Training All Chemical Engineers in Computing and Data Science

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These slides are on the LAPSE archive: http://psecommunity.org/LAPSE:2019.1133
Research: Molecular-to-Systems Engineering

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

Funding: Multi-institution Projects:
### Chemical Engineering Suggested 4 Year Curriculum University of Notre Dame entering FA18

<table>
<thead>
<tr>
<th>Year 1</th>
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<th>Year 3</th>
<th>Year 4</th>
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<td><strong>Fall</strong></td>
<td><strong>Spring</strong></td>
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<td><strong>Spring</strong></td>
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<td>Intro to Chem CHEM 10171 (3)</td>
<td>Phys 1 PHYS 10310 (4)</td>
<td>O Chem 1 CHEM 10172 (3)</td>
<td>Transport I* CBE 20255 (3)</td>
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<td>Chem Lab CHEM 11171 (1)</td>
<td>Calculus II MATH 10550 (4)</td>
<td>Calculus III MATH 20550 (3.5)</td>
<td>Materials CBE 30361 (3)</td>
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<td>Intro. Eng. EG 10111 (3)</td>
<td>Intro to Che CBE 20255 (3)</td>
<td>Linear ODE MATH 20580 (3.5)</td>
<td>Thermo I CBE 20260 (3)</td>
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<td>COE Requirements</td>
<td>Physics 2 PHYS 10320 (4)</td>
<td>Num Stats CBE 20258 (3)</td>
<td>Transport II CBE 30367 (3)</td>
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<td>A Chem Lab CHEM 30333 (3)</td>
<td>O Chem Lab CHEM 31333 (1)</td>
<td>Diff Eq MATH 30560 (3)</td>
<td>A Chem Lab I CBE 31358 (3)</td>
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<td>P Chem CBE 30324 (3)</td>
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<td>Controls CBE 30338 (3)</td>
<td>ChE Lab I** CBE 41459 (3)</td>
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**Course Description**

- **Prerequisite**: course only offered in semester shown
- **Concurrent prerequisite**: course offered both spring and fall semesters

**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

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**LA 4: art/lt/lang/culture**

**LA 5: hist/soc sci**

**LA 6: int/WoK**

**Theology 1: found**

**Theology 2: develop**

**Philosophy 1: intro**

**Philosophy 2: philo/CAD**

**Writing 1: university seminar (satisfy with one of above)**

**University Core Curriculum**

**UCore 1** (3)

**Writing 2** (3)

**UCore 2** (3)

**Writing 1 Satisfy with other UCore**

**UCore 3** (3)

**UCore 4** (3)

**UCore 5** (3)

**UCore 6** (3)

**UCore 7** (3)
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

**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?

**labs**
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

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 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
Making your time more effective

**Traditional Class (plan)**

- Lecture: 3 hr / wk
- Tutorial: 1 hr / wk
- Studying: 2 hr / wk
- Homework: 3 hr / wk

Initial exposure: Practice
But how?: Builds on lectures

Total: 9 hr / wk

**Traditional Class (reality for many)**

- Lecture: 3 hr / wk
- Tutorial: 1 hr / wk
- Studying: 1 hr / wk
- Homework: 10+ hr / wk

Difficult to focus 100% of time
Too busy to start homework before
Either skipped or not effective
Really difficult if not comfortable with lecture examples

Total: 15+ hr / wk

I show this slide on day 1.
Making your time more effective

This Semester

- **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

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

- **Class**: 3 hr / wk
  - I’ll teach you how to do this & give extra practice problems

- **Problem solving together**

**Total**: 9 - 11 hr / wk

This is 100% on task time… i.e., Facebook closed, not watching Netflix, not texting.

*We’ll start some homework problems during class.*
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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Supports plagiarism detections (if you want it)

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

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**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

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**Final Project: Heavy Metal Water Treatment**

- **Fit Isotherm Model & Estimate Uncertainty**
- **Calculate Filter Lifespan**
- **Draw Conclusions with Uncertainty**

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