Python for HPC

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Jupyter Notebook

Data exploration in your browser

What is the notebook?

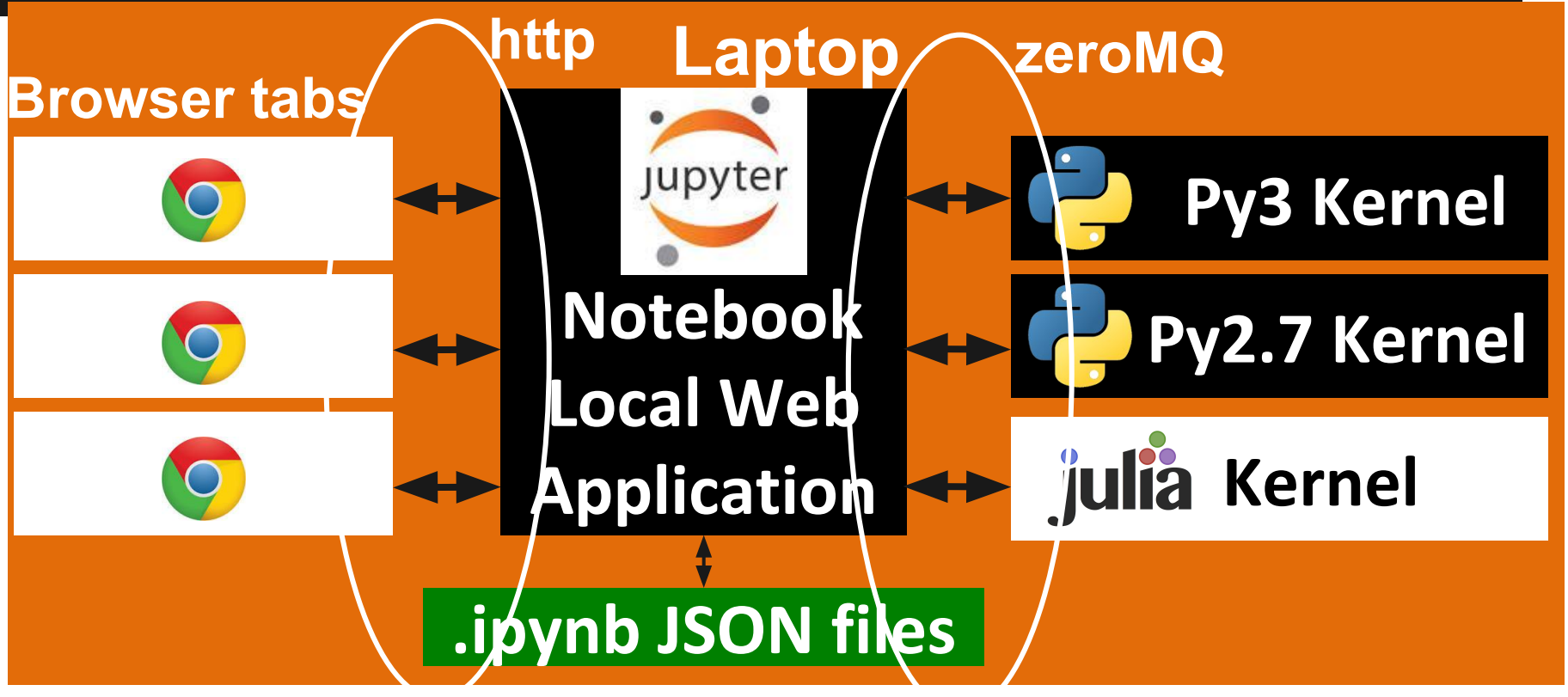
- Browser based interactive console
- Supports multiple sessions in browser tabs
- Each session has a Kernel executing computation
- Saved in JSON format

Notebooks for LIGO

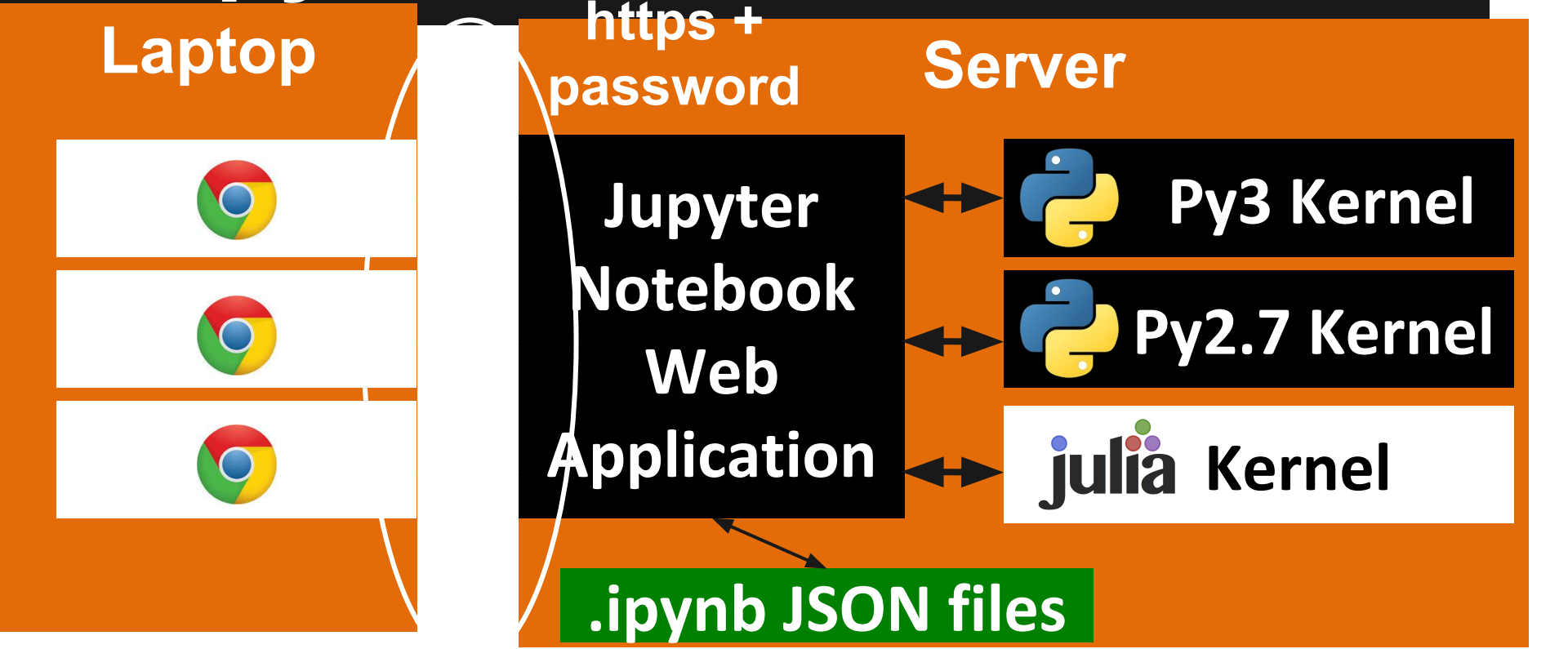
Interactive data analysis of gravitational waves from black holes merging:

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

Jupyter notebook local



Jupyter notebook remote



Clone workshop repository

ssh into comet with training account

`git clone URL`

URL is https://github.com/sdsc/sdsc-summer-institute-2018

Launch notebook job

- cd hpc0_python_hpc/
- sbatch notebook_singularity.cmd

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

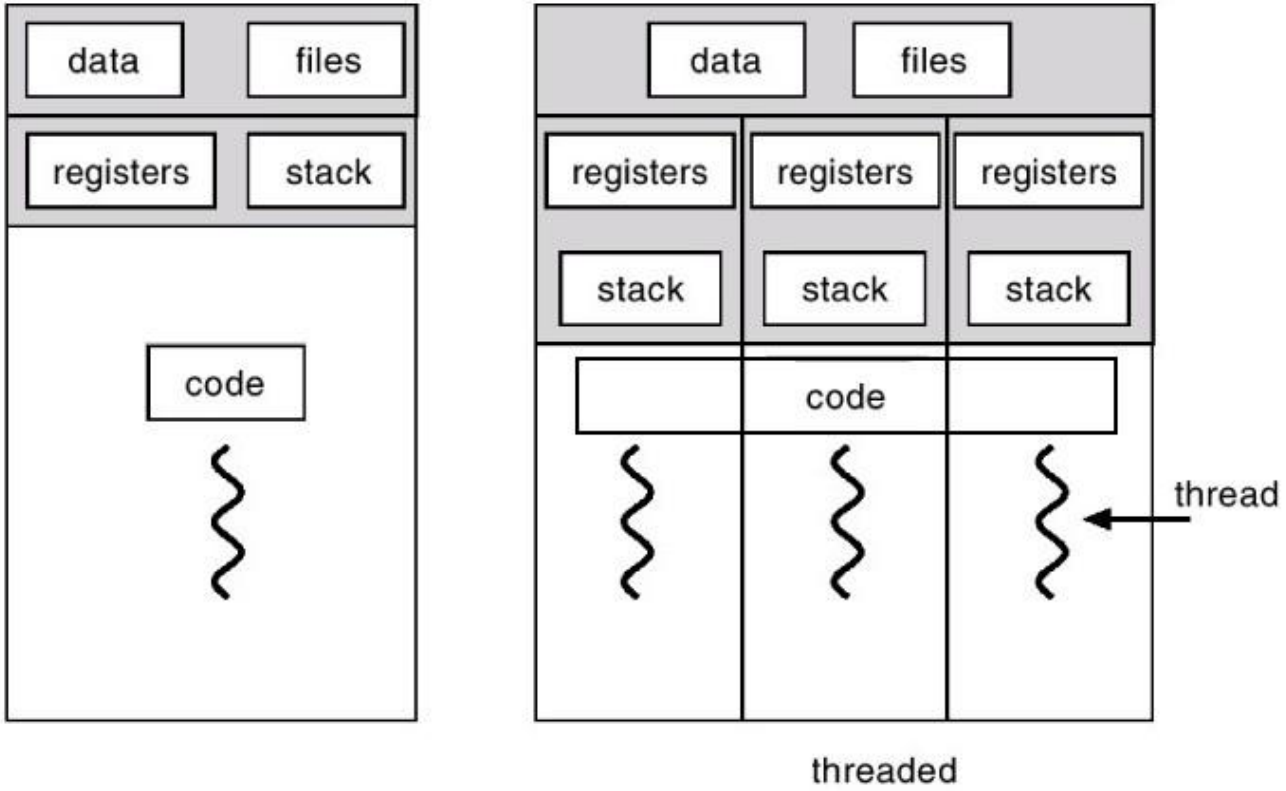
- JSON format
- includes plots in binary format
- easy to convert to .html/.pdf for sharing
- http://nbviewer.ipython.org
- Recently rendered automatically on Github

HPC: interactive notebooks

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

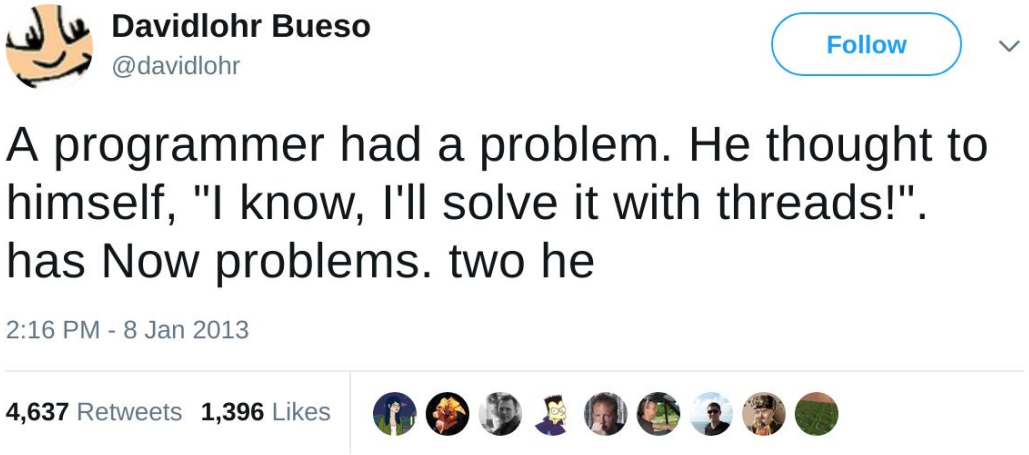
Threads and processes

Threads vs processes



Out of order execution

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



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

PyTrilinos

Distributed linear algebra with Python

Distributed linear algebra

Large complete C++ packages with Python support:

- PETSC, petsc4py
- Trilinos, PyTrilinos

Both use C++ for MPI communication and LAPACK/BLAS for local computing

Both subclass numpy arrays

PyTrilinos example

See pytrilinos.ipynb