

Training All Chemical Engineers in Computing and Data Science



Prof. Alexander Dowling

adowling@nd.edu dowlinglab.nd.edu

Department of Chemical and Biomolecular Engineering

University of Notre Dame, Notre Dame, IN

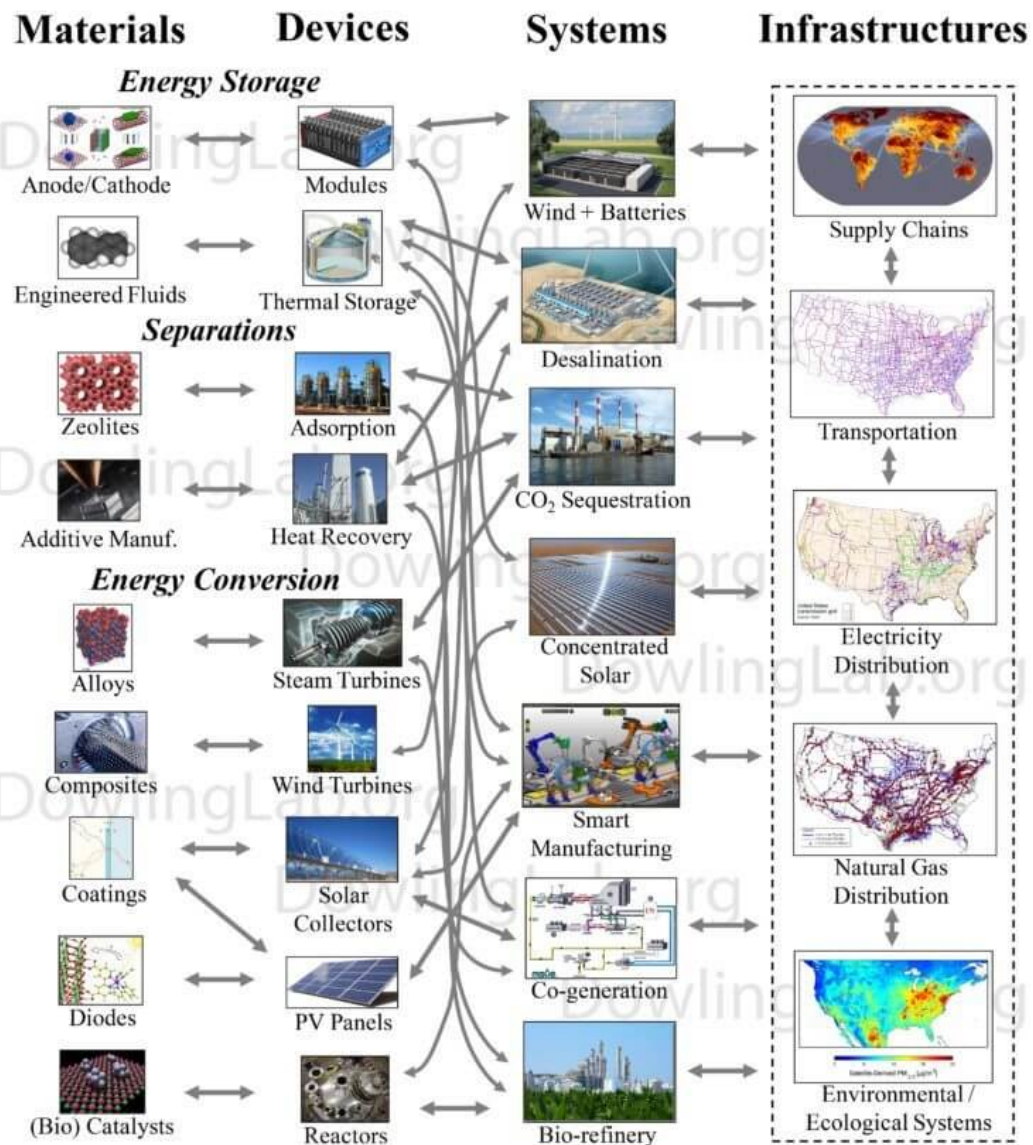
November 11, 2019 AIChE Annual Meeting Orlando, FL

colab

vocareum

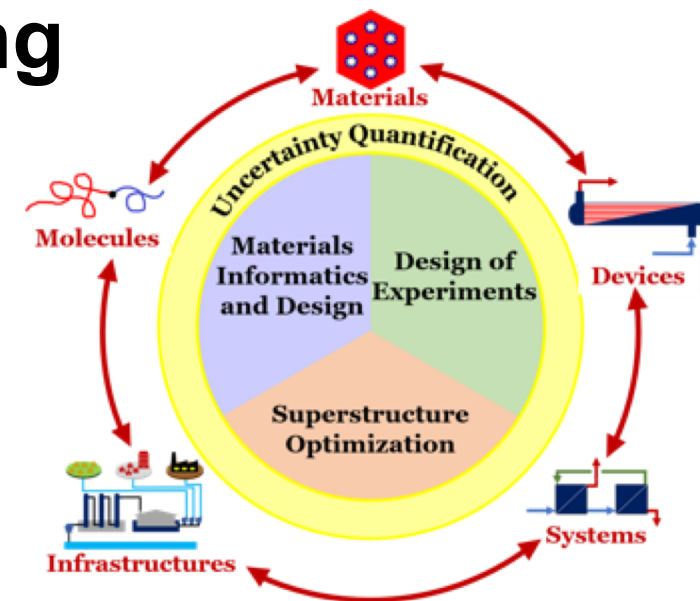


Research: Molecular-to-Systems Engineering



Themes

- Mathematical Modeling
- Computational Optimization
- Applied Bayesian Statistics & 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)

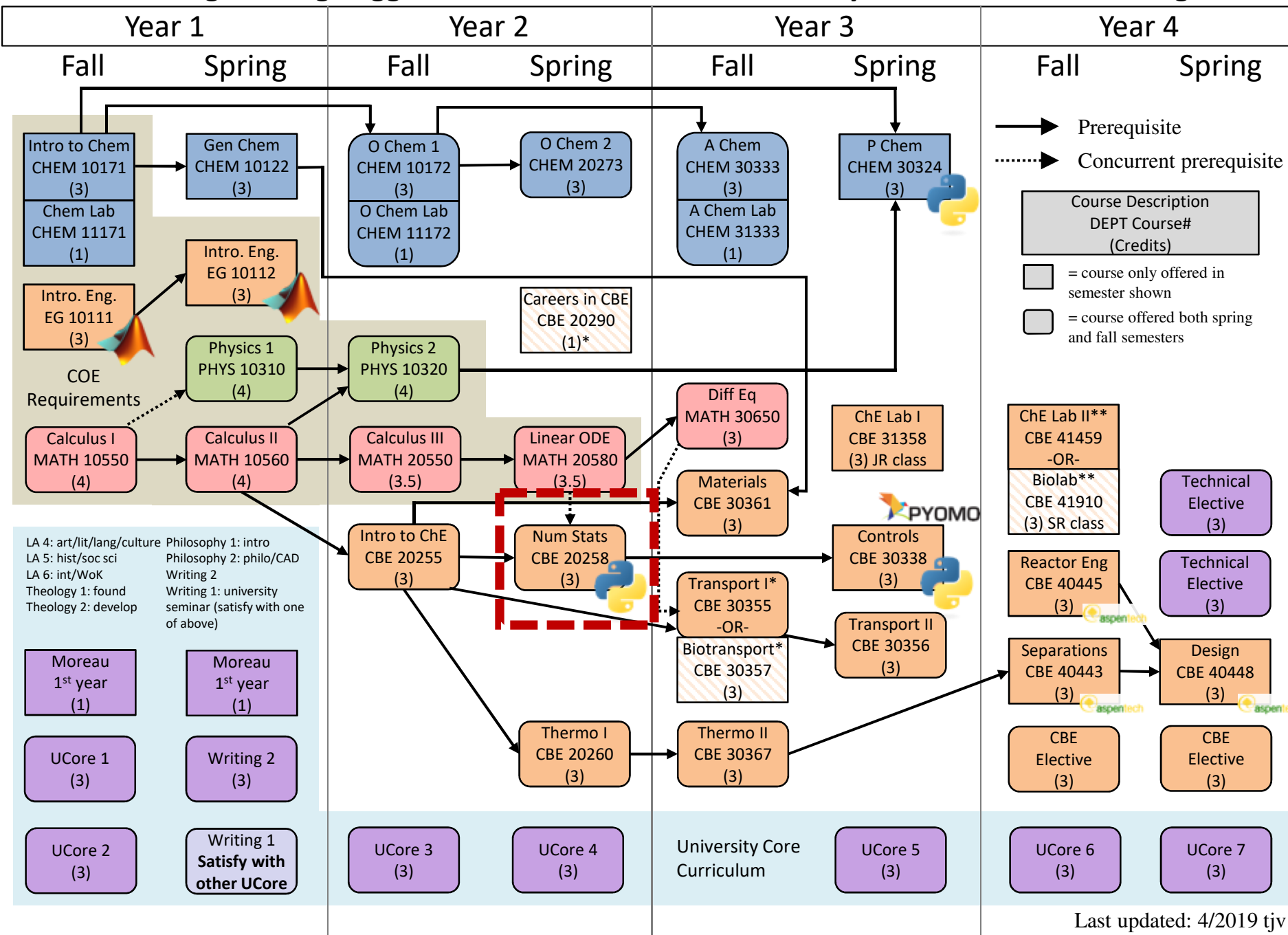
Ad-hoc computing & statistics in upper-level classes:

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

Vision

Vertically integrate computing and statistics throughout the undergraduate curriculum

Last updated: 4/2019 tjv



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)

“Brain 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

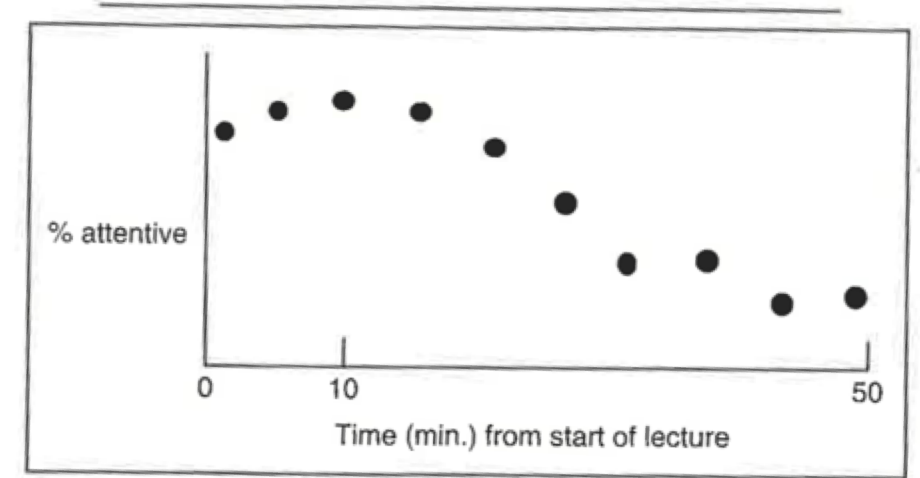


Figure 6.3-1: Attentiveness versus Time in Lecture—No Activities

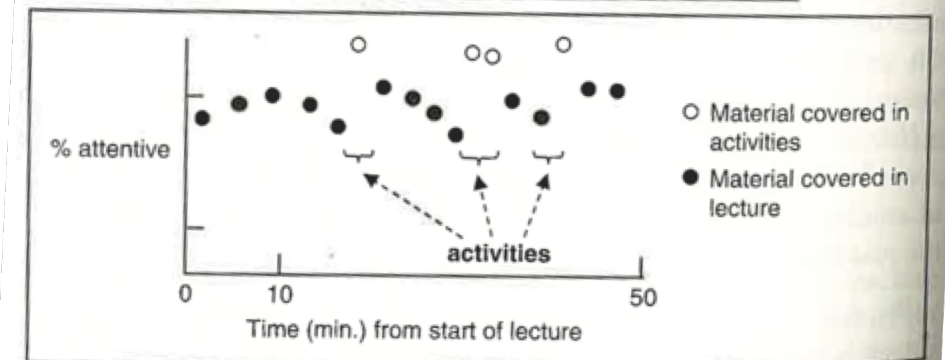


Figure 6.3-2: Attentiveness versus Time in Lecture—Activities Interspersed

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

colab.research.google.com

Benefits of Google Colaboratory:

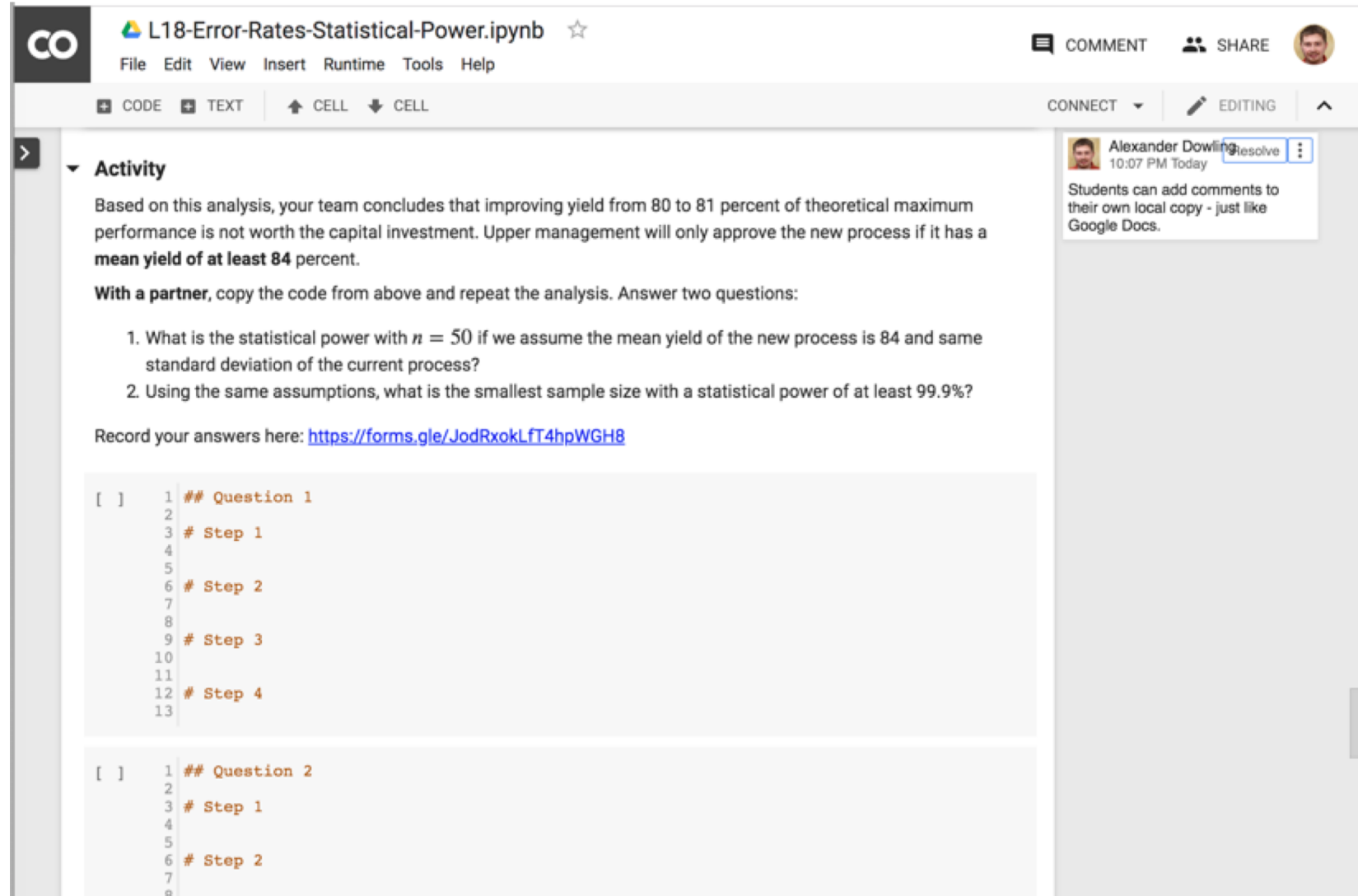
Like Google Docs, but for code

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



The screenshot displays the Google Colaboratory interface for a Jupyter Notebook titled "L18-Error-Rates-Statistical-Power.ipynb". The interface includes a top menu bar with options like File, Edit, View, Insert, Runtime, Tools, and Help. Below the menu, there are tabs for CODE, TEXT, and CELL. The main content area shows an "Activity" section with a text-based problem involving statistical power calculations. The problem asks for the statistical power with $n = 50$ and the smallest sample size for a given power. A link to a Google Form for recording answers is provided. Below the text, there are two code input cells, each containing a placeholder for a question and its steps. On the right side, there is a sidebar with a "COMMENT" button, a "SHARE" button, and a user profile for Alexander Dowling. A notification bubble indicates that students can add comments to their own local copy, similar to Google Docs.

co L18-Error-Rates-Statistical-Power.ipynb ☆

File Edit View Insert Runtime Tools Help

CODE TEXT CELL CELL

CONNECT EDITING

Activity

Based on this analysis, your team concludes that improving yield from 80 to 81 percent of theoretical maximum performance is not worth the capital investment. Upper management will only approve the new process if it has a mean yield of at least 84 percent.

With a partner, copy the code from above and repeat the analysis. Answer two questions:

1. What is the statistical power with $n = 50$ if we assume the mean yield of the new process is 84 and same standard deviation of the current process?
2. Using the same assumptions, what is the smallest sample size with a statistical power of at least 99.9%?

Record your answers here: <https://forms.gle/JodRxokLT4hpWGH8>

```
[ ] 1 ## Question 1
    2
    3 # Step 1
    4
    5 # Step 2
    6
    7 # Step 3
    8
    9 # Step 4
   10
   11
   12
   13
```

```
[ ] 1 ## Question 2
    2
    3 # Step 1
    4
    5 # Step 2
    6
    7
    8
```

Alexander Dowling 10:07 PM Today

Students can add comments to their own local copy - just like Google Docs.

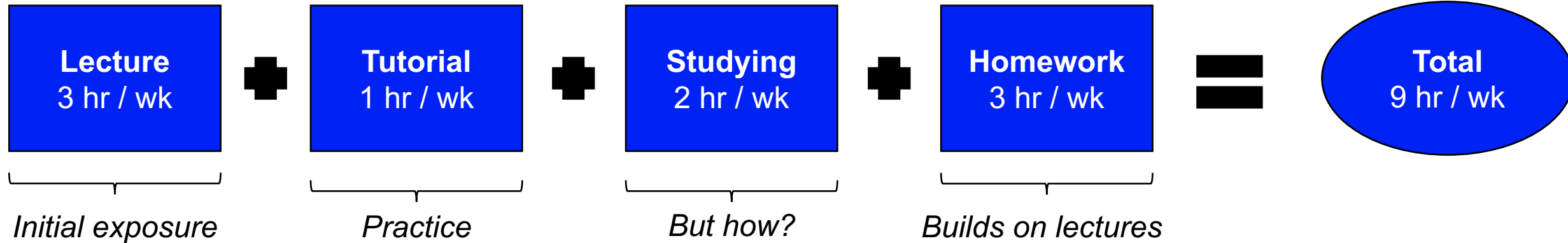
Making your time more effective

Easy

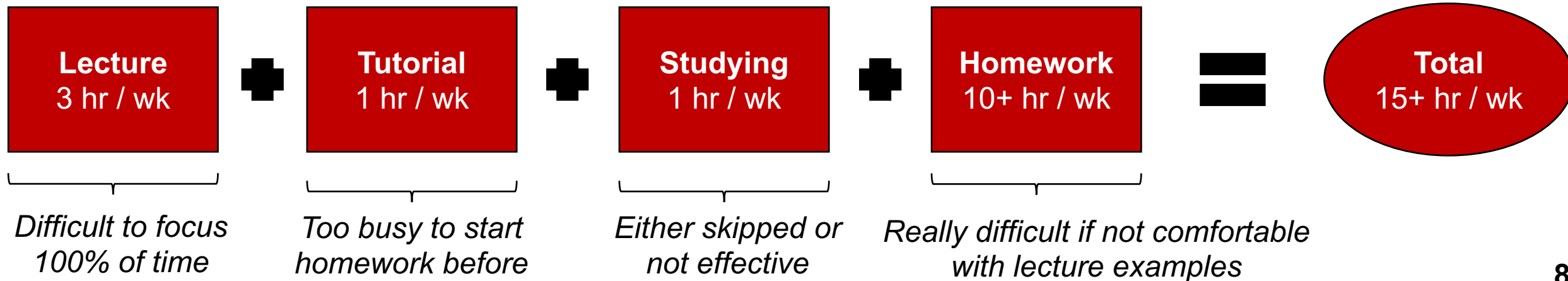
Complexity of Concepts and Applications

Difficult

Traditional Class (plan)



Traditional Class (reality for many)



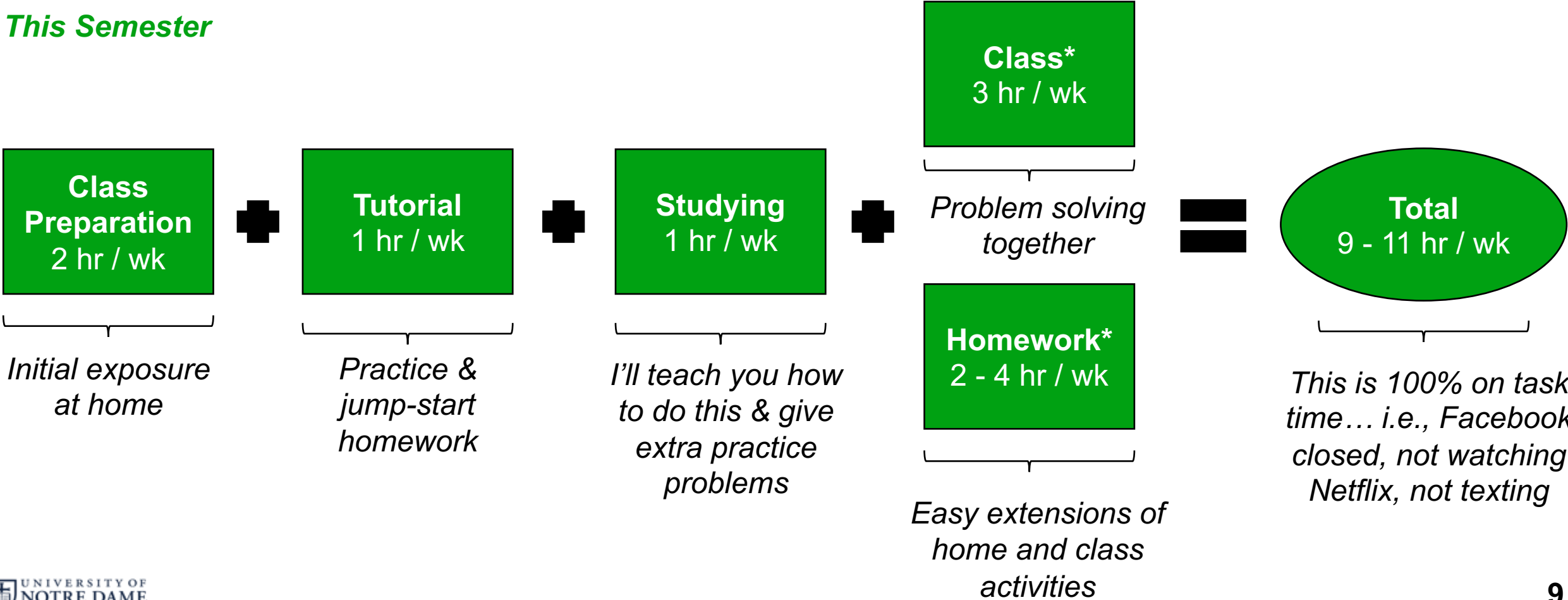
Making your time more effective

I show this slide on day 1.



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

This Semester



Fall 2019: Cloud-based Vocareum (Jupyter Notebooks)

www.vocareum.com

Benefits of Vocareum:

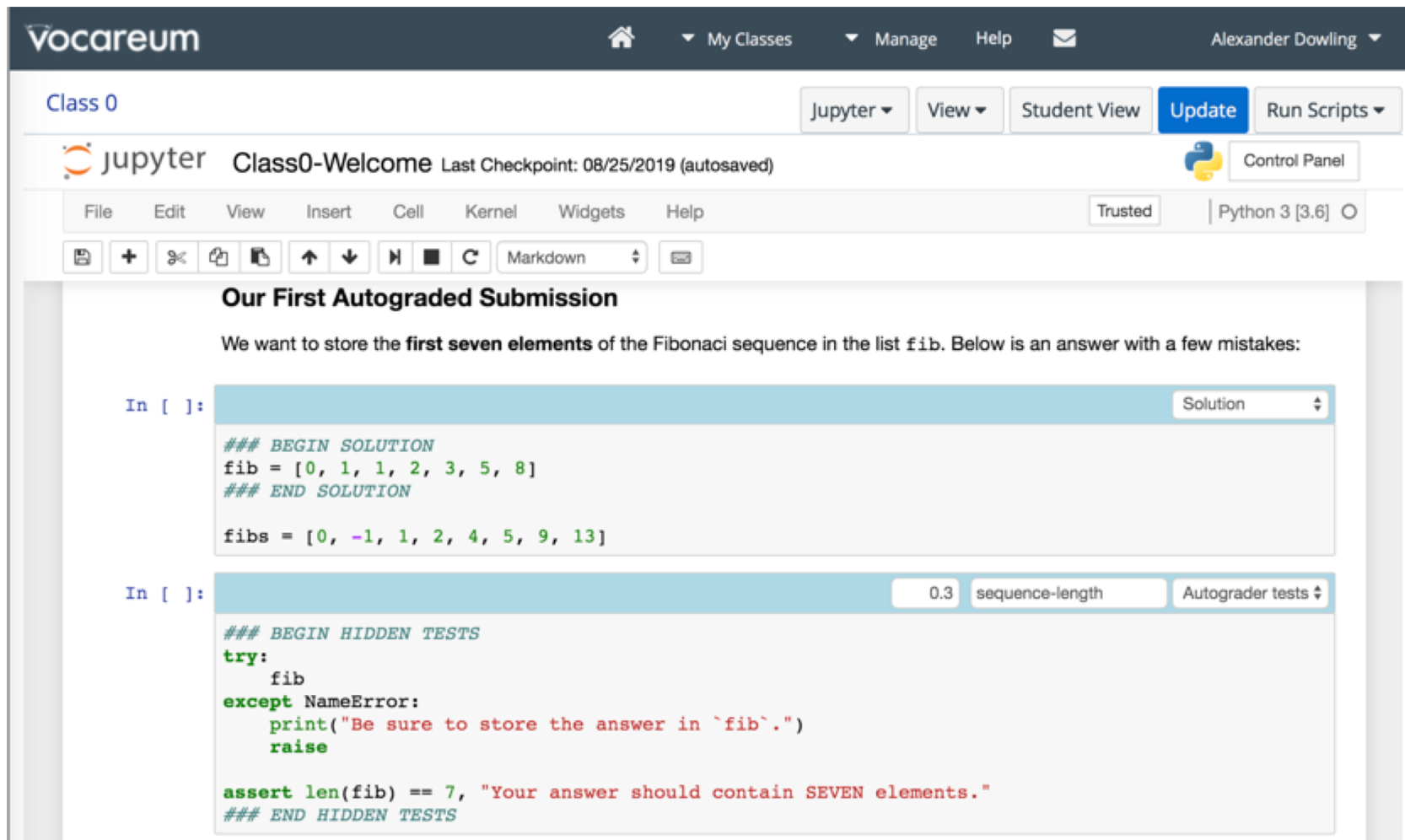
Many of the same cloud-based benefits as Colaboratory

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



The screenshot displays the Vocareum web interface for a Jupyter Notebook. The top navigation bar includes the Vocareum logo, a home icon, and links for 'My Classes', 'Manage', 'Help', and a user profile 'Alexander Dowling'. Below this, the notebook is titled 'Class 0' with buttons for 'Jupyter', 'View', 'Student View', 'Update', and 'Run Scripts'. The Jupyter interface shows a 'Class0-Welcome' header with a 'Last Checkpoint: 08/25/2019 (autosaved)' and a 'Control Panel' button. The main toolbar includes 'File', 'Edit', 'View', 'Insert', 'Cell', 'Kernel', 'Widgets', and 'Help', along with a 'Trusted' status and 'Python 3 [3.6]' kernel information. The notebook content is titled 'Our First Autograded Submission' and includes a text prompt: 'We want to store the **first seven elements** of the Fibonacci sequence in the list `fib`. Below is an answer with a few mistakes:'. The first code cell, labeled 'In []:', contains a solution attempt:

```
### BEGIN SOLUTION
fib = [0, 1, 1, 2, 3, 5, 8]
### END SOLUTION

fibs = [0, -1, 1, 2, 4, 5, 9, 13]
```

. The second code cell, also labeled 'In []:', shows hidden tests:

```
### BEGIN HIDDEN TESTS
try:
    fib
except NameError:
    print("Be sure to store the answer in `fib`.")
    raise

assert len(fib) == 7, "Your answer should contain SEVEN elements."
### END HIDDEN TESTS
```

. The output of the second cell shows a score of '0.3', the test name 'sequence-length', and 'Autograder tests'.

Fall 2019: Cloud-based Vocareum (Jupyter Notebooks)

www.vocareum.com

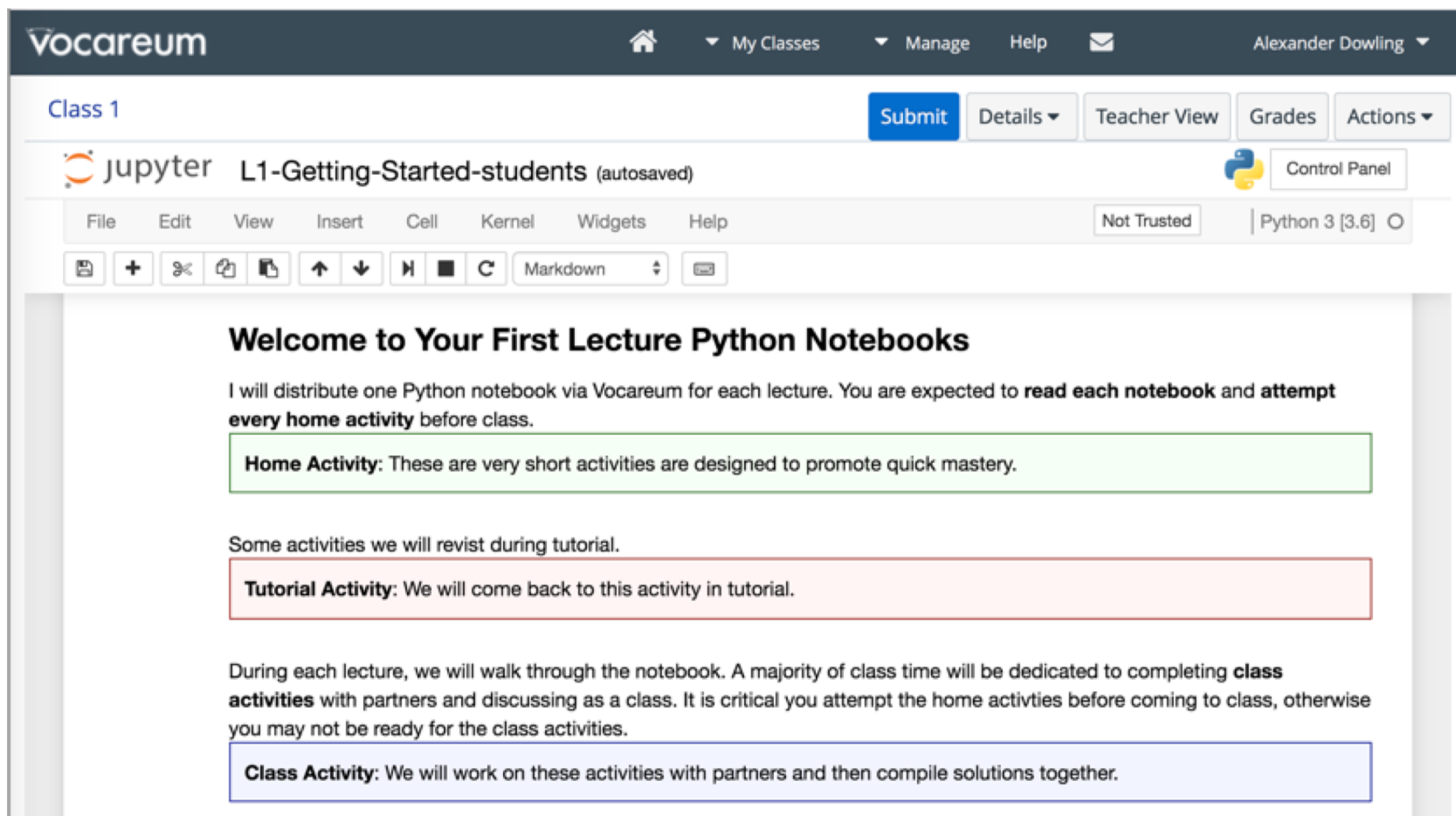
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The screenshot displays the Vocareum web interface. At the top, the Vocareum logo is on the left, and navigation links for 'My Classes', 'Manage', 'Help', and a user profile 'Alexander Dowling' are on the right. Below the header, a 'Class 1' section contains buttons for 'Submit', 'Details', 'Teacher View', 'Grades', and 'Actions'. The main content area is a Jupyter Notebook titled 'L1-Getting-Started-students (autosaved)'. It features a standard Jupyter menu (File, Edit, View, Insert, Cell, Kernel, Widgets, Help) and a toolbar with icons for saving, undo, redo, and other editing functions. The notebook content includes a heading 'Welcome to Your First Lecture Python Notebooks' followed by a paragraph: 'I will distribute one Python notebook via Vocareum for each lecture. You are expected to **read each notebook** and **attempt every home activity** before class.' Below this, there are three highlighted activity boxes: a green box for 'Home Activity' (designed to promote quick mastery), a red box for 'Tutorial Activity' (to be revisited during the tutorial), and a blue box for 'Class Activity' (to be worked on with partners and compiled together).

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

Excited Students 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**

Set them up for **early success**

- Require pseudocode
- Embrace the autograder

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

Extension Assignments

Watch TED talk, listen to podcast, etc.

Answer brief reflection questions

Completion grade, counts towards dropped homework

Examples:

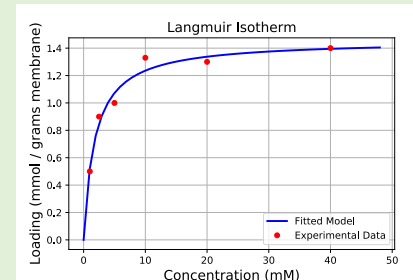
Planet Money, “What Causes What?”

Hidden Brain, “The Scientific Process”

TED Talks: Bias and Algorithms

Final Project: Heavy Metal Water Treatment

Fit Isotherm Model & Estimate Uncertainty



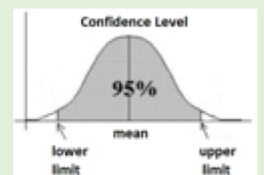
Calculate Filter Lifespan



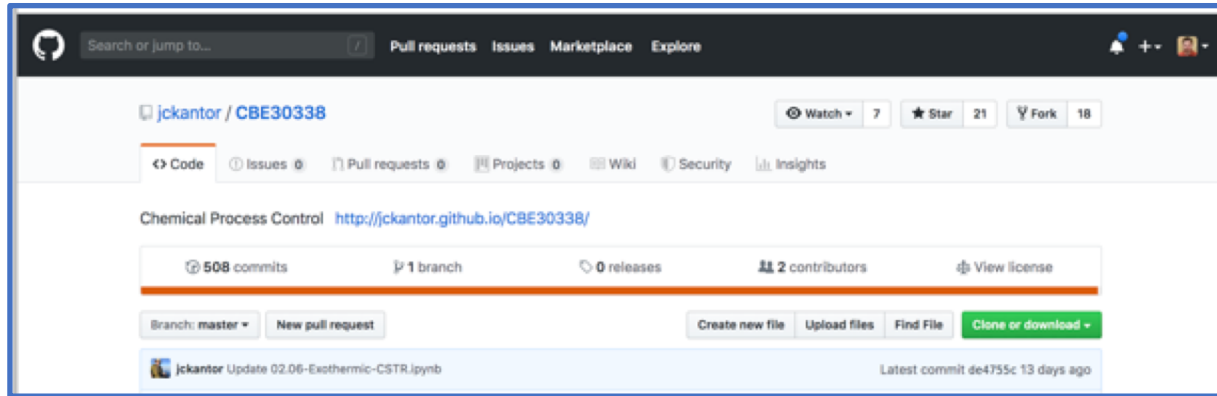
$$\frac{d}{dt}q(t) = \frac{F}{m}(c_{in} - c(t))$$



Draw Conclusions with Uncertainty



Special Thanks to Prof. Jeff Kantor



<https://github.com/jckantor>

Chemical Process Control

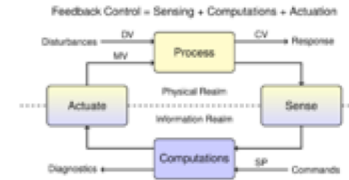
Introduction to Chemical Engineering Analysis

Introduction to Operations Research

Process Operations



CBE 30338



Chemical Process Control

[View the Project on GitHub](#)
jckantor/CBE30338

CBE 30338 Chemical Process Control

This repository comprises a collection of Jupyter/Python notebooks in support of **CBE 30338 Chemical Process Control** taught at the University of Notre Dame.

The links below display the notebooks as regular HTML web pages. From there you can run the notebook on [Google Colaboratory](#) or download to run on your own laptop. To run on your own laptop you will need to install Jupyter and Python 3, such as the excellent [Anaconda distribution from Continuum Analytics](#).

Please let me know (jeff at nd.edu) if you any thoughts or suggestions on how these notebooks could be improved for teaching and learning the principles of Chemical Process Control.

Table of Contents

Chapter 1.0 Getting Started

- 1.1 Getting Started with Python and Jupyter Notebooks
- 1.2 Python Basics
- 1.3 Python Conditionals and Libraries
- 1.4 Python Numeric Integration Revisited

Chapter 2.0 Process Modeling

- 2.1 Process Variables

This project is maintained by [jckantor](#)

Hosted on GitHub Pages — Theme by [orderedlist](#)



JUPYTER FAQ </> [Menu] [Refresh] [Download]

CBE30338 / notebooks

This notebook contains course material from **CBE30338** by Jeffrey Kantor (jeff at nd.edu); the content is available [on GitHub](#). The text is released under the [CC-BY-NC-ND-4.0 license](#), and code is released under the [MIT license](#).

< [Simulation and Optimal Control](#) | [Contents](#) | [Soft Landing a Rocket](#) >

[Open in Colab](#)

Simulation and Optimal Control in Pharmacokinetics

Installations and Initialization

Pyomo and IPOPT are now preinstalled on [Google Colaboratory](#). On MacOS and Windows PC, a one-time installation of pyomo and IPOPT is required. The following commands will perform the needed installation when using the Anaconda distribution of Python.

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