

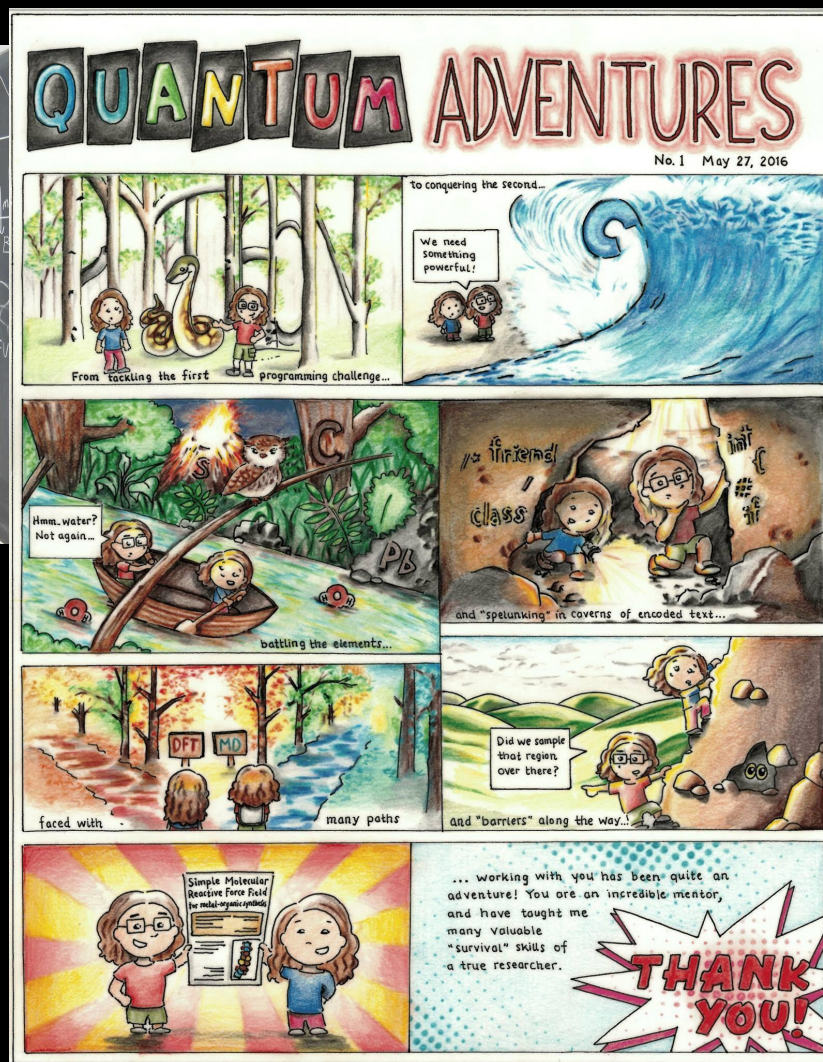
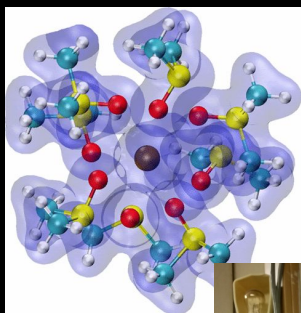
ChE352  
Numerical Techniques for Chemical Engineers  
Professor Stevenson

# Lecture 1

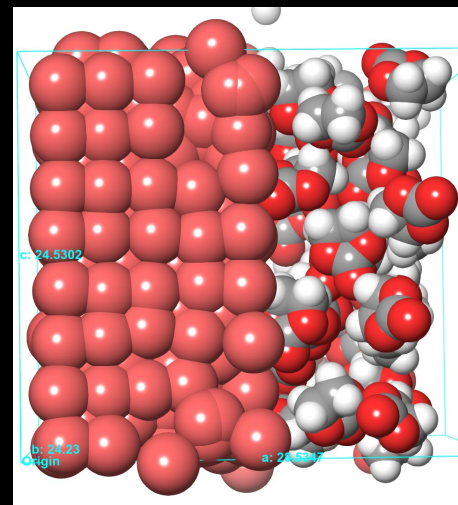
# Professor Stevenson



Cooper Union 2011



Cornell 2016





# My day job: Schrödinger, Inc

Maestro Materials Science - Scratch Project

Quick Select: ADD Invert Expand Fit: AUTO STYLE PRESETS BUILD TABLE JOBS TASKS

Minimize Selected A Measure

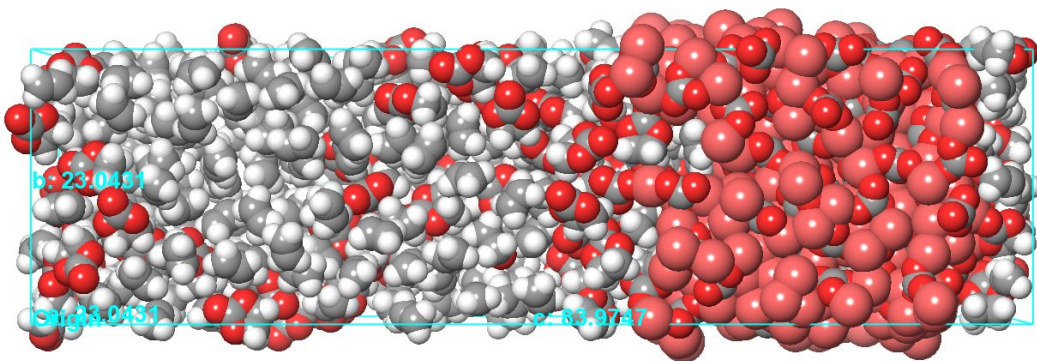
Workspace Navigator

ENTRY LIST

Row	In	Title
1	<input checked="" type="radio"/>	MD: Li001_300EC...
1	<input checked="" type="radio"/>	Li_BCC P1-00...
2	<input type="radio"/>	MD: Li001_300EC...
2	<input type="radio"/>	Li_BCC P1-00...
3	<input type="radio"/>	MD: Li001_300EC...
3	<input type="radio"/>	Li_BCC P1-00...
4	<input type="radio"/>	PBE_QRRN_start_...
5	<input type="radio"/>	MD: Li001_300EC...
5	<input type="radio"/>	wB97_QRRN_start_...

Title: Li\_BCC P1-001-surface + Li\_BCC P1-001-surface

## Electrolyte reacting with lithium metal



x: 23.0451 y: 34.0481 z: 85.9747

Schrödinger

SELECTED 0 atoms ATOMS 3490 ENTRIES 1 CHARGE 0 CELL: 1 x 1 x 1 P 1

DISPLAYED 3490 of 3490 RPT. UNITS 709 MOLS 509

Commands:

Entries: 5 total, 1 selected, 1 included

# 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?

*James Stevenson*  
*he/him*

*Coding comfort: 10/10*

*I want to learn more about biochemistry*

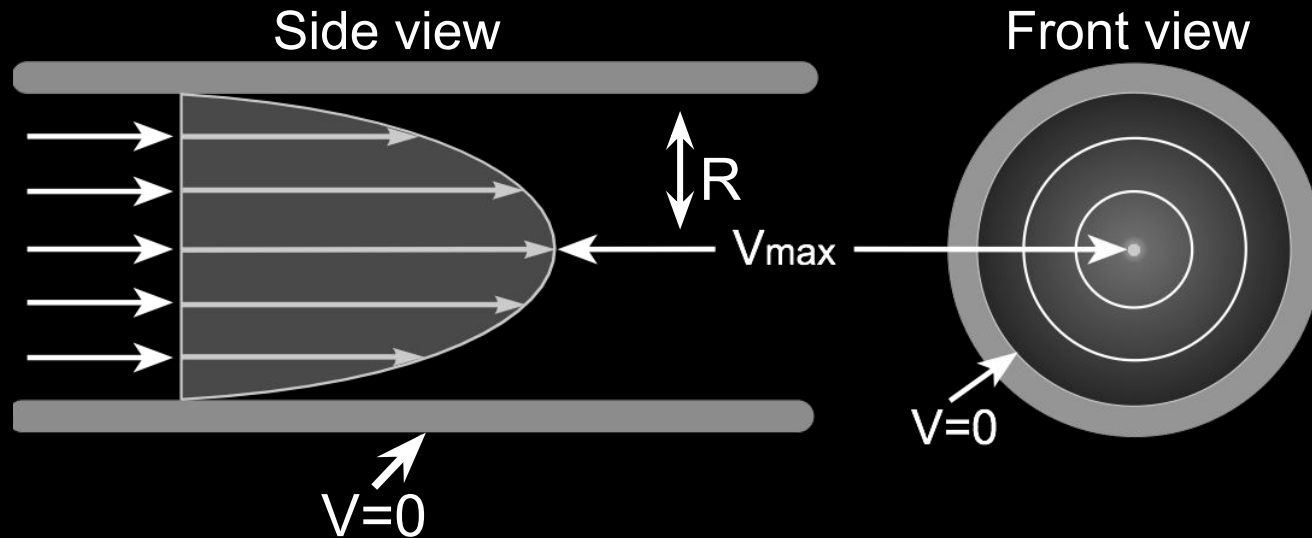
# Things I Would Like From You

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?

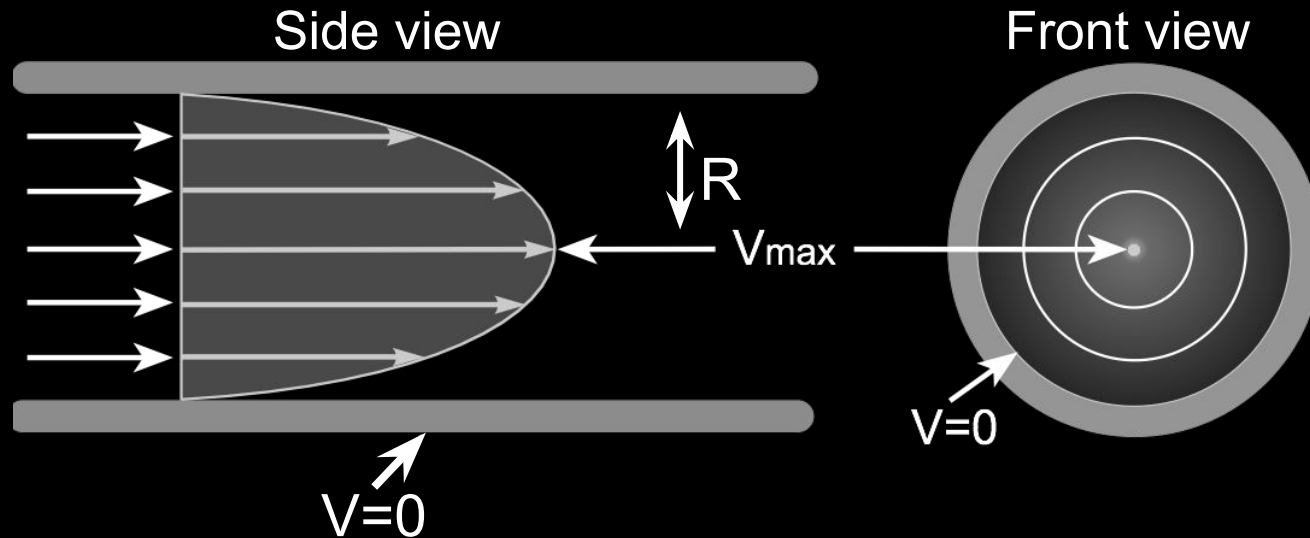
# A familiar kind of problem



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

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

General analytic solution

$$v = A + Br^2$$

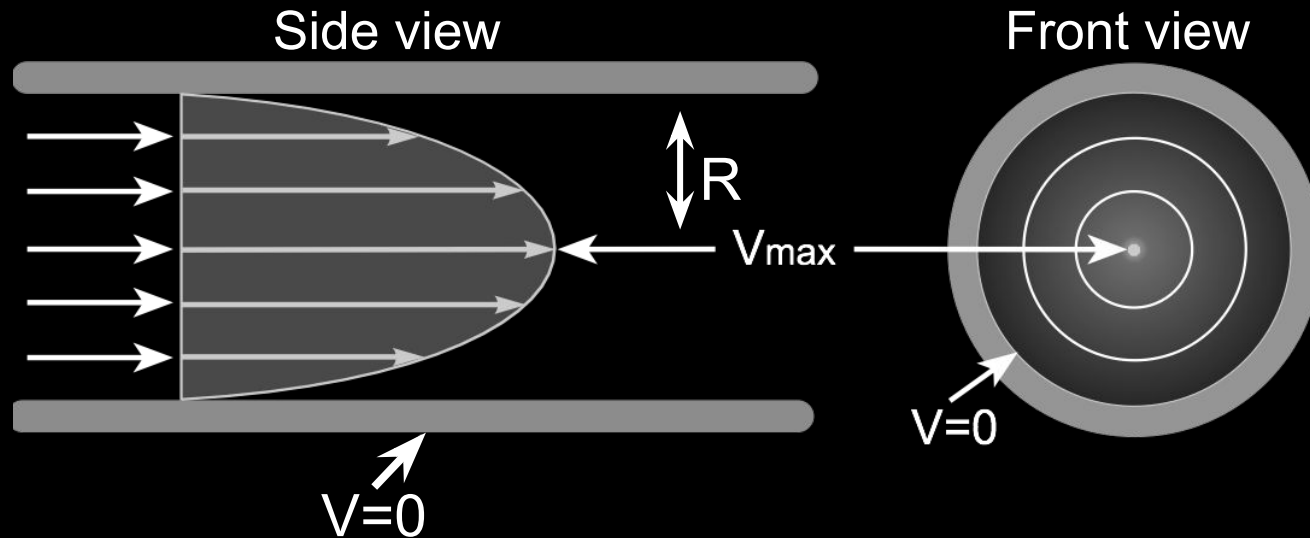
Solve for A & B

Boundary conditions

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



# A familiar kind of problem



Differential equation

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

Boundary conditions

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

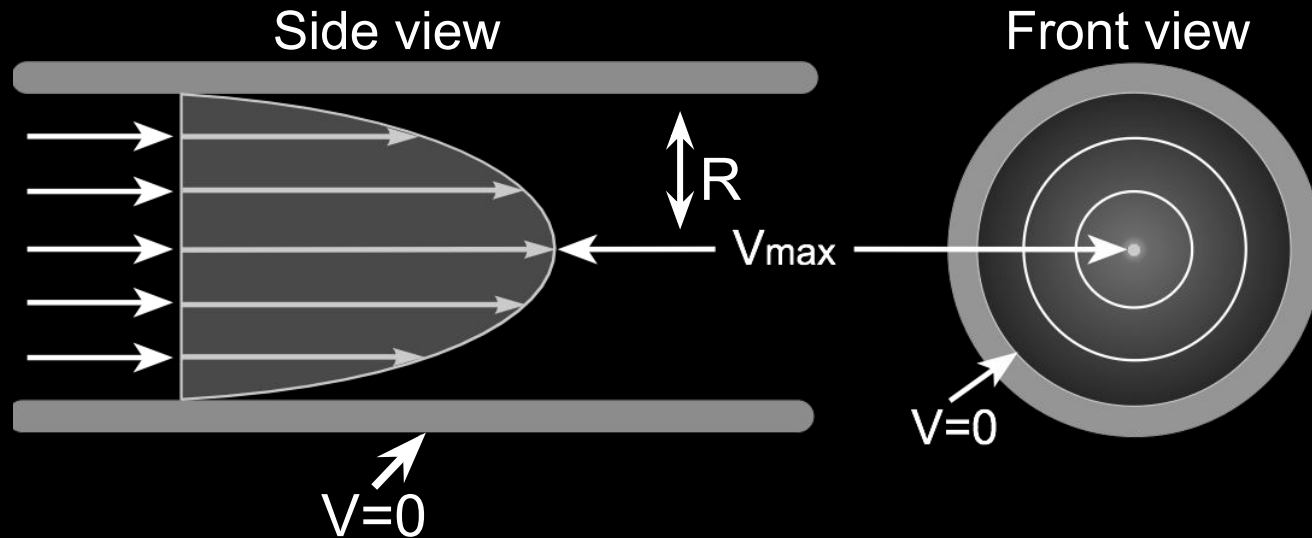
General analytic solution

$$v = A + Br^2$$

Solve for A & B

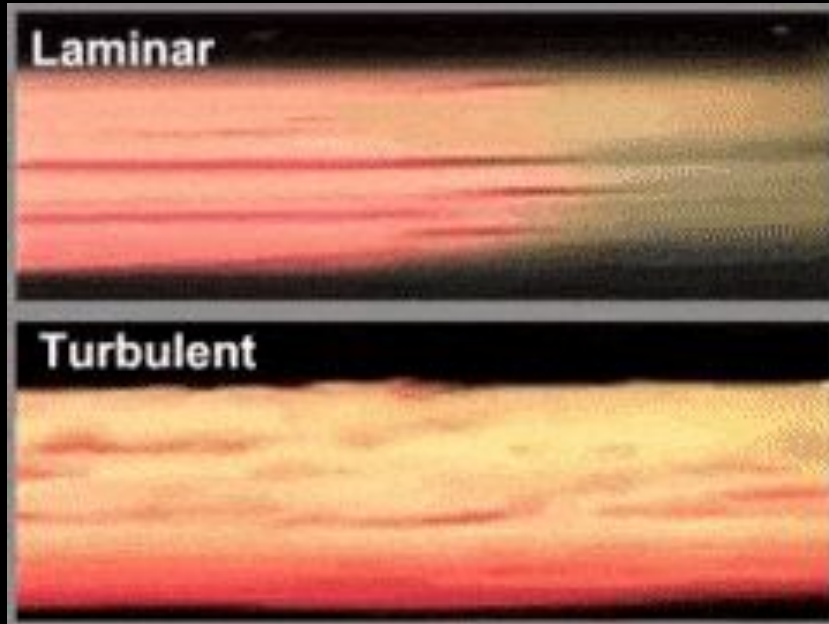
$$v = V_{max} \left( 1 - \frac{r^2}{R^2} \right)$$

# 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



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

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

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](mailto: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](https://kaggle.com)
- Send me your Kaggle handle via Teams
  - Mine is **allaboutchemistry**
- Go to [kaggle.com/learn/python](https://kaggle.com/learn/python)

## Python

Learn the most important language for data science.

5 hours to go

Begin Course

Course

Discussion



Lessons

Tutorial

Exercise



1

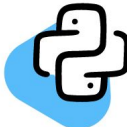
**Hello, Python**  
A quick introduction to Python syntax, variable assignment, and numbers



2

**Functions and Getting Help**  
Calling functions and defining our own, and using Python's builtin documentation





# 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](https://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