Training All Chemical Engineers in Computing and Data Science

colab

vocareum

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November 11, 2019   AIChE Annual Meeting   Orlando, FL

python™

pandas

NumPy

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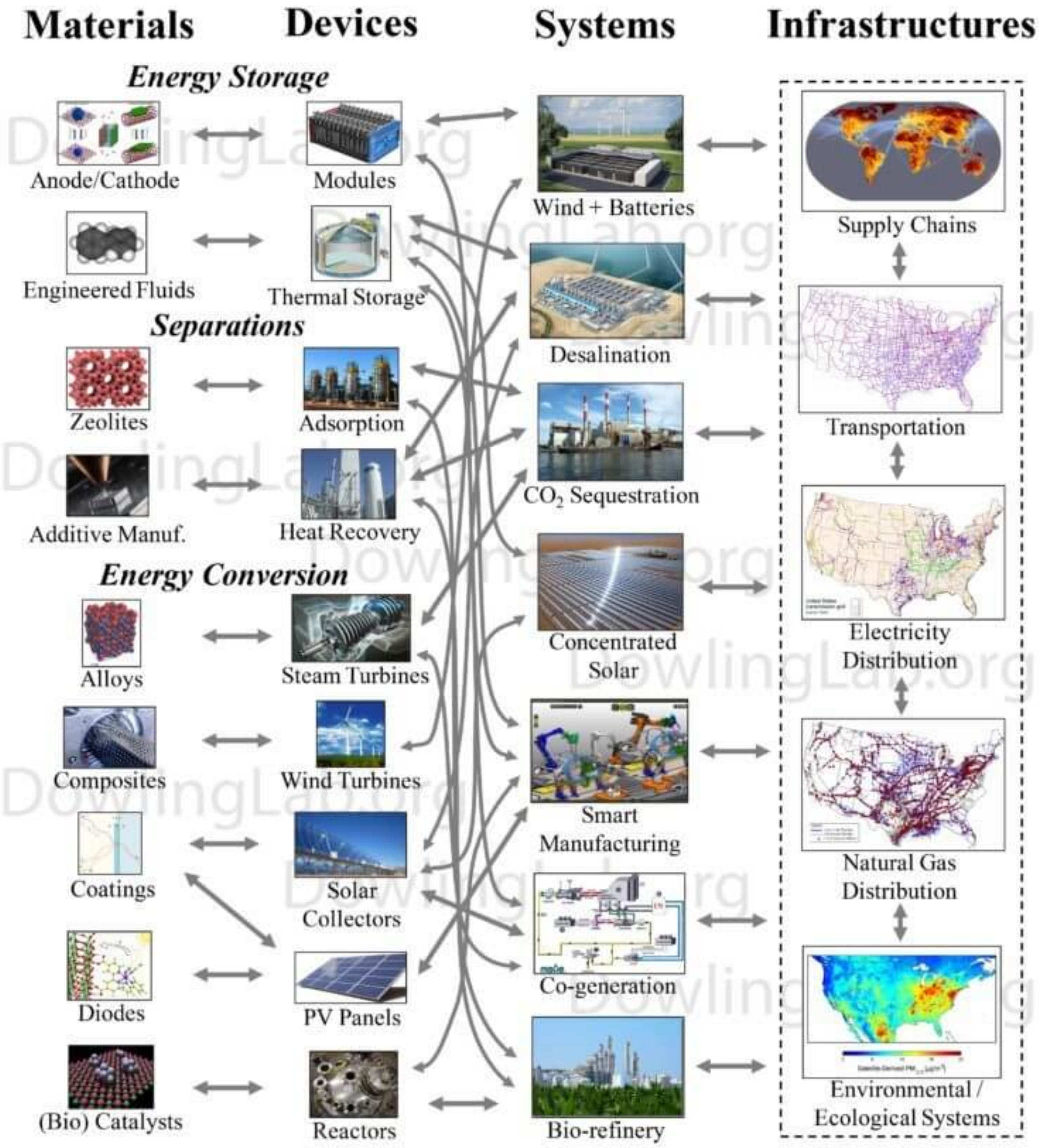
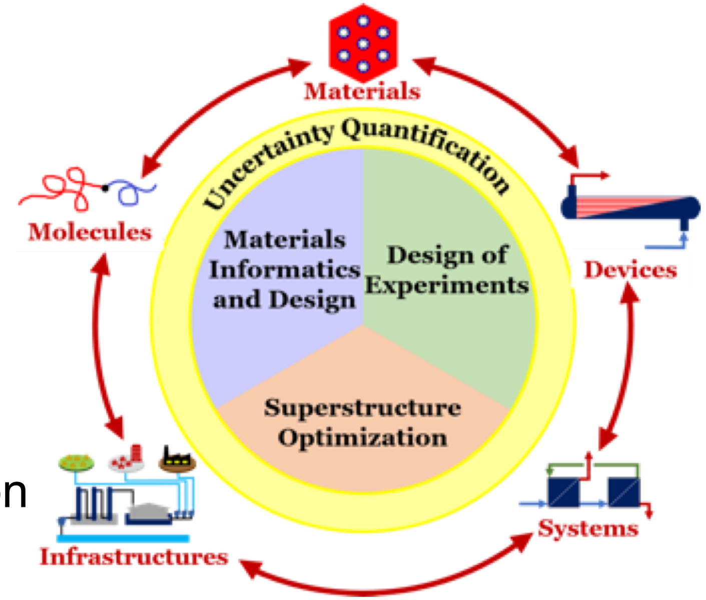
Research: Process Systems Engineering

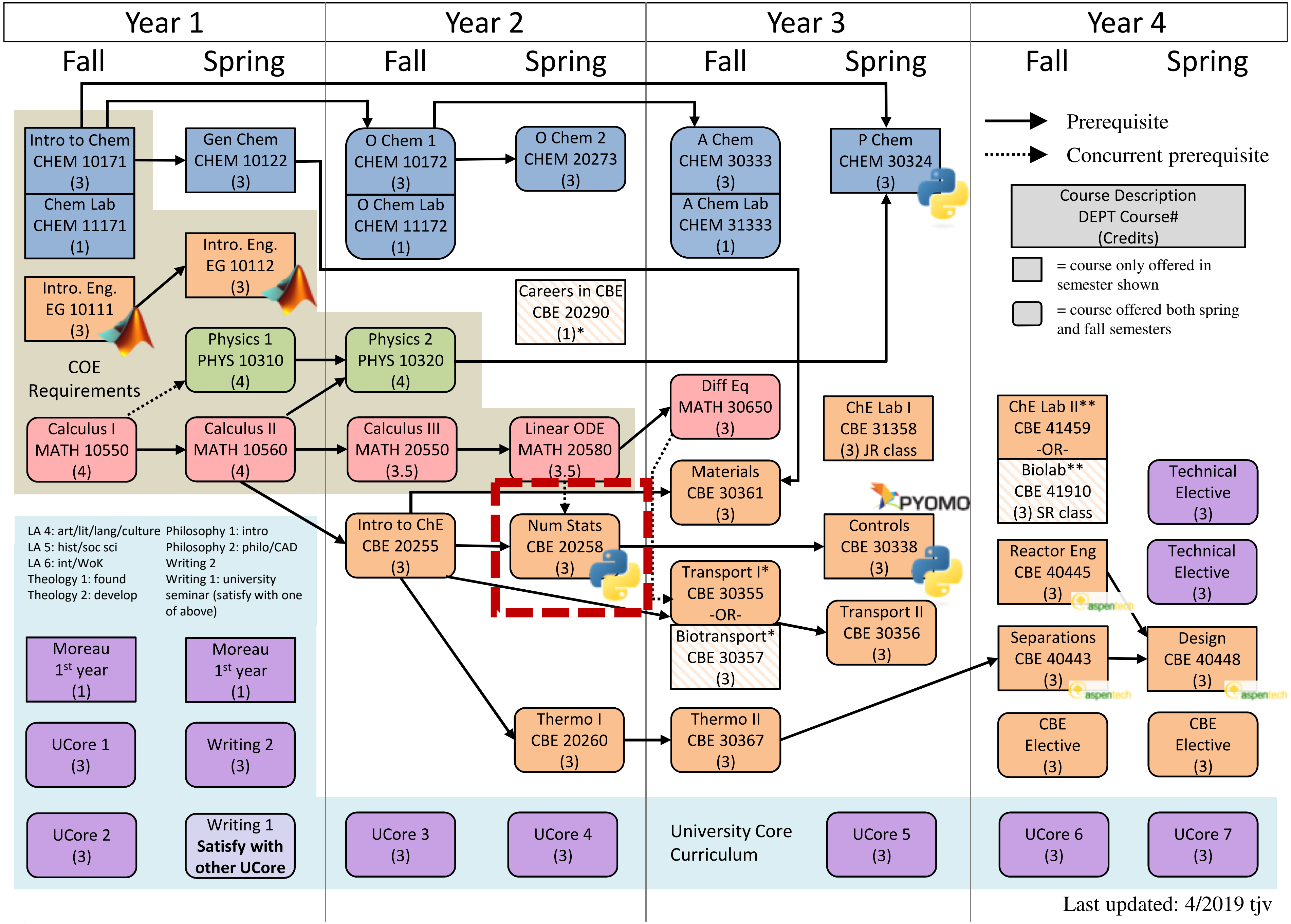


Themes

- Mathematical Modeling
- Computational Optimization
- Applied Bayesian Statistics and Uncertainty Quantification
- Energy & Sustainability Applications



Chemical Engineering Suggested 4 Year Curriculum University of Notre Dame entering FA18



Current Practice: Computing & Statistics

MATLAB in freshman engineering sequence

Sophomore-required **Numerical & Statistical Analysis** (NSA)

Ad-hoc computing & statistics in upper-level classes:

"You learned this as sophomores… just figure it out" – Prof. Anonymous

Vision

Vertically integrate computing and statistics throughout the undergraduate curriculum

Vertical Integration: Opportunities and Challenges

Numerical Methods
Equation solving (thermo., separations)
Optimization (controls, design)
Numeric integration (transport, reactions)

Statistics and Data Analysis
Probability (physical chemistry)
Visualization
Regression
Error Analysis
Uncertainty Propagation
} labs

Challenges
Difficult to learn advanced topics sophomore year (e.g., PDEs, BVPs)

"Brian drain" without repeated exposure

Common software tools?

How to avoid burdening all faculty?

Modernizing Numerical and Statistical Analysis

Backward Course Design
Set Clear Learning Objectives

At the end of the semester, you should be able to…

1. **Create mathematical models** and **apply computational methods** to analyze systems using basic principles of chemical engineering (e.g., mass and energy balances, thermodynamic equilibrium, etc.)

2. **Analyze data** and **quantify uncertainty** using standard statistical techniques and mathematical models grounded in engineering fundamentals

3. Independently plan, implement, and debug short (100 to 300 lines) **Python computer programs** to analyze data, solve engineering mathematical models, and visualize results

Major Changes

Reorganized class topics

- Removed advanced topics (QR factorization, compression with SVD, trust regions, BVPs, PDEs)
- Emphasized fundamentals, especially probability & statistics
- Added mass and energy balance examples

Switched to **Python**, with great student buy-in

Incorporated **active learning** into lectures

Shortened assignments

Active Learning is Essential for Computing and Statistics

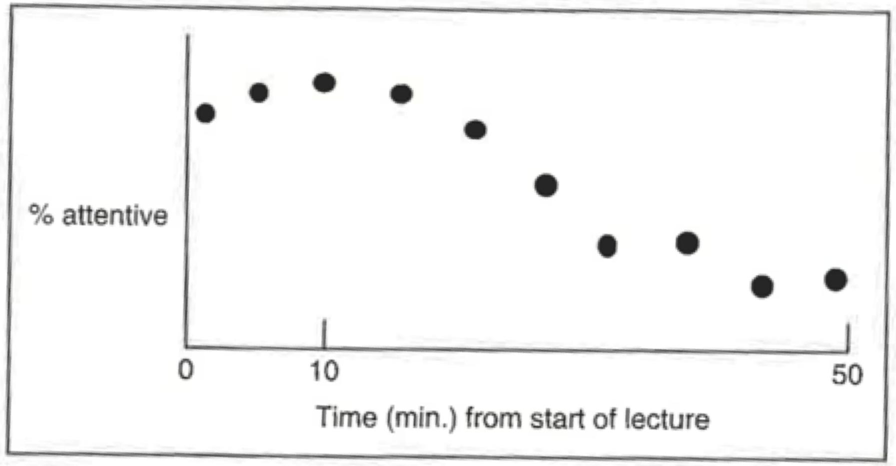


Figure 6.3–1: Attentiveness versus Time in Lecture—No Activities

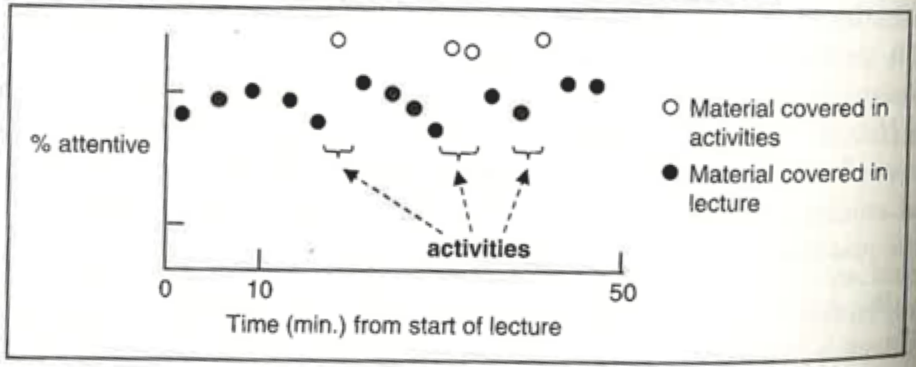


Figure 6.3–2: Attentiveness versus Time in Lecture—Activities Interspersed

Right: Felder and Brent (2015), *Teaching and Learning STEM: A Practical Guide*

Spring 2019: Cloud-based Google Colaboratory (Jupyter Notebooks)

colab.research.google.com

Benefits of Google Colaboratry:

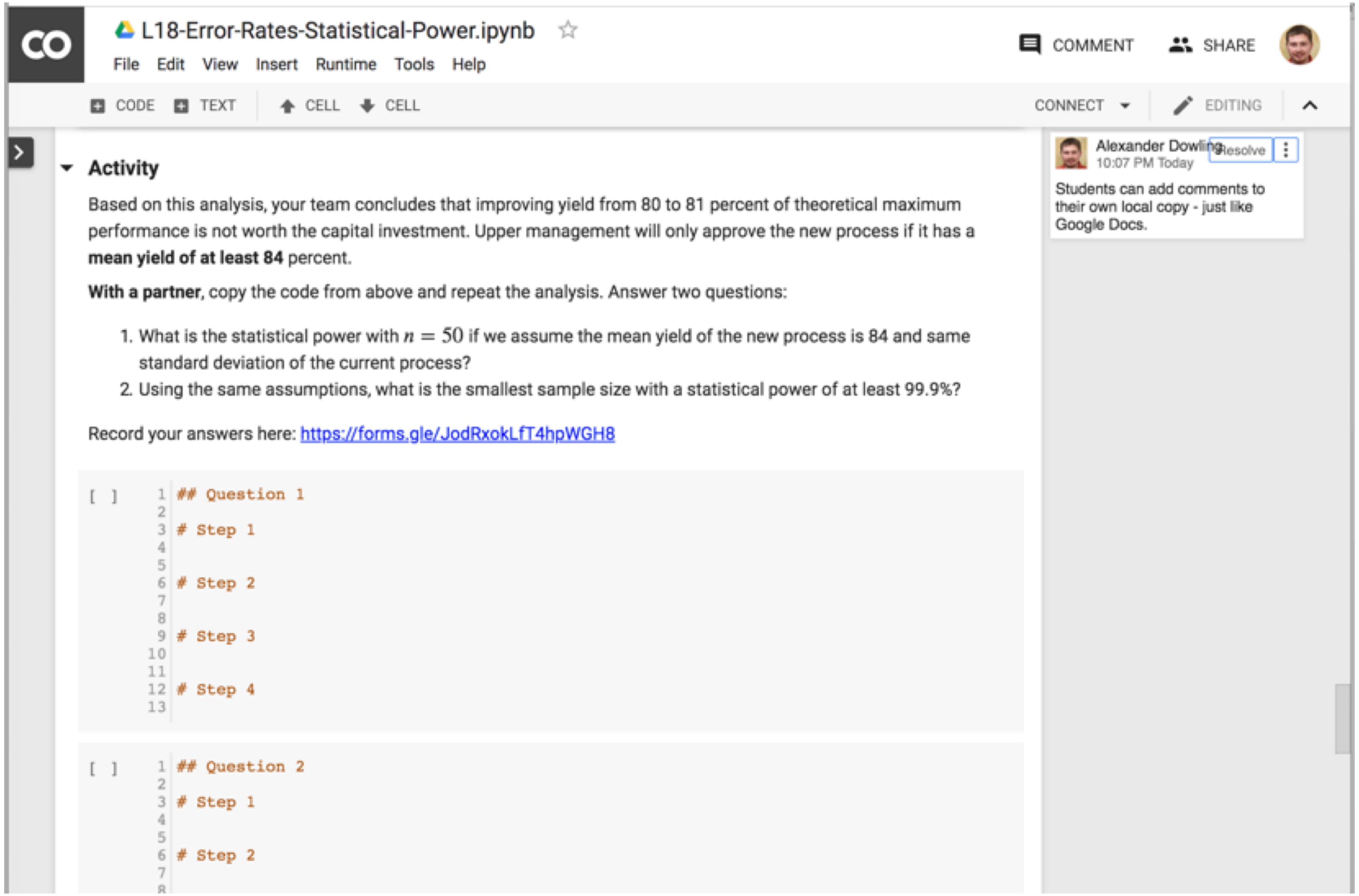
Like Google Docs, but for code

Integrated with **Google Drive**: automatic versioning, easy sharing

Removes barriers to access: students can complete assignments from **any internet connect computer** – no need to support 80+ local Python installations

Facilitates **active learning**

Free



I show this slide on day 1.

Making your time more effective

Easy — Complexity of Concepts and Applications — **Difficult**

Traditional Class (plan)

Lecture 3 hr / wk + **Tutorial** 1 hr / wk + **Studying** 2 hr / wk + **Homework** 3 hr / wk = **Total** 9 hr / wk

- Lecture: *Initial exposure*
- Tutorial: *Practice*
- Studying: *But how?*
- Homework: *Builds on lectures*

Traditional Class (reality for many)

Lecture 3 hr / wk + **Tutorial** 1 hr / wk + **Studying** 1 hr / wk + **Homework** 10+ hr / wk = **Total** 15+ hr / wk

- Lecture: *Difficult to focus 100% of time*
- Tutorial: *Too busy to start homework before*
- Studying: *Either skipped or not effective*
- Homework: *Really difficult if not comfortable with lecture examples*

Making your time more effective

I show this slide on day 1.

Easy Complexity of Concepts and Applications **Difficult**

This Semester

**We'll start some homework problems during class.*

Class Preparation
2 hr / wk
Initial exposure at home

+

Tutorial
1 hr / wk
Practice & jump-start homework

+

Studying
1 hr / wk
I'll teach you how to do this & give extra practice problems

+

Class*
3 hr / wk

Problem solving together

Homework*
2 - 4 hr / wk
Easy extensions of home and class activities

=

Total
9 - 11 hr / wk
This is 100% on task time… i.e., Facebook closed, not watching Netflix, not texting

Fall 2019: Cloud-based Vocareum (Jupyter Notebooks)

`www.vocareum.com`

Benefits of Vocareum:

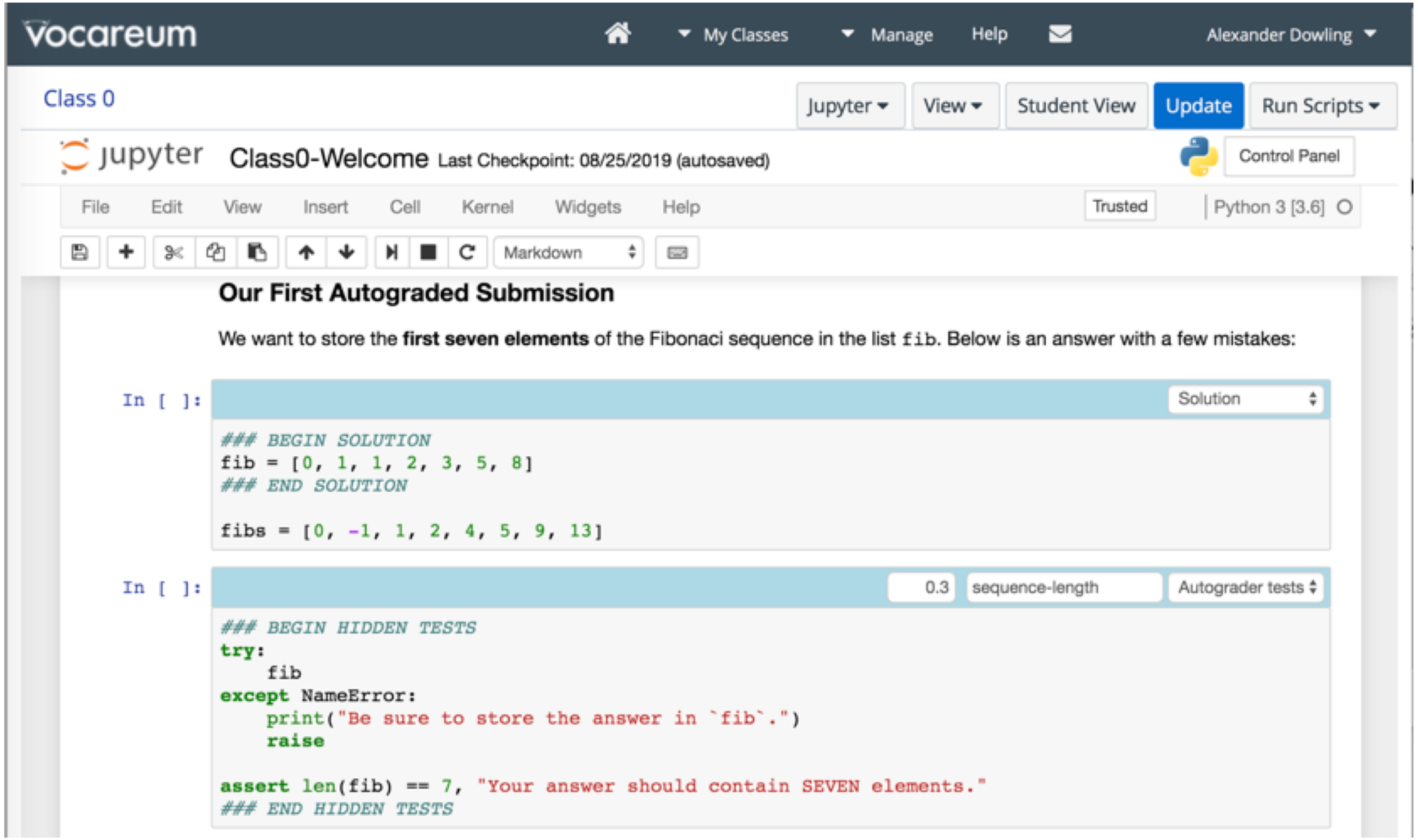
Many of the same cloud-based benefits as Colaboratory

Integrated with **Learning Management System** (e.g., Sakai) and gradebook

Supports **autograding** via nbgrader (with some enhancements)

Supports plagiarism detections (if you want it)

Paid service, but responsive technical support



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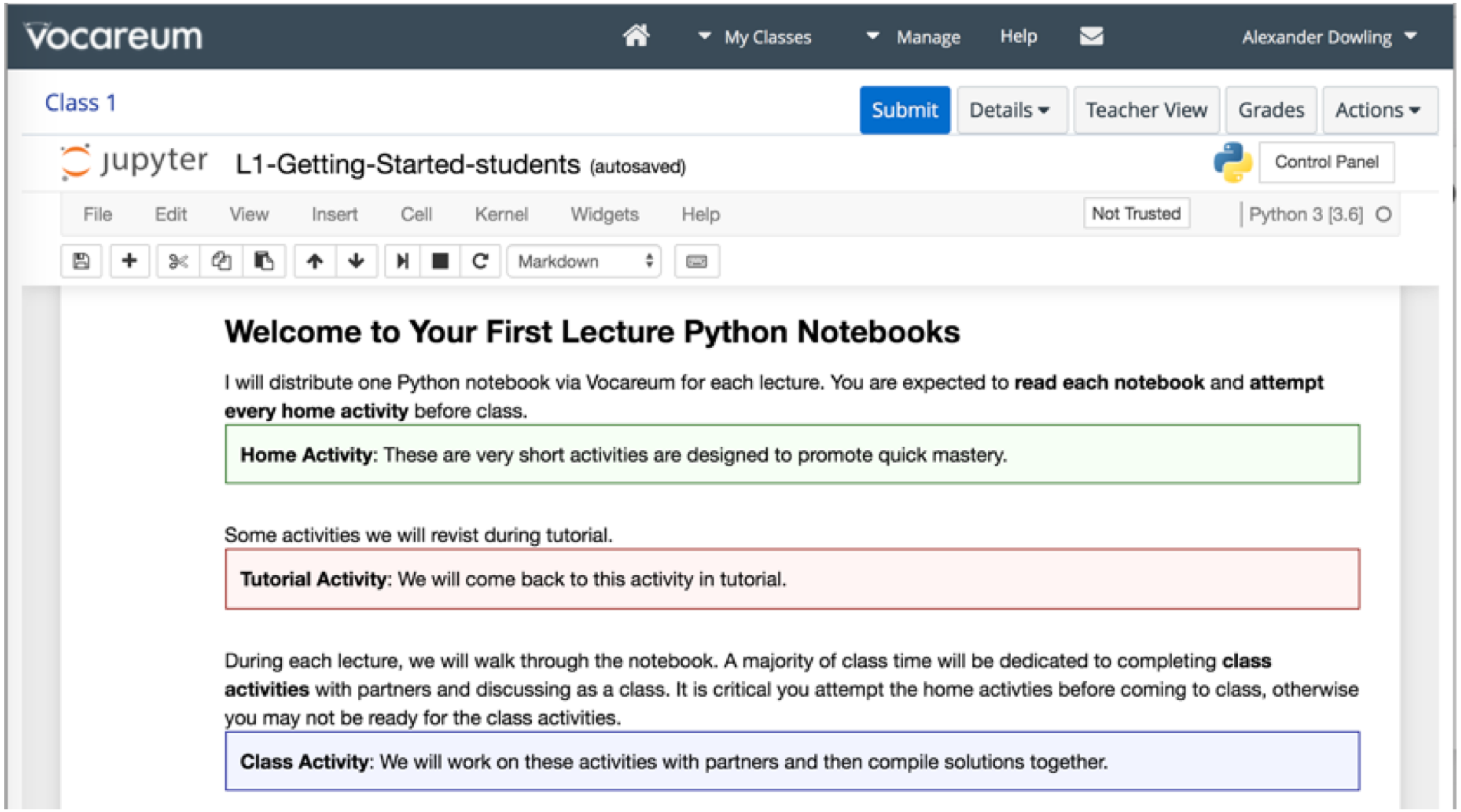


Bottom Line: Autograder (Vocareum) enables accountability for meaningful home activities before class, which translates to more engaging class sessions.

Excited Students to Become Long-Term Learners

Success Stories and Lessons Learned

Show students how computing and statistics:
- Makes them competitive for jobs
- Helps them in future classes & career
- **Connects to chemical engineering & society**

Extension Assignments

Watch TED talk, listen to podcast, etc.

Answer brief reflection questions

Completion grade, counts towards dropped homework

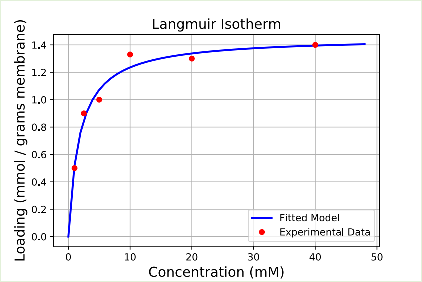
Examples:
Planet Money, "What Causes What?"
Hidden Brain, "The Scientific Process"
TED Talks: Bias and Algorithms

Set them up for **early success**
- Require pseudocode
- Embrace the autograder

Show them how to **study & learn independently**

Final Project: Heavy Metal Water Treatment

Fit Isotherm Model & Estimate Uncertainty

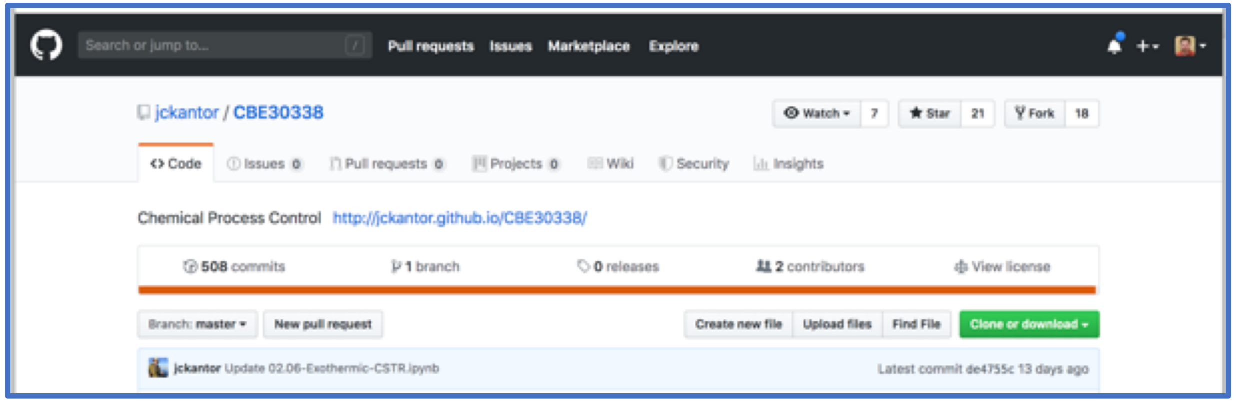


Calculate Filter Lifespan

$$\frac{d}{dt}q(t) = \frac{F}{m}(c_{in} - c(t))$$

Draw Conclusions with Uncertainty

Special Thanks to Prof. Jeff Kantor



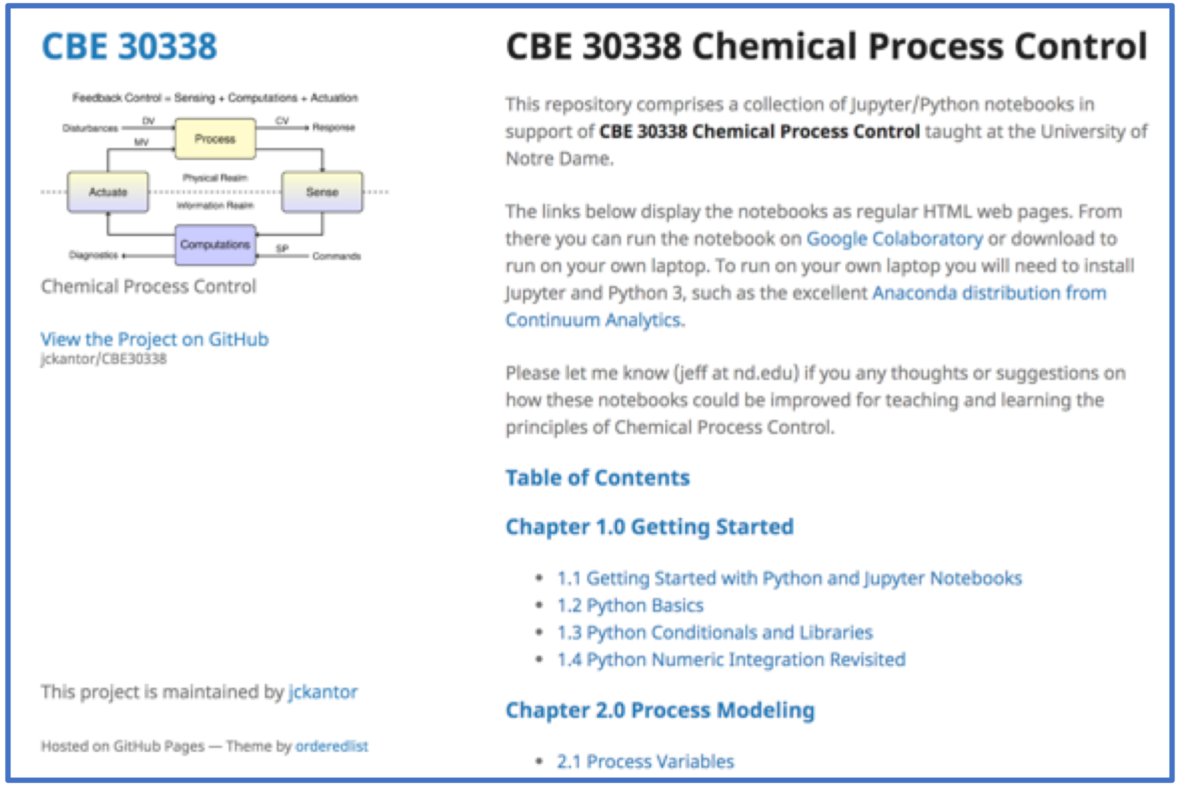
https://github.com/jckantor

Chemical Process Control

Introduction to Chemical Engineering Analysis

Introduction to Operations Research

Process Operations



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These slides are on the LAPSE archive: http://psecommunity.org/LAPSE:2019.1133