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Computational instruction with Jupyter notebooks

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Notebook available at https://github.com/phaustin/mcgill_2019_talk
(https://github.com/phaustin/mcgill_2019_talk).

Part 1 – Infrastructure

- Linux/git
- Conda-forge
- Jupyter/JupyterText
- Cocalc
- nbgrader
- nbsphinx
- pangeo

Part 2 – Examples

- 2nd year course, 48 students
 - Jupyter/chrome/cocalc
- 3rd/4th year course, 26 students
 - Jupyter/laptops/conda-forge
- Grad/postdoc workshop, 20 students,
 - pangeo with dask/xarray,zarr on an HPC cluster

Some history

July, 1997: BAMS article: John Stockie, Susan Allen, Phil Austin

An Interactive Course in Numerical Methods for the Earth Sciences

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In [2]: Image(filename='figures/bams_ref.png')
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Out[2]:

tial project planning stage. Undergraduates meet with the graduate students in the weekly discussion sessions and participate in the graduate course mailing list discussions. The first-year computer language used in the UBC computer science department is C++, so in this sense the undergraduates may be better prepared than graduate students arriving with a background in Pascal or FORTRAN.

A more detailed discussion of the lab templates, the software and hardware requirements for our labs, and access to the labs themselves are available at <http://www.geog.ubc.ca/numeric>. Readers are invited to forward comments/questions to us at numerical_methods@geog.ubc.ca. We would be interested in sharing experiences with others who are beginning to explore instruction via the Internet.

5. Discussion

Our first venture into Web-based instruction has met the objectives we set for ourselves in the winter of 1995. We were particularly impressed by the undergraduate student interns hired to develop the

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Infrastructure

Linux kernel

- developed by 19,000 unique committers
- 65,000 files
- 25 million lines of code

Git and Github

- 2005: Linus Torvalds (https://en.wikipedia.org/wiki/Linus_Torvalds), begins Git development (<https://en.wikipedia.org/wiki/Git>).
- 2008: Github founded (<https://en.wikipedia.org/wiki/GitHub>), in 2018 it hosted 28 million users and 57 million repositories
- Distributed version control makes possible the
 - pull request workflow (<https://yangsu.github.io/pull-request-tutorial/>).

Conda-forge

- Software packaging using conda
(<https://conda.io/projects/conda/en/latest/index.html>).
- Supported by numfocus (<https://numfocus.org/project/conda-forge>) -- provides scientific software for linux, macos and windows 10 ~ 3500 separate packages
 - netcdf-fortran feedstock (<https://github.com/conda-forge/netcdf-fortran-feedstock>).
 - gdal feedstock (<https://github.com/conda-forge/gdal-feedstock>).

Jupyter and jupyterx

- Jupyter (<https://blog.jupyter.org/jupyter-receives-the-acm-software-system-award-d43>)
 - Origins -- began in 2001 as ipython: repl (read, evaluate, print, loop)
 - Hosts 100 language kernels (<https://github.com/jupyter/jupyter/wiki/Jupyter-kernels>)
 - jupyterx (<https://github.com/mwouts/jupyterx>)
 - round trip conversion between jupyter notebooks written in javascript and
 - python, R, markdown, Julia, bash scripts
 - Allows collaborative notebook development using pull-requests
 - Example: this talk
(https://github.com/phaustin/mcgill_2019_talk/blob/master/talk_dir/python/mc)
-

Cocalc, nbgrader and nbsphinx

- cocalc.com (<https://cocalc.com>): jupyter notebook hosting for classes
- nbgrader (<https://github.com/jupyter/nbgrader>): autograded jupyter notebooks
- nbsphinx (<https://github.com/spatialaudio/nbsphinx>): build a webstie from notebooks

Examples

Inspiration

- Cliburn Chan's Stat 663 (<http://people.duke.edu/~ccc14/sta-663-2018/index.html>).
- Berkeley's data 8 (<https://data.berkeley.edu/education/courses/data-8>).

Large class, 2nd year

- Computational Methods in Geological Engineering (<https://phaustin.github.io/eosc213/>).
 - co-taught with Roger Beckie and Nicolas Seigneur
 - 48 2nd year geological engineering students
 - Prereqs: vector calculus, linear algebra, C
 - students use: cocalc.com notebooks

Smaller class, 3rd and 4th year

- 3rd/4th year: Radiation and remote sensing
(https://phaustin.github.io/a301_code/).
 - taught to 26 students in EOSC and other departments
 - open to any student with 1st year calculus, physics, programming
 - includes both jupyter notebooks and course libraries
 - students use: conda environments on laptops or lab desktops

Grad/post-doc workshop

- Parallel python tutorial (https://phaustin.github.io/parallel_python_course/).
 - Introduce the pangeo software stack (<https://docs.google.com/presentation/d/1evNXCddIIIXUt4a5jKfmlO2197sp8T6I9L650> particularly dask (<https://medium.com/pangeo/dask-jobqueue-d7754e42ca53>), xarray (!zarr (<https://zarr.readthedocs.io/en/stable/>)). (see this pangeo notebook server (https://mybinder.org/v2/gh/pangeo/pangeo-notebook/HEAD?filepath=notebooks/pangeo_notebook_server.ipynb))
 - 20 UBC HPC focussed grad students/postdocs
 - Half day, using notebooks and Compute Canada cluster
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Take home points

Jupyter notebooks plus conda-forge and github.

- Make active learning possible at scale. Costs to students are similar to the price they are paying for textbooks (cocalc plus a tablet/chromebook)
- In-class sessions and assignments deal with working examples of realistic problems and best-practices for production computing
- Use the same workflow for both research and teaching, and make research reproducible by default.

What's next?

- I am writing an instructor's guide to teaching with Jupyter notebooks
- EOAS is creating a github repository for collaborative notebook development focussing on UCAR/ACCRU institutions, watch the UCAR members/ACCRU mailing lists
- Questions/interest/want to help? Email me at paustin@eoas.ubc.ca

*"The future is already here — it's just not very evenly distributed." --
William Gibson*