

Python for HPC

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github.com/zonca/python_hpc_tutorial

Code of Conduct

XSEDE has an external code of conduct for XSEDE sponsored events which represents XSEDE's commitment to providing an inclusive and harassment-free environment in all interactions regardless of gender, sexual orientation, disability, physical appearance, race, or religion. The code of conduct extends to all XSEDE-sponsored events, services, and interactions.

Code of Conduct: <https://www.xsede.org/codeofconduct>

Contact:

- Event organizer: Mary Thomas (mthomas@sdsc.edu)
- XSEDE ombudspersons:
 - Linda Akli, Southeastern Universities Research Association (akli@sura.org)
 - Lizanne Destefano, Georgia Tech (lizanne.destefano@ceismc.gatech.edu)
 - Ken Hackworth, Pittsburgh Supercomputing Center (hackworth@psc.edu)
 - Bryan Snead, Texas Advanced Computing Center (jbsnead@tacc.utexas.edu)

Jupyter Notebook

Data exploration in your browser

What is the notebook?

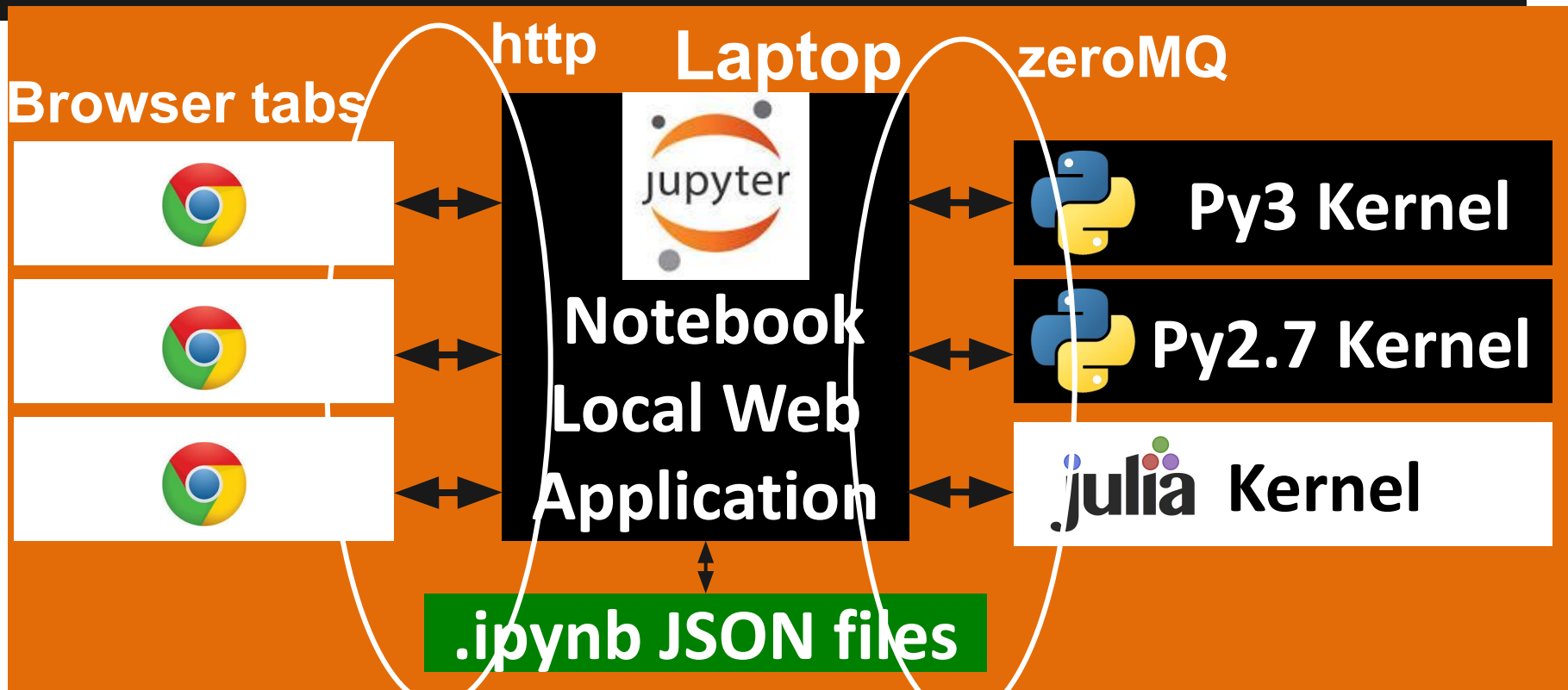
- Browser based interactive console
- Supports multiple sessions in browser tabs
- Each session has a Kernel executing computation
- Saved in JSON format

Notebooks for LIGO

Interactive data analysis of gravitational waves from black holes merging:

http://beta.mybinder.org/repo/losc-tutorial/LOS_C_Event_tutorial

Jupyter notebook local



Jupyter notebook remote

Laptop



https +
password

Server

Jupyter
Notebook
Web
Application



Py3 Kernel



Py2.7 Kernel



Julia Kernel

.ipynb JSON files

Clone workshop repository

ssh into comet with training account

```
git clone URL
```

URL is

```
https://github.com/zonca/python\_hpc\_tutorial
```


Launch notebook job

- `cd python_hpc_tutorial/`
- `sbatch notebook_singularity.slm`

connect with browser

Open browser on your laptop and connect to

```
cat jupyter-notebook*.out
```

New -> Notebook

```
!hostname
```

IPython notebook demo

- Python code
- Formatted text
- Equations
- Plots
- Cells execution, cells order
- Clear output

Why the notebook?

- Literate programming: code and explanation together
- Reproducible science: document easily every step
- Easy to share computations: send one single notebook instead of scripts/plots/.doc

ipynb documents

- JSON format
- includes plots in binary format
- easy to convert to .html/.pdf for sharing
- <http://nbviewer.ipython.org>
- Recently rendered automatically on Github

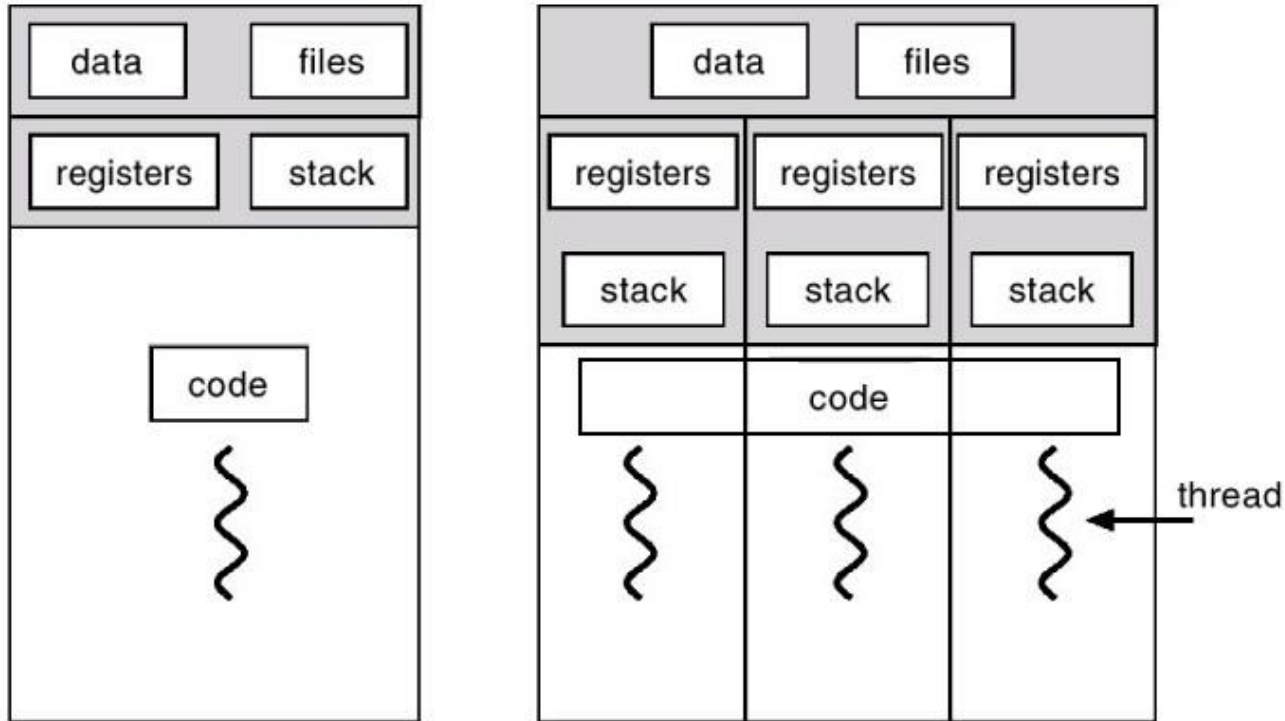
HPC: interactive notebooks

- Analyze large amount of data
- In-situ visualization
- Centralized Python stack
- Check long-running computations
- Prepare and submit batch jobs

Threads and processes



Threads vs processes



threaded

Out of order execution

Some people, when confronted with a problem, think "I know, I'll use regular expressions." Now they have two problems.



Davidlohr Bueso

@davidlohr

Follow



A programmer had a problem. He thought to himself, "I know, I'll solve it with threads!".
has Now problems. two he

2:16 PM - 8 Jan 2013

4,637 Retweets 1,396 Likes



Numba

Run code on GPU with Python

JIT compiler for Python

- based on LLVM (compiler infrastructure behind clang, Apple's C++ compiler)
- turns Python code into machine code
- on-the-fly