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Computational notebooks in chemical engineering curricula

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28

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33

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36 Advanced Studies in Mathematics from the University of Cambridge in 2010, and a Ph.D. in
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39 nanotube devices and sensors under the supervision of Michael S. Strano and Richard
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43

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51

52 ABSTRACT

53

54 Computational notebooks are an increasingly common tool used to support student learning in
55 a variety of contexts where computer programming can be applied. These notebooks provide
56 an easily distributable method of displaying text, images, as well as sections of computer code
57 that can be manipulated and run in real-time. This format allows instructors to introduce
58 content and methodologies to students in a single document that can be copied and
59 manipulated. In this paper we outline case studies of computational notebook usage at a
60 variety of institutions. These notebooks have been successfully used in required and elective
61 courses from the undergraduate sophomore-level to the graduate level. In each case study,
62 implementation, pedagogical strategies, and results are discussed.

63

64 INTRODUCTION

65

66 Computational notebooks are documents that can be read similarly to a textbook section or
67 journal paper, but can be run as computer code. The genesis of these notebooks has come
68 from the continual evolution of computer programming methodology to make programs more
69 comprehensible. This is by no means a new notion and is described by Knuth in his article on
70 “literate programming” from 1984 (1). Traditional computing environments such as MATLAB
71 and Mathematica to name only a few have evolved to offer interactivity, unique toolboxes and
72 well-documented help resources. These may be strong arguments to teach with such
73 languages, however, studies contrasting teaching in Python and Matlab have generally found
74 Python to be more effective for novice programmers, although there are advantages and
75 disadvantages to each language (2,3). Proprietary environments also have a significant

76 downside for students due to their expensive licensing fees which may make it difficult for
77 students to apply the codes they have developed after their studies or to share code with
78 colleagues who do not have a license.

79 Jupyter notebooks is a tool introduced in 2015 that advances the notion of narrative in
80 programming (4). Jupyter's main aims were to create a system to ensure that computational
81 tools can be used in a wide variety of contexts, be created in collaboration, and be easily
82 understood and reproduced. Jupyter offers a web-based interactive computing platform. The
83 web-based nature allows for relatively quick and easy use of these notebooks and
84 programming capabilities, the user needs only a web browser to interact and code. However,
85 all functionality can also be used offline if desired. Jupyter notebooks can combine live code,
86 text, equations, interactive user interfaces and other rich media. Jupyter supports a number of
87 programming languages including Python, Julia and R.

88

89 Within this article we present five case studies for the use of Jupyter notebooks in the
90 chemical engineering curriculum at a variety of institutions. In each case we describe how the
91 notebooks are implemented, used in classroom, and the impact on students and instructors.

92

93 **Georgia Institute of Technology: Teaching Data-Driven Decision-Making for Chemical** 94 **Process Engineering**

95 Optimization problems can be found everywhere in engineering, in both industry and academia.
96 However, most chemical engineering programs do not offer a course that discusses optimization
97 specifically in the context of chemical engineering case studies. At the same time, over the past
98 few years we have observed a tremendous increase in interest on data-analytics and machine
99 learning across all areas of chemical engineering (5, 6). In academia data-analytics is being
100 used to enable or expedite scientific discovery in materials science, pharmaceuticals, process

101 systems engineering and more. Similarly, industry is entering an era of digitalization, which has
102 led to an explosion of chemical, process, and manufacturing and operations data. It is
103 undoubtable that a large fraction of chemical engineering graduates will be faced with design,
104 control, or operations optimization problems that will also involve handling of data sets. As a
105 result, incorporation of such concepts in our curriculum will make our graduates competitive in
106 today's market.

107

108 The above tasks (i.e., data-analytics for decision making) require proficiency in computer
109 programming for data processing, analysis, visualization, modeling and optimization. In this
110 case study, a new elective course was developed to introduce chemical engineers to various
111 techniques for data-driven decision-making in chemical process engineering, as well as Python
112 programming. The course was taught primarily using Jupyter notebooks. The versatility and
113 flexibility of Jupyter notebooks facilitated the instruction of optimization and machine-learning
114 theory, but also enabled: (i) the students to learn and practice their programming skills in the
115 classroom; (ii) the creation of a very interactive, hands-on lecture where the data and results
116 were visualized; and finally (iii) the incorporation of active-learning group exercises and
117 discussion in the lecture.

118

119 The main learning outcomes of this course are (a) understanding of basic theory of linear,
120 nonlinear and mixed-integer optimization, (b) introduction to sampling, regression, validation
121 and data-reduction techniques, (c) understanding of how to use data-driven techniques for
122 optimization, and (d) comprehension of the dangers and ethics of the use of data for decision
123 making. Overall, the course maintained a balance between theory, tools and applications, such
124 that the students obtain key knowledge on how to efficiently formulate their optimization
125 problem, know it's mathematical characteristics, have the ability to select the appropriate

126 software/tool and, if needed, be able to create a customizable tool to solve the given problem
127 at hand. This balance was enabled through the use of open source Python tools for data
128 processing, machine-learning, visualization and optimization and most importantly, Jupyter
129 notebooks.

130

131 Each lecture started with the review of the background, theory and mathematical representation
132 of a specific type of optimization or machine-learning algorithm, followed by the loading of a
133 data-set and the formulation of the computer program that employed the theory to the specific
134 data set, and concluded with the visualization and discussion of the results. Students followed
135 the lecture through projection of the Instructor's screen and their personal laptops, which
136 allowed them to keep notes on their own version of the Jupyter notebook, as well as participate
137 in active learning exercises. In 80% of the lectures, an active-learning exercise was included,
138 during which the students were asked to complete a short assignment in small groups of 2-3
139 members, followed by an in-class open discussion of the solution (7). These active-learning
140 exercises ranged from purely conceptual questions, to purely computer programming
141 assignments. For example, the students were asked to generate a computer program from
142 scratch that would optimize a function, or most frequently, they were asked to make a
143 modification to a provided code to obtain the result (e.g., correct an error, fill in a few missing
144 coding lines, change some parameters and observe the sensitivity of the outcome, etc).

145

146 The student feedback on the usefulness and effectiveness of Jupyter notebooks has been very
147 positive. Students found that hands-on programming in class and visualization of the results
148 were crucial towards understanding hard concepts, such as the use of derivatives for searching
149 for an optimum, the effects of lack of data, noise and outliers on data-driven modeling and
150 optimization, the representation of data in reduced-dimensions, and many more.

151

152 At the beginning of the course, almost 70% of the students did not have any prior Python
153 programming experience and almost 90% of the students had not used Jupyter notebooks
154 before. All of the students had previous programming experience in MATLAB or other
155 programming languages. Three lectures at the beginning of the course were dedicated to
156 tutorials in Python and Jupyter notebooks. One of the challenges pointed out by students with
157 minimal prior Python programming expertise was the steep learning curve of the course, which
158 included learning optimization theory, machine learning and statistics concepts at the same time
159 as learning to program in a new language. However, none of the students found that it was
160 challenging to learn how to use, read and modify Jupyter notebooks. In fact, several students
161 recognized that the use of Jupyter notebooks is by itself a skill that can be beneficial in other
162 aspects of their careers. For example, students now use Jupyter notebooks for research
163 projects and research communication within their lab, with industry and as supplementary
164 material to accompany their publications. Despite the challenge of learning a new programming
165 language, all students passed the course and were able to complete challenging projects using
166 programming in Python.

167

168 Overall, through this experience it became clear that a course on topics that involve modern
169 data analytics, machine learning, realistic data sets and decision-making was effective mainly
170 because of this new medium that enables the combination of theory, images, programming,
171 plotting and more within a single lecture. The instructor plans to make the lectures as stand-
172 alone teaching modules that can be shared with the community, and this points to another
173 advantage of the use of this flexible teaching medium.

174

175 **University of Notre Dame: Numerical Methods, Applied Statistics, and More**

176 Over the past few years, Jupyter notebooks have become an integral part of at least eight
177 chemical engineering courses at Notre Dame taught by three faculty (8):

- 178 1. CBE 20255 Introduction to Chemical Engineering Analysis (sophomore, required) (9)
- 179 2. CBE 20258 Numerical and Statistical Analysis (sophomore, required) (this article)
- 180 3. CHE 30324 Physical Chemistry for Chemical Engineers (junior, required) (10)
- 181 4. CBE 30338 Chemical Process Control (junior, required) (11)
- 182 5. CBE 40455 Process Operations (senior, elective) (12)
- 183 6. CBE 60499 Nonlinear and Stochastic Optimization (graduate, elective) (this article)
- 184 7. CBE 60547 Computational Chemistry (graduate, elective) (13)
- 185 8. CBE 60553 Advanced Chemical Engineering Thermodynamics (graduate, required) (14)

186 This article highlights pedagogical advantages and shortcomings of Jupyter notebooks in the
187 context of teaching numerical methods and applied statistics in CBE 20258 and CBE 60499
188 with Python.

189

190 Most importantly, Jupyter notebooks facilitate active learning by co-locating code and diverse
191 outputs (text, error messages, and graphics) into a single, living document. Previously, when
192 teaching CBE 20258 with MATLAB, it was difficult to engage students with examples as code
193 (script), text output (console) and graphics were all separate windows. This can be resolved in
194 MATLAB by using the live editor feature. Moreover, text (markdown) cells in Jupyter notebooks
195 allow descriptive text, equations (through LaTeX), and embedded images to be easily
196 interspersed between computer code and output. Though the equivalent can also be done in
197 MATLAB it is not as intuitive as in Jupyter. The latest iteration of CBE 20258 is organized with
198 one notebook for each class meeting. Before each class, students are required to i) read the
199 notebook and any assigned book sections and ii) and complete brief home activities. The
200 notebook also includes several more complex, often multipart, class activities. During class

201 session, we work through the class activities individually, in partners, or as a large group. While
202 scrolling between class activities in the notebook, we stop to answer questions on the reading
203 and home activities. As needed, 5 to 10-minute mini-lectures are given on important and difficult
204 concepts. Jupyter notebooks are a key enabling technology for this class structure because
205 examples, activities (with detailed instructions), and reading material are integrated into a single
206 living document.

207

208 Cloud-based hosting platforms for Jupyter notebooks can eliminate barriers for access, simplify
209 class administration, and further facilitate active learning. CBE 60499 was last taught using
210 Jupyter locally installed on each students' personal laptop. Although Python distribution
211 anaconda simplifies installation process for students, this local installation works best with small
212 classes. During the last two iterations of CBE 20258, we have experimented with two cloud-
213 based Jupyter systems: Google Colaboratory and Vocareum. Both systems allow students to
214 complete all class assignments through a web-browser on any internet connected computer.

215

216 Google Colaboratory ("Colab" for short) is a free computing environment built for research.
217 Colab is best described as "Google Docs but for code" with similar comments and editing from
218 multiple users. At Notre Dame, we shared all class notebooks with students in a read-only
219 Google Drive folder. Colab would then prompt students to save a copy of the notebook in their
220 own Google Drive. This facilitates easy sharing, interactive editing, and automated back-ups
221 with revision history. To submit assignments, students would create a shareable URL, add the
222 URL to the top of their notebook, and save the notebook as a PDF.

223

224 Vocareum is a paid-for-use hosted Jupyter server built for education. A key advantage of
225 Vocareum is that it integrates directly with learning management systems (LMS) including

226 Sakai. Most importantly, Vocareum supports auto-grading scripts including the open-source
227 nbgrader platform for Jupyter notebooks. Auto-grading has two main advantages: i) it gives
228 students instant feedback on their work and ii) dramatically reduces time required to grade the
229 assignment. However auto-grading also has significant drawbacks in that it can be time-
230 consuming to set up and cannot give qualitative feedback (for example in assessing figures or
231 code for readability). For CBE 20258, the auto-grader allows for accountability with the home
232 activities before each class, which is not feasible otherwise due to time constraints. Although
233 Vocareum allows for manually grading of Jupyter notebooks, the interface is cumbersome.
234 Instead, students are required to submit both i) notebook to Vocareum for auto-grading sections
235 and ii) PDF printout to Gradescope to assess coding style (comments, etc.), figures, and
236 pseudocode or model derivations. In summary, neither Colab or Vocareum are perfect. Colab
237 offers more flexible sharing and is free, but Vocareum has education-focused features including
238 LMS integration and auto-grading that can greatly streamline classes.

239

240 **University of British Columbia: Interactive Notebooks in Reactor Design and Process**

241 **Control**

242 At the University of British Columbia (UBC), Reactor Design (CHBE 355), and Process Control
243 (CHBE 356) are junior-level chemical engineering courses taken in the same term that require
244 significant mathematical and computational backgrounds. The reactor design course focuses
245 on homogeneous chemical reactor design and modelling. The process control course focuses
246 on modelling chemical processes in order to design effective control strategies. Engineering
247 undergraduates with limited mathematical knowledge and programming skills have the most
248 difficulty with these courses. Engineers working in industry often need to solve poorly-defined
249 problems that require proficiency with advanced computational and design tools. Engineering

250 graduates who lack design and programming experience can face difficulty in the job market as
251 they have little exposure to these types of problems.

252

253 Guzman et al. highlighted the use of interactive tools to encourage active participation and
254 facilitate student-focused learning in engineering education (15). These tools allow students to
255 understand difficult mathematical concepts through manipulatable figures. Students can
256 develop a comprehensive understanding of course materials and obtain design experience
257 through interactive tools and integrated projects that requires content from multiple courses to
258 solve. In order to develop students' design, analysis and problem-solving skills, computational
259 tools for these two courses using Python were introduced through Jupyter notebooks.

260

261 Syzygy is an online Jupyter notebooks hosting service offered by the Pacific Institute of
262 Mathematical Sciences, Compute Canada and Cybera to researchers and educators across
263 Canada. This tool is free for instructors, students and researchers and allows notebooks to be
264 easily run and shared. During tutorial sessions the teaching assistant leading the tutorial
265 would work through a notebook with their screen mirrored on a projector as students worked
266 in their own copy of a Jupyter notebook. The communication tool Slack was used as a
267 discussion board to facilitate student question during the tutorial period.

268

269 Students in these courses had prior experience with MATLAB, but were assumed to have no
270 prior experience with Python. In order to introduce students to Python and its application in
271 solving a variety of mathematical problems, six tutorial notebooks were created to introduce
272 students to relevant functions for solving a variety of mathematical systems. These were used
273 in tutorials in both courses during the first third of the course. The following six tutorials in each
274 course then focused on the use of computational tools to solve relevant problems. In addition

275 to notebooks used in the tutorials, students were given take home assignments (two in reactor
276 design and one in process control) and one final project in each course. The final projects
277 applied the skills students had learned in previous tutorials to address a complex problem in an
278 industrial context. All of these tutorial notebooks can be accessed online through a GitHub
279 repository (16).

280

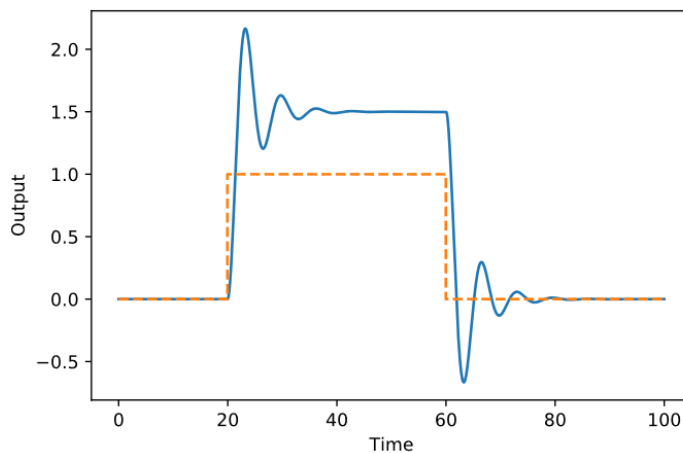
```
In [82]: # Generate a step response
T = np.linspace(0,100,1000)

# Our input is one between t=20 and t=60
U = np.zeros(len(T))
U[200:600] = 1

t, yout, _ = control.forced_response(G_s, T, U)

# Plot
plt.figure()
plt.xlabel('Time')
plt.ylabel('Output')
plt.plot(t,yout)
plt.step(t,U, linestyle='--')
```

```
Out[82]: [<matplotlib.lines.Line2D at 0x11e2085c0>]
```



281

282 Figure 1. A screenshot from a Jupyter notebook from the process control course showcasing
283 coding input that can be manipulated and corresponding graphical output for a step change in
284 a control process.

285

286 A survey was run at the end of the courses focusing on student experience in the final projects.
287 Responses, found in Table 1, were received from 19 students out of the roughly 120 unique

288 students in both classes (note that about 95% of students are common between the two
 289 courses). This low turnout was perhaps due to having no incentive for survey completion as well
 290 as the survey being at the end of the term when students are busy with other projects and
 291 studying for final exams. Given the small number of responses, no overall conclusion can be
 292 reached, but the students who did respond indicated they saw the benefit of learning
 293 programming to their future careers. Open comments from students at the end of the survey
 294 point to the range of background programming abilities of students. Many comments focused
 295 on the pace of the tutorials and programming content with some saying the pace was too fast,
 296 and others saying the opposite.

297

298 Table 1: Student survey results from reactor design and process control Jupyter-based terms
 299 projects.

Survey Question	Strongly Agree	Agree	Neutral	Disagree	Strongly Disagree
The project enhanced my learning of the course material. I can see the relevance of the project to the course material	4	7	4	4	0
The project content was interesting	3	6	8	2	0
I can see the benefit of learning programming and Python to my future career	11	5	3	0	0

300

301

302 **Carnegie Mellon University: Integrating Jupyter into the Master of Science Program**

303 Jupyter and related methods have been used extensively in the Master of Science (MS)
 304 program in the Department of Chemical Engineering at Carnegie Mellon University (CMU). The
 305 MS program was designed to give chemical engineering students specialization in numerical
 306 methods and computational skills to tackle more complicated and realistic problems in industrial
 307 settings. The students come from diverse educational backgrounds. Most of these students
 308 have ChE undergraduate degrees, but background varies and includes large US research

309 universities, small liberal arts colleges, and foreign universities including China, India, and
310 Japan, among others). Most but not all undergraduate programs integrate a small amount of
311 programming exercises into the core curriculum, typically as MATLAB assignments and labs.
312 Informal polls of this population of these students indicate that about 10% have no programming
313 experience at all from their undergraduate curriculum, and less than half have been introduced
314 to python. This diversity of backgrounds presents a challenge to teaching a course completely
315 in python but by the end of their first semester with two python-intensive courses all students
316 are able to solve technical numerical programming problems.

317

318 Although chemical engineering instruction with Jupyter is quite recent, similar approaches have
319 been used for some time at CMU. Two of the first-semester core classes in the CMU MS
320 program are taught entirely with computational methods, including a numerical methods course
321 (06-623) and a reactor engineering course (06-625). The format for both courses was pioneered
322 and developed by Prof. John Kitchin who has described extensively how Emacs org-mode can
323 be used for education (17). Emacs is a powerful open source text editor, and org-mode is a
324 package that can be run within emacs. Org-mode allows a number of features including a simple
325 document markup syntax, the capability to embed interactive code and data in a document and
326 the capability to export a document into another format such as PDF or LaTeX. From 2015 to
327 2017, 06-625 was taught with all lecture notes, homework, and exams using the org-mode
328 structure. In 2017, Prof. Zack Ulissi transitioned to Jupyter notebooks based on their increasing
329 popularity and relevance to other fields. In 2018 and 2019, both Fall core classes (06-623 and
330 06-625) were taught in the Jupyter format. Lecture notes, assignments, and exams, are
331 available for 06-623 (18). This approach was also adopted for one semester for the
332 undergraduate reaction engineering course 06-634. Email surveys of students one semester
333 after taking these courses indicate that 80% of the students are using Jupyter in their

334 research/classes, suggesting that the skills are transferable to broader chemical engineering
335 challenges.

336

337 **Course Format:**

338 06-623 and 06-625 at CMU are relatively unique among numerical methods courses in that
339 nearly 100% of in-class lectures, exercises, homework, and exams are in the form of Jupyter
340 notebooks. Lectures are given by projecting the instructor's laptop screen with the interactive
341 notebook. Lecture notes are distributed before class, and students are expected to bring their
342 own laptops and follow along. This format is interactive as the instructor can develop python
343 solutions to engineering problems as a live demonstration, can adjust and interact with existing
344 solutions (e.g. change initial conditions or tolerances and observe the effect on solutions), and
345 answer student questions about the methods or ideas with additional examples. All homework
346 and exams are distributed in the form of jupyter notebooks, and students complete the
347 notebooks and submit them as the notebook file and a PDF. This significantly simplifies the
348 evaluation process since the exams/homeworks are in exactly the same format as the daily
349 lectures.

350

351 **Intro to python on-ramp:**

352 In the context of a one-semester course for students using python and jupyter for the first time,
353 the on-ramp process is extremely important. Various strategies that have been used in teaching
354 06-623 and 06-625 include: (i) introduction through the first two weeks of class (with in-class
355 demonstrations and exercises) (ii) use of tailored on-line python materials as out-of-class
356 exercises in week 1, and (iii) a short half-day python-intensive workshop before the first week
357 of class. (ii) was implemented using the Open Learning Initiative (OLI) system at CMU with help
358 from the Eberly Center and a Wimmer teaching fellowship for Prof. Ulissi. (iii) was implemented

359 as a single 5-hour session using the established Software Carpentry “Introduction to
360 Programming” module (19) the week before classes started. In all cases, nearly all students
361 were able to complete the courses, and most students were comfortable with the format by the
362 end of the third week of lectures. Self-reported homework and out-of-class study times in the
363 first two weeks were considerably lower with (ii)/(iii) instead of (i), suggesting that these methods
364 helped with the on-ramp experience.

365

366 **Grading:**

367 Grading of Jupyter notebooks is still imperfect. Distributing and collecting notebooks can be
368 performed with some packages such as nbgrader, but this relies on special json code embedded
369 in the documents. Json is a standard data format often used in web programming which
370 structures data such that it can be easily read by a number of programming languages. LMS
371 integration of nbgrader is dependent on the Jupyter platform and LMS being used. Furthermore
372 nbgrader does not have support for standard/repeated feedback (e.g. different students making
373 the same mistakes). Prof. Ulissi is currently using Gradescope to grade the notebooks submitted
374 as PDFs. Students simply print their notebook to PDF and upload to gradescope. Note that the
375 default Jupyter to PDF conversion which works via pdflatex is less favorable as equation errors
376 in the markdown cells, which often display correctly within Jupyter, frequently break the pdflatex
377 conversion. Teaching assistants (TAs) then use the Gradescope interface to quickly grade the
378 assignment as they would a normal engineering homework. Students are also expected to
379 submit a copy of the jupyter notebook in case the TAs wish to manually check the solution/code
380 or for plagiarism detection (detailed below).

381

382 **Plagiarism:**

383 An obvious concern in programming-heavy courses is the possibility of plagiarism. These
384 challenges are not unique to chemical engineering or Jupyter notebooks. Since students submit
385 copies of their notebooks, standard methods such as Measure Of Software Similarity (MOSS)
386 can be used (20). Collected jupyter notebooks are batch-converted to python scripts, which are
387 then submitted to MOSS for analysis. This process is not perfect, but quickly flags the most
388 flagrant violations. A secondary benefit of this approach is that this process also identifies
389 students who copied and modified particularly relevant examples from the lecture notes. While
390 not academically dishonest if disclosed, this method of solution is less desirable and often
391 correlated with students who struggle to creatively solve engineering problems in formats they
392 have not seen before. Finally, with an exam format of every student working on a laptop and
393 submitting their own notebook, it is very difficult to guarantee students are not messaging each
394 other with solutions. Standard approaches (random seating, TAs roaming the room, etc) can
395 partially address this challenge.

396

397 **Installation/usage:**

398 Most students do not have experience installing and using python and jupyter notebooks. We
399 have used pre-installed anaconda installations, docker images, and on-line hosted instances
400 such as Google Colab or Microsoft Azure Notebooks. All were sufficient for the needs of the
401 classes, but the hosted solutions have had the fewest technical difficulties. Prof Kichin has
402 developed a flask web app interface (Techela) to jupyter notebook distribution and submission
403 that largely hides many of these difficulties if a local python installation is used (21).

404

405 **University of Wisconsin-Madison: Teaching Advanced Optimization Techniques to**

406 **Undergraduate Students using Julia and Jupyter Notebooks**

407 Optimization has traditionally been a difficult topic to teach to undergraduate students. The
408 mathematics behind it (and associated software tools) are rather abstract and sophisticated.
409 Commercial optimization tools (e.g., AMPL, AIMMS, GAMS) are computationally powerful but
410 they are targeted towards graduate-level students and industrial practitioners. These tools
411 also have proprietary syntax and stand-alone implementations that complicate integration with
412 other tools (e.g., visualization). On the other hand, Matlab (the most popular scientific
413 computing package for undergraduate education) provides a flexible environment but its
414 optimization tools are computationally inefficient and difficult to use (e.g., translating an
415 optimization problem into matrix-vector form and/or computing derivatives is difficult). As a
416 result, instructors that teach optimization using such tools can spend significant amounts of
417 time (weeks to months) teaching students how to use software tools, as opposed to teaching
418 students how to properly formulate the problem at hand and analyze the results. Moreover,
419 students tend to lose motivation if they feel that the tools learned cannot solve industrially-
420 relevant problems.

421 Recent developments in open-source modeling languages such as Pyomo (in Python) and
422 JuMP (in Julia) have dramatically changed the landscape of optimization software. In
423 particular, these tools are much more accessible to students (22, 23). Pyomo and JuMP also
424 largely benefit from the fact that they reside in a flexible computing environment (as Matlab),
425 which facilitates the use of supporting tools (e.g., linear algebra, data, statistics, visualization)
426 in the modeling and analysis process. Such tools are also under active development by the
427 open-source Julia and Python communities.

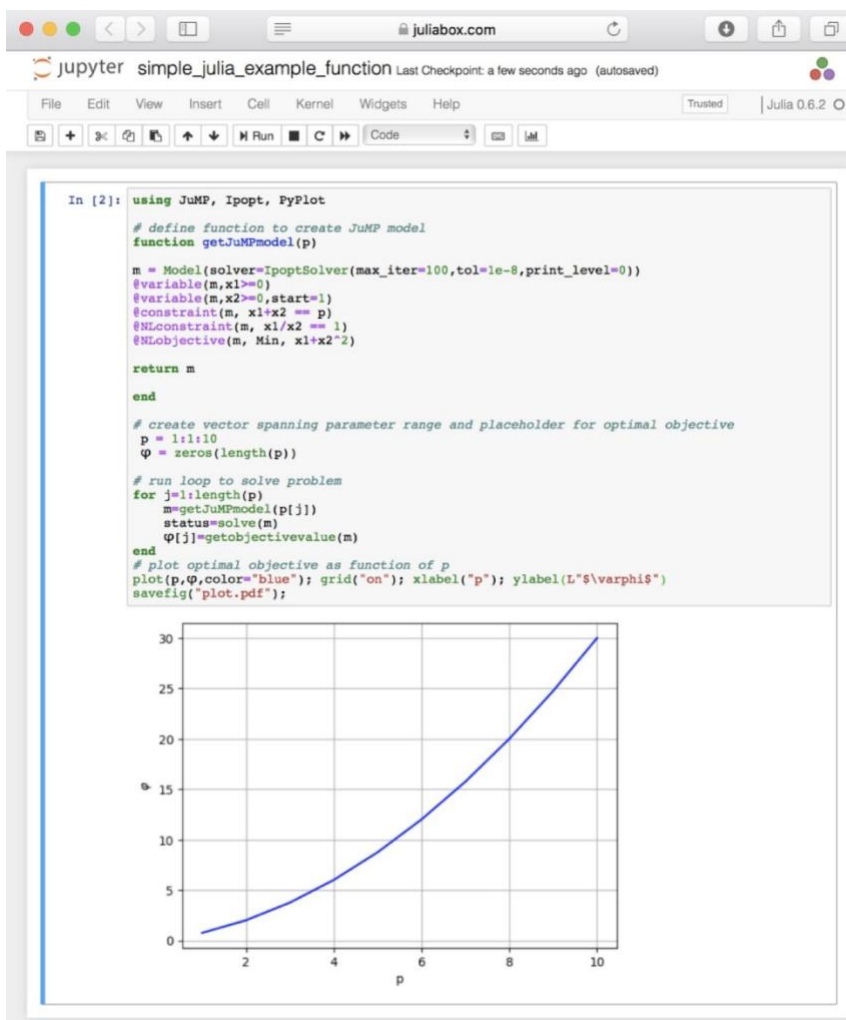
428 Jupyter notebooks is a premier example of how open-source software benefits undergraduate
429 education. At UW-Madison, we have been using JuMP and Jupyter notebooks to teach
430 optimization to undergraduate students. In the Chemical and Biological Engineering
431 Department, Jupyter notebooks are being used to teach the senior Process Design course

432 (CBE 450) while, in the Electrical and Computer Engineering Department, Jupyter notebooks
433 are being used to teach the Introduction to Optimization course (CS/ECE/ISyE 524). In CBE
434 450, the instructor spends a total of 4 hours teaching students the basics of optimization
435 modeling and implementations in JuMP (the students have no previous background in
436 optimization). This is possible because the syntax of JuMP is compact and intuitive (the
437 software implementation of a model looks similar to that in paper). For instance, a simple but
438 powerful feature of JuMP is the ability to express variables as unicode symbols, which allows
439 students to define variables using letters from the Greek alphabet. JuMP also incorporates set
440 notation and allows indexes to take names (e.g., chemical formulas to identify components).
441 Jupyter notebooks provided to the students are executed in the public portal
442 <https://www.juliabox.com> (students do not have to install new software in their computers).
443 Learning JuMP allows students to tackle complex optimization problems rather easily. For
444 instance, we teach them how to optimize a flowsheet, how to design water and heat recovery
445 networks, how to design compressor trains, and how to conduct equilibrium calculations.
446 These examples are non-trivial (e.g., involve difficult sets of nonlinear equations) and are
447 sufficient for students to start comprehending the concepts of objective functions, constraints,
448 trade-offs, and nonlinearity as well as to understand the power of modern optimization tools.
449 Specifically, JuMP is not an educational package but is in fact actively used in academic and
450 industrial research (JuMP can tackle problems with millions of variables) (24). The objective is
451 thus to help students appreciate the tools learned in their undergraduate education do solve
452 real problems.

453 It is important to emphasize that all these benefits are largely enabled by Jupyter notebooks.
454 Implementing JuMP models as plain Julia scripts, while doable, does not provide an
455 interactive experience and can be frustrating to students that are not familiar with the
456 language. Specifically, Jupyter allows students to experiment with their code and quickly see

457 the outcomes (i.e., execute pieces of code on-the-fly). This feature is particularly important
458 when building and debugging complex optimization models. Moreover, students are asked to
459 submit their homework assignments as Jupyter notebooks and this teaches them how to
460 properly document and share code. Jupyter notebooks also enable students to learn and
461 appreciate the benefits of LaTeX (an advanced type-setting system). The use of Jupyter
462 notebooks also helps students understand the computational workflow behind their code (an
463 insight that gets lost when executing a script all-at-once). The use of embedded visualization
464 tools in notebooks has also proven to be of high value, as most students prefer to visualize
465 data and like to perform sensitivity analyses (see Figure 2). Notebooks thus provide a natural
466 segway to the use of data analysis, uncertainty quantification, and visualization techniques.

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468

469 Figure 2. Snapshot of Jupyter notebook implementing sensitivity analysis for a simple
470 optimization problem.

471 Conclusions

472 Computational notebooks are powerful and versatile tools that can be used at a variety of
473 instructional levels. They have become relatively easy to implement, and can be leveraged to
474 help students understand physical, chemical and biological phenomena that chemical
475 engineers deal with on a daily basis. Furthermore, their use helps promote data and
476 programming literacy, which is becoming increasingly important for all engineering disciplines.

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