Easy Interactive Supercomputing on Maxwell

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Scientific perspective

1. Open Laptop
2. ...
3. ...
4. ...
n. Do Science

Scientific perspective

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We do not care & it should be easy!

Easy | Interactive | Supercomputing on Maxwell

Easy Interactive Supercomputing on Maxwell

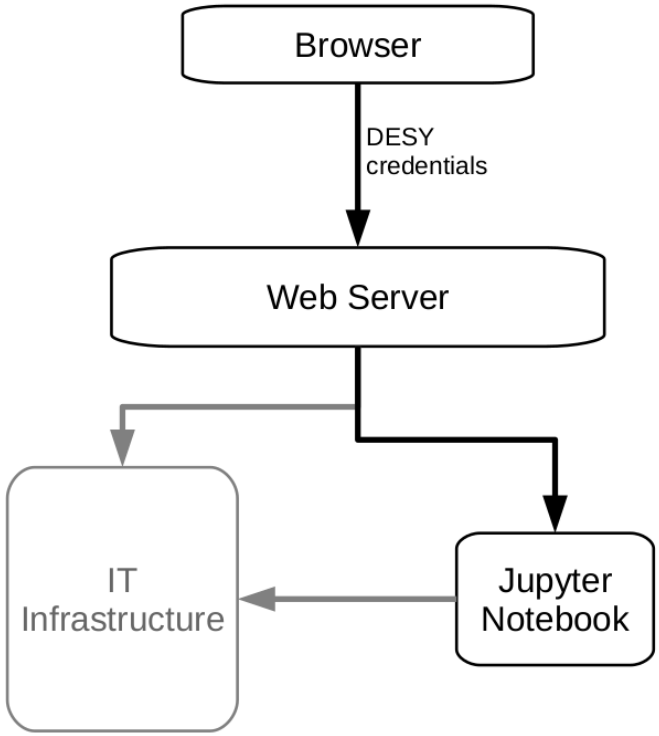
- Slurm scheduler for batch processing [1]
- Slurm submission nodes:
  - max-fsc | max-fsc
  - max-display
  - max-jhub

```
# simple job which prints hostname
[@max-wgs ~]$ cat hostname.sh
#!/bin/bash
#SBATCH --partition=maxwell
#SBATCH --time=00:10:00                                  # Maxi
#SBATCH --nodes=1                                        # Numb
##### note: from SLurm news file 17.11.0rc1:
##### Change --workdir in sbatch to be --chdir as in all
#####SBATCH --workdir   /home/mmuster/slurm/output    # 
#SBATCH --chdir   /home/mmuster/slurm/output      # dire
#SBATCH --job-name  hostname
#SBATCH --output    hostname-%N-%j.out            # File
#SBATCH --error     hostname-%N-%j.err            # File
#SBATCH --mail-type END                           # Type
#SBATCH --mail-user max.muster@desy.de            # Emai

/bin/hostname

# submit to batch queue for one node with one task
# requesting 10 mins of wall time
[@max-wgs ~]$ sbatch hostname.sh
Submitted batch job 2163

[@max-wgs ~]$ ls
hostname.sh  slurm-2163.out

[@max-wgs ~]$ cat slurm-2163.out
max-wn004.desy.de
```

Easy Interactive Supercomputing on Maxwell

- IPython Console
- Jupyter Notebooks
- JupyterLab

- JupyterHub @DESY [2]



Easy Interactive Supercomputing on Maxwell

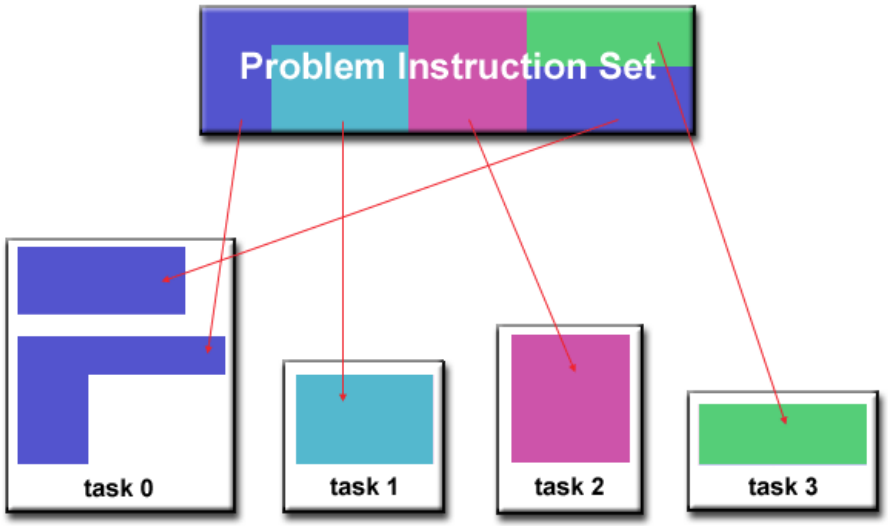
- Anaconda: venvs
  - requirements.txt

You shall not

- import mpi4py

Use external framework

- Dask for parallel computing.
  - Dynamic task scheduling
  - "Big Data" collections for distributed environments or larger-than-memory



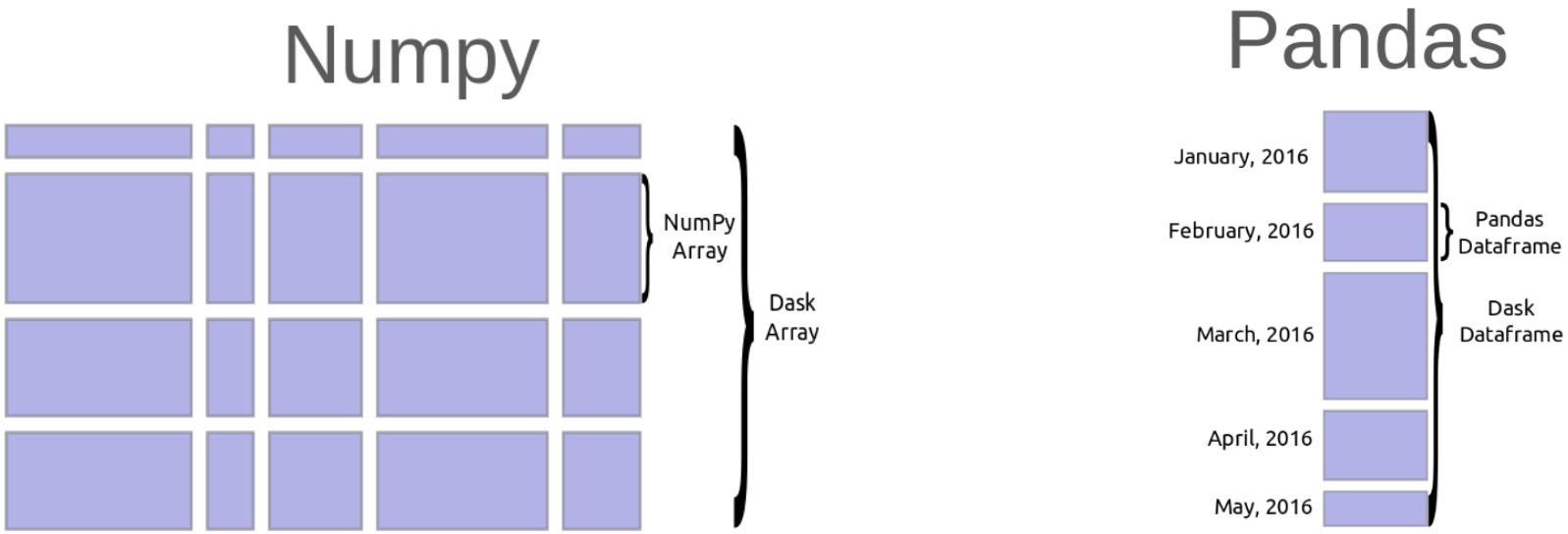
computing.llnl.gov

Demo

Demo #1

- DESY's JupyterHub
- *dask.delayed* as way to parallelize existing code
- fetch via:
  git clone `https://github.com/chrispassow/dask_demo.git`

dask.array & dask.dataframe



https://dask.org/

- for distributed environments or larger-than-memory
- most of *Numpy* & *Pandas* methods are implemented

Demo

Demo #2

- using a single node on Maxwell via *sbatch*
- compare *numpy.array* and *dask.array*

Demo

Demo #3

- using multpile nodes on Maxwell interactivly via *dask_jobqueue*

Terminate Idle Slurm Jobs

Danger Zone

"With great power there must also come – great responsibility!" [3]

Below is an (automatically generated) list of partitions and the limits applying

Partition	# of nodes	Nodes/Job	Max Number of Jobs	Default Time	Maximum Time	Allowed groups
ps	35	1	5	1:00:00	14-00:00:00	max-ps2-users
psx	16	1	5	1:00:00	7-00:00:00	max-psx2-users

Emergancy Commands [4]

scancel -u your_uid

Summary and Outlook

Current situation

- manual work is lengthy and prone to error
- Conda envs already simplify
- Slurm batch procession

The other side of the fence

- Frameworks to speed up analytics or scale to large data
- Dask as a state-of-the-art solution
- Jupyter notebooks for interactive data exploration
- JupyterHub as easy to use gateway

Great responsibility

Be careful about the resources you allocate.

References

[1] https://confluence.desy.de/display/IS/Running+Jobs+on+Maxwell

[2] https://confluence.desy.de/display/IS/JupyterHub+on+Maxwell

[3] Uncle Ben, Amazing Fantasy #15, Marvel Comics

[4] https://www.rc.fas.harvard.edu/resources/documentation/convenient-slurm-commands/