

SciNet Jupyter Hub for Researchers

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10 February 2021

Common computational research scenario

- 1 Get a research idea
- 2 You roughly know what computation it needs
- 3 *Prototype/development:*
 - ▶ You write your computation or analysis code
 - ▶ Try: It does not work
 - ▶ Try a small case: still does not work
 - ▶ Debug code line-by-line (repeat)
- 4 Fix performance bottlenecks.
- 5 Need more resources: SciNet
 - ▶ *preprocess* (prep data)
 - ▶ test small case
 - ▶ submit large computations
 - ▶ *postprocess* results
- 6 Write paper/thesis

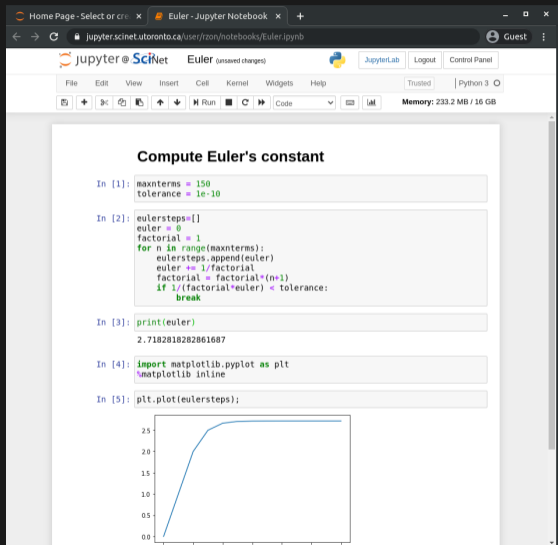


Many steps are easier in an interactive environment.

1

Jupyter = Interactive Research Computing

Interactive computing with Jupyter Notebooks



The screenshot shows a Jupyter Notebook titled "Euler (unsaved changes)" running on SciNet. The notebook contains five input cells:

```
In [1]: maxterms = 150
        tolerance = 1e-10

In [2]: eulersteps=[]
        euler = 0
        factorial = 1
        for n in range(maxterms):
            eulersteps.append(euler)
            euler += 1/factorial
            factorial = factorial*(n+1)
            if 1/(factorial*euler) < tolerance:
                break

In [3]: print(euler)
        2.7182818282861687

In [4]: import matplotlib.pyplot as plt
        %matplotlib inline

In [5]: plt.plot(eulersteps);
```

The output of the fifth cell is a line plot showing the convergence of Euler's constant. The x-axis represents the step number (0 to 150), and the y-axis represents the value of the constant (0.0 to 2.5). The plot shows a curve that starts at (0,0) and rises steeply, then levels off to a horizontal line at approximately 2.718.

Supports different languages: **Julia**, **Python**, **R**.

Interface runs in your webbrowser

Computation can run elsewhere.

- Notebook consists of cells which can have code or text and output.
- You can jump around in the notebook, and execute different cells:
- You can rerun parts of your code.
- You can add text portions, making your notebook more like an article.

2

Large Scale Research Computing = SciNet

Large compute = shared compute

- **Demand for computing and storage** beyond the desktop comes from all fields of research.
- Better use of research money is to have **shared national resources** that are always busy.
- In general, that means large **computer clusters** doing **batch processing** using the **command line** and **non-interactive applications**.
- In Canada: national resources coordinated by **Compute Canada** (→ **NDRIO**).

SciNet HPC Consortium

- A special department at UofT hosting:
 - ▶ **Niagara** 80,000 supercomputer
 - ▶ **Mist** 200+ GPU cluster (with SOSICIP)
- With scientific computing specialists.
- Training+education: <https://scinet.courses>
- User support: support@scinet.utoronto.ca



www.scinethpc.ca/getting-a-scinet-account

- Get a Compute Canada account, PI first (ccdb.computecanada.ca).
- Opt-in to Niagara.
- Read docs.scinet.utoronto.ca/index.php/Niagara_Quickstart.
- Attend “Intro to Niagara” session.

FREE

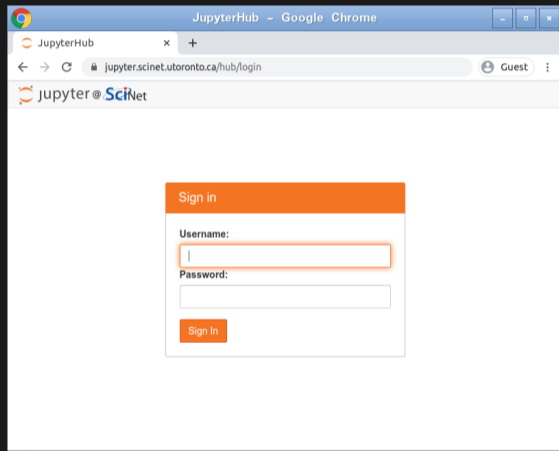
3

Jupyter Hub = Easy Interactive Access to Niagara

SciNet's Jupyter Hub

<https://jupyter.scinet.utoronto.ca>

- Log in with your Compute Canada username and password.
- No need to install your own jupyterhub and setup port forwarding.
- Shared resource with other researchers.



SciNet's Jupyter Hub Features

<https://jupyter.scinet.utoronto.ca>

- Work with your data on Niagara.
- Work with your virtual environments on Niagara.
- Share notebooks with collaborators.
- Python 3.8.3, R 3.4.3 and 4.0.2, Julia 1.5.2.
- Single-click to Jupyter Lab.
- Software modules can be loaded.
- Some limits: 16GB RAM, 6 hours of CPU time.

For teaching?

- UofT has a **separate JupyterHub** for teaching, <https://jupyter.utoronto.ca>.
- No access to SciNet data, but can login with UTORID: no need for students to get extra accounts.
- Also has a desktop and RStudio.
- Each student runs in a virtual machine isolated from all others.

Need a teaching cluster?

If, instead of Jupyterhub, you actually want to teach using a cluster environment in your course, SciNet has a **Teach cluster** that you can use as well.

SciNet JupyterHub Links

Get an account:

<https://www.scinethpc.ca/getting-a-scinet-account>

JupyterHub for research:

<https://jupyter.scinet.utoronto.ca>

Documentation:

<https://docs.scinet.utoronto.ca>

Training:

<https://scinet.courses>

Question about anything SciNet: support@scinet.utoronto.ca

