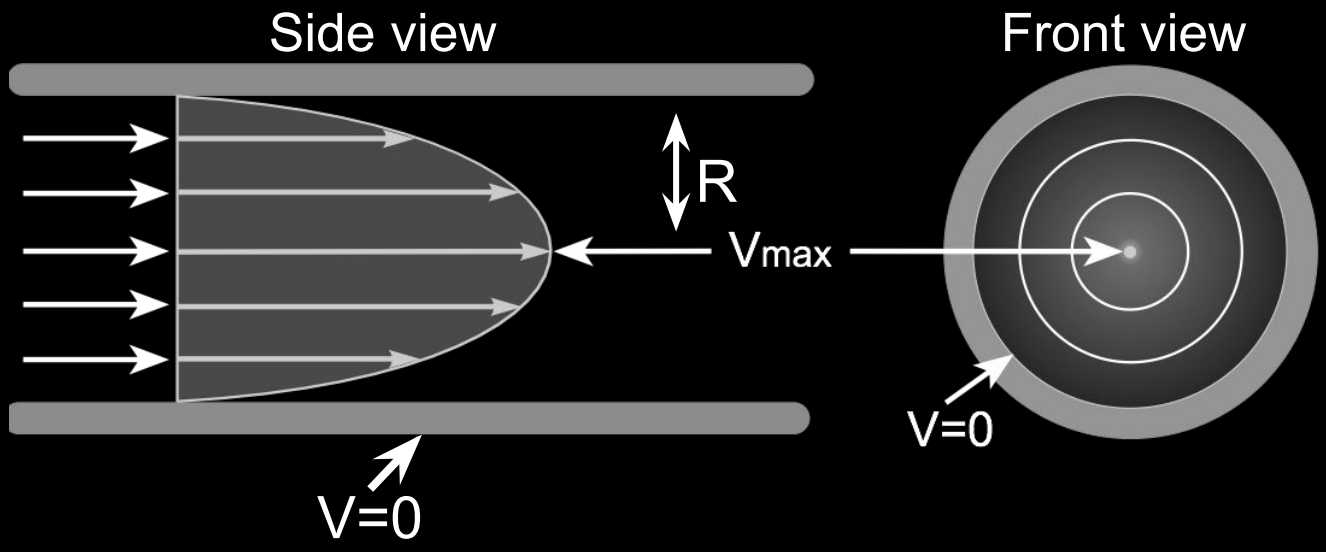
Things I Would Like From You

1. Bring problems to me ASAP
   - Especially if you feel unprepared
   - I might assume pre-reqs wrong
2. Remind me about jargon
   - Some rare terms are common in my work
   - Raise your hand when I use them in class
3. Be honest

In 16 months, you will have a degree that says “Chemical Engineering” on it

1. What does that mean?
2. What should you be able to do?
3. How do numerical methods & process simulation fit in?

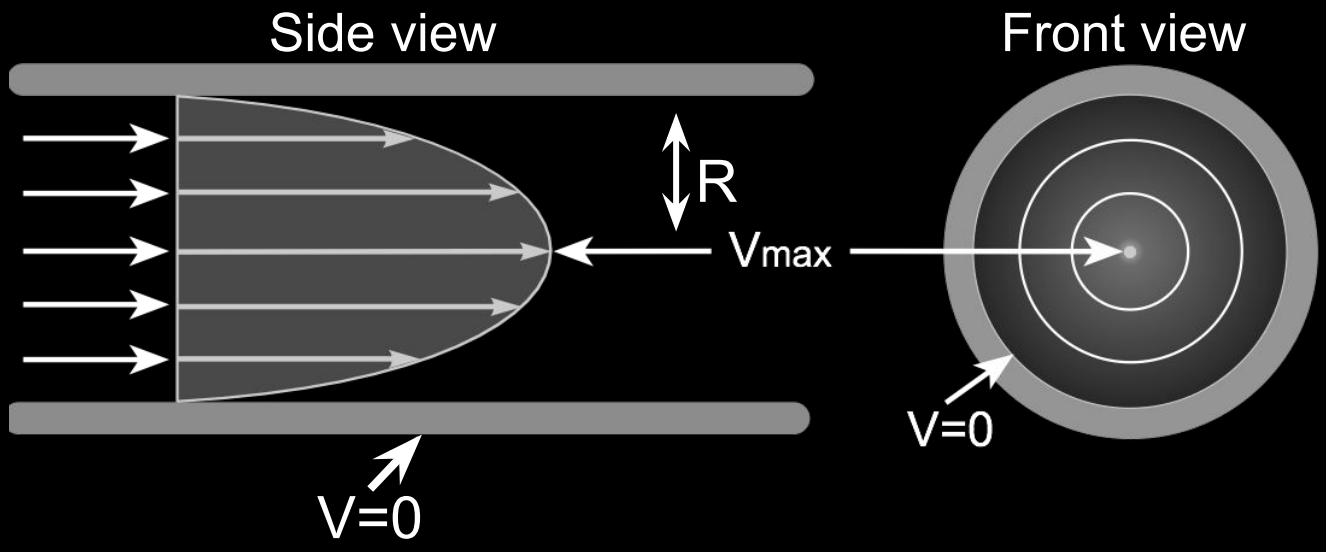
A familiar kind of problem



What is the velocity profile v(r) of a viscous fluid flowing in a pipe?

Assume radially symmetric, v=0 at the edges, v_{max} is at center

A familiar kind of problem



Differential equation

$$\frac{d^2v}{dr^2} + \frac{1}{r}\frac{dv}{dr} = -\frac{1}{\eta}\frac{\Delta P}{\Delta z}$$

General analytic solution

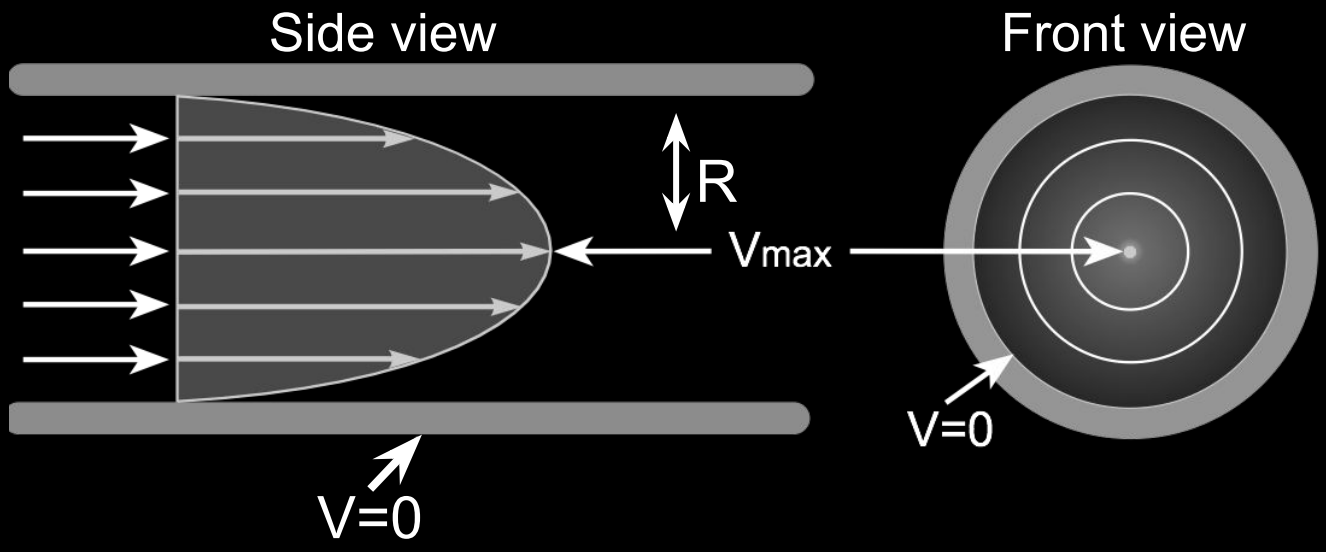
$$v = A + Br^2$$

Solve for A & B

Boundary conditions

$$v(R) = 0, v(0) = v_{max}$$

A familiar kind of problem



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$$v = A + Br^2$$

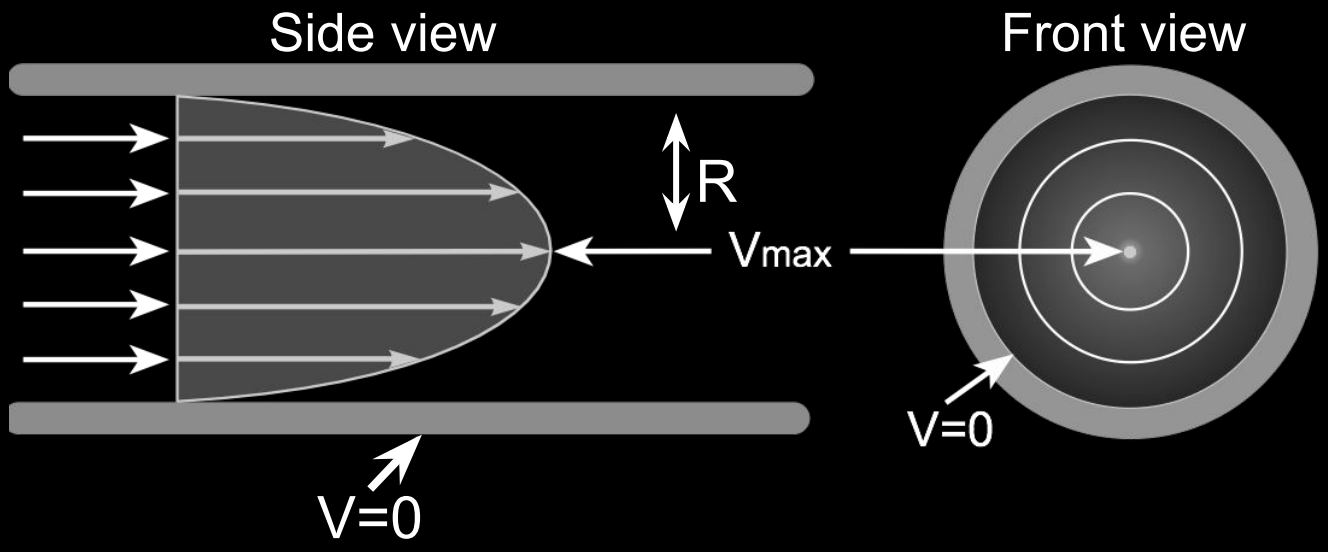
Solve for A & B

Boundary conditions

$$v(R) = 0, v(0) = v_{max}$$

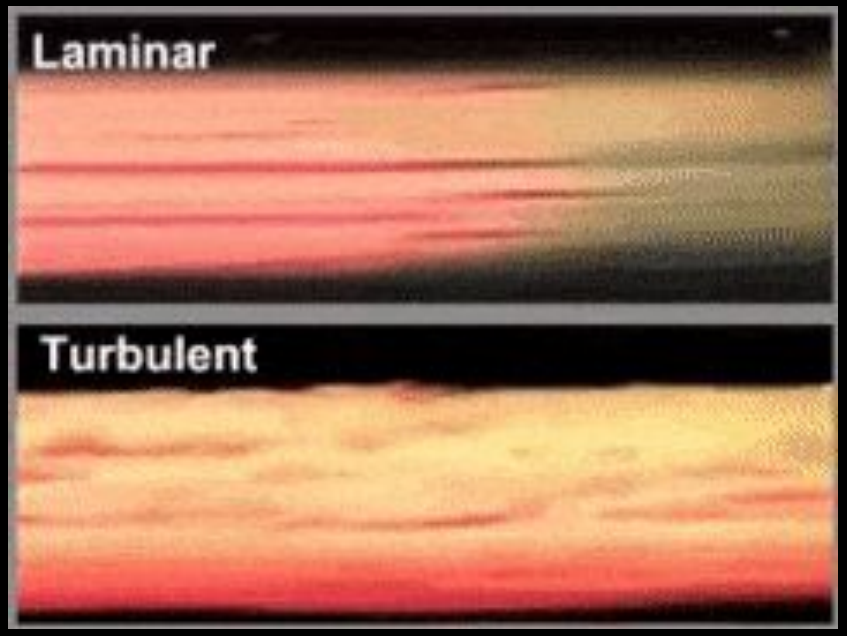
$$v = v_{max}\left(1 - \frac{r^2}{R^2}\right)$$

Slight change to the problem



What is the velocity profile v(r) of a **low-viscosity** fluid flowing in a pipe?

Slight change to the problem



$$\frac{d^2v}{dr^2} + \frac{1}{r}\frac{dv}{dr} = -\frac{1}{\eta}\frac{\Delta P}{\Delta z}$$

$$\frac{d\mathbf{v}}{dt} + \mathbf{v}\cdot\nabla\mathbf{v} + \frac{\nabla P}{\rho} = 0$$

No general analytic solution exists outside of the simple laminar flow case

Why not use existing software?

- Whenever possible, you should!
- But...

Why not use existing software?

- Whenever possible, you should!
- But...
- Numerical methods have hidden assumptions
- All software has unknown bugs, especially technical software (narrow user base)
- Software **makers** are often more in demand than software **users**

What to expect from this class

- ~Weekly homework assignments
- One midterm exam
- One final project

Homework	Midterm	Final Project	Class participation
30%	30%	30%	10%

- No more code than we need (but still a lot)
- Tools: Python language, Kaggle & Google Colab notebooks

Class materials

- Most topics are in your textbooks
- Topics that are part of the course, but NOT in the textbooks, are labeled “Supp:” on the syllabus
  - I will give you supplemental sources as needed
- Bring a laptop or tablet to class which you are comfortable using to type code
- If you have issues getting a textbook or laptop to use, let me know ASAP and I will help

Office Hours

Wednesdays after class, 5:50pm - 6:20pm

Or by appointment (message me on Teams)

Email: james.stevenson@cooper.edu

Coding environments

- Behind the scenes: in previous years, this class has used a Python environment called Spyder
  - Spyder runs on your laptop
  - Each install is a little different
  - Usually that doesn't matter, but in this class we deal with *error propagation*



Previous software experience

Show of hands:

- Who has used Google Colab?
- Who has used Kaggle?
- Who has used Github?
- Who has used Matlab (effectively)?

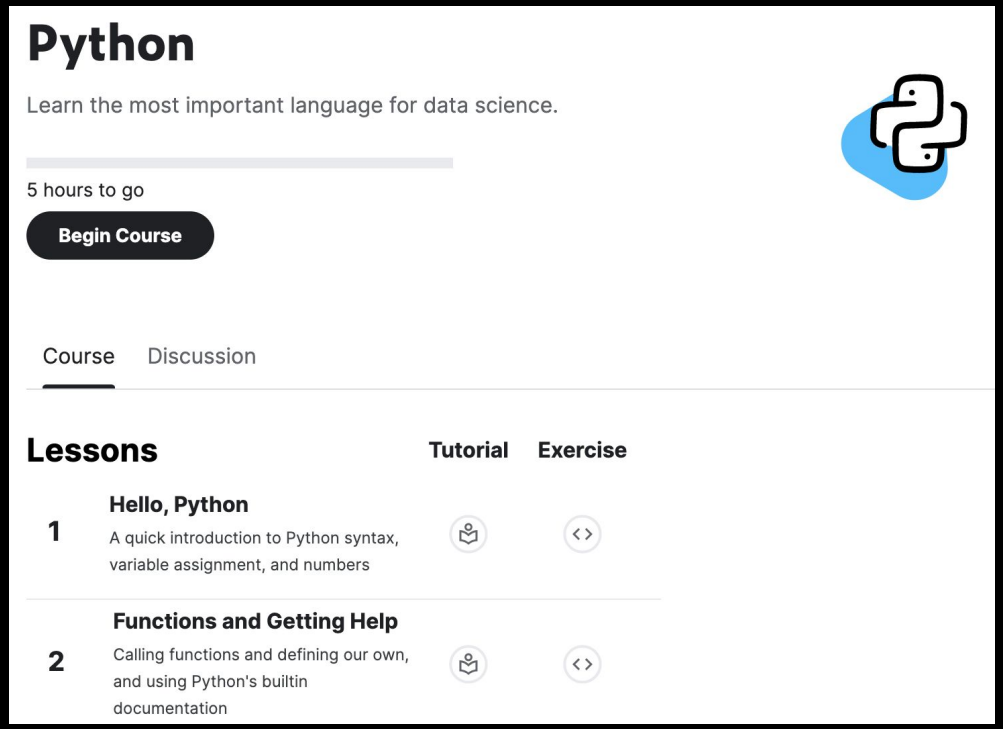
Any other software experience that might be common among Cooper ChemEs?

Coding with online notebooks

- Google Colab & Kaggle are based on a popular Python environment called "Jupyter notebooks"
- Can write plain code, or embed chunks of runnable code (called "cells") inside an interactive document
- Code runs on the remote server, so everyone's environment can be identical
  - Used for machine learning competitions
  - Also great for this kind of class

Set up Kaggle

- Make a free account at kaggle.com
- Send me your Kaggle handle via Teams
  - Mine is **allaboutchemistry**
- Go to kaggle.com/learn/python



Python warmup

- We need a baseline of Python skills for the remainder of the course
- I will provide class time and help to work on kaggle.com/learn/python - today, next class, and at office hours
- Graded by automated tests: you need all right answers, but the only penalty is to keep trying
- Any parts you don't finish in class will become HW #1