SDSC Summer Institute 2022

Title: Python for HPC

Instructor: Mahidhar Tatineni

Date: 09:45AM-12:00 (PT), August 3, 2022

Slack support channel: main-room

Slack general support: help-desk

Outline

- Introduction to Jupyter notebooks and JupyterLab
- Single-node Python code optimization with numba
- Dask tutorial: overlap functions, introduction to dask array, distributed scheduler
- Dask array in-depth tutorial for multi-core, out-of-core, multi-node computing

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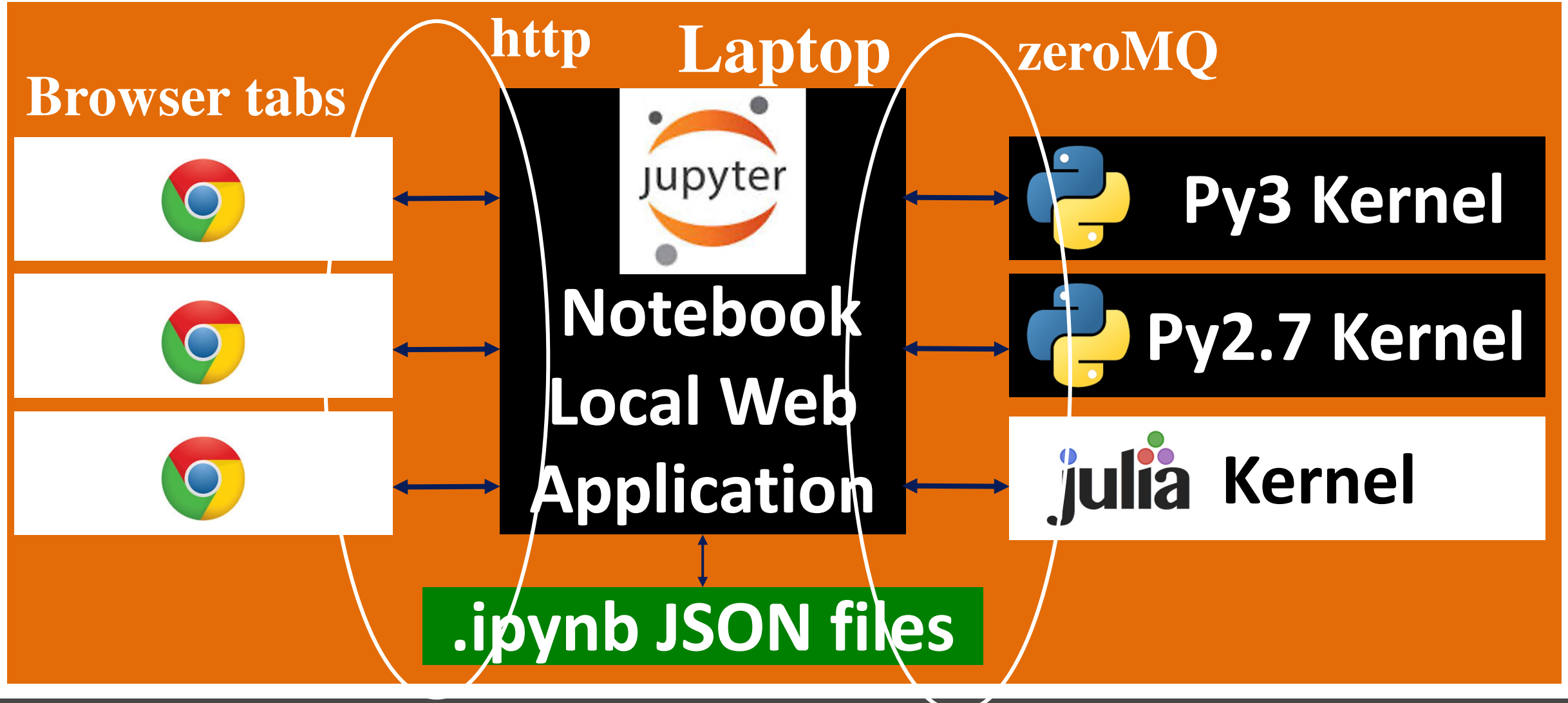
Overview of Jupyter notebooks and JupyterLab

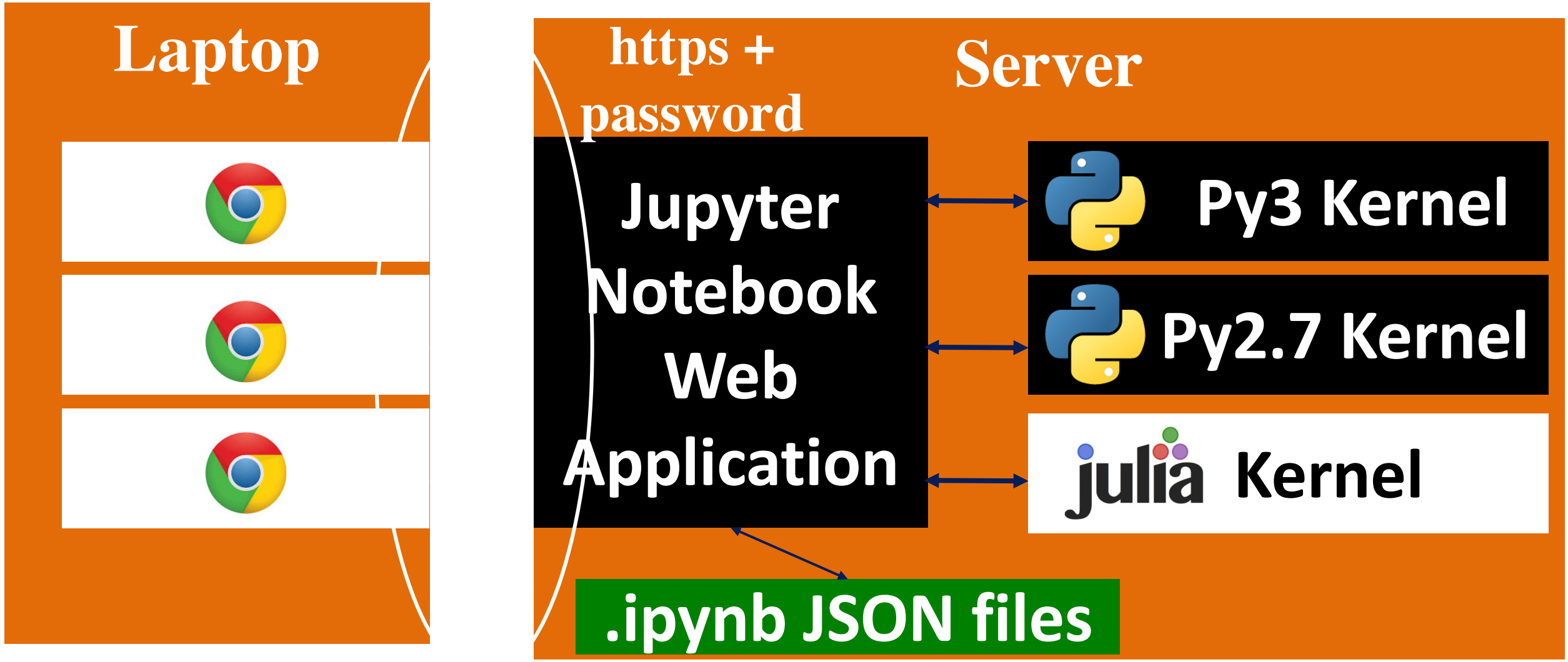
- Browser based interactive console
- Supports multiple sessions in browser tabs
- Each session has a Kernel executing computation
- Saved in JSON format
- LIGO notebook examples for interactive data analysis of gravitational waves from black holes merging:

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

Jupyter notebook local



Jupyter notebook remote



Clone workshop repository

ssh into Expanse with training account

git clone https://github.com/sdsc/sdsc-summer-institute-2022
cd sdsc-summer-institute-2022

Launch notebook job

- Change to python HPC directory and launch job:

  ```
  cd  4.2a_python_for_hpc
  bash  launch_jupyter_singularity.sh
  ```

  (note: this is using galyleo)
- Check your job status with:

  ```
  squeue -u $USER
  ```
- Open browser on your laptop and connect to URL

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Numba: JIT compiler for Python

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

Synchronization with content on YouTube (Andrea Zonca's Channel)

- Terminal on Expanse with training account
- Browser window or phone with Youtube videos: https://bit.ly/pythonhpc2021 (also linked from repo)
- #main-room Slack open for questions
- Start to watch the first video (Introduction) [you can speed up to 1.25x]
- Reconvene for questions in 15 min

Numba

- Watch numba 0 : basics, 10 minutes

https://www.youtube.com/watch?v=-aUkLZmrasA

- Watch numba 1 : numpy, 10 minutes

https://www.youtube.com/watch?v=ET372Rq1i8I

Numba

- Watch numba 2: threads, 10 minutes

  https://www.youtube.com/watch?v=Tfaoy6x2CJg

- Watch numba 3: groupby pixels, 10 minutes

  https://www.youtube.com/watch?v=4VxHd2qwkro

Dask Tutorial

- Dask 1 delayed: 15 minutes

  https://www.youtube.com/watch?v=oaUwrw_WDAI

- Break: 5 minutes

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Dask Tutorial

- **Dask 3 Arrays: 20 minutes**

  https://www.youtube.com/watch?v=5hH--5EuBek

- **Dask 5 Distributed: 20 minutes**

  https://www.youtube.com/watch?v=NEHxLjMed7I

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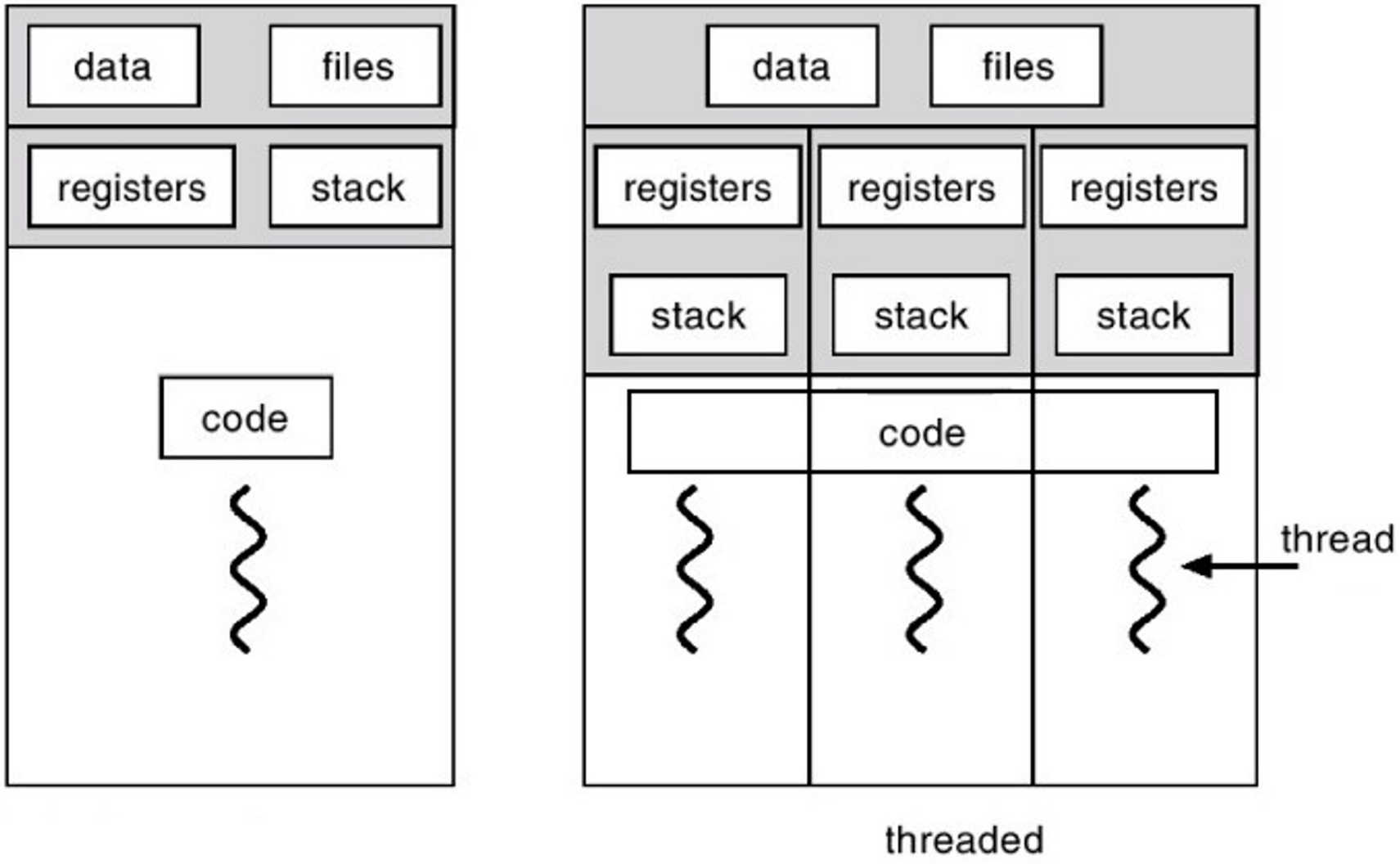
Threads vs processes



Dask array

- Watch dask array 0-2: 15 minutes

https://www.youtube.com/watch?v=2__dbnm6nCk

Note: We are not doing the multi-node example (setup needed) but the video is available.