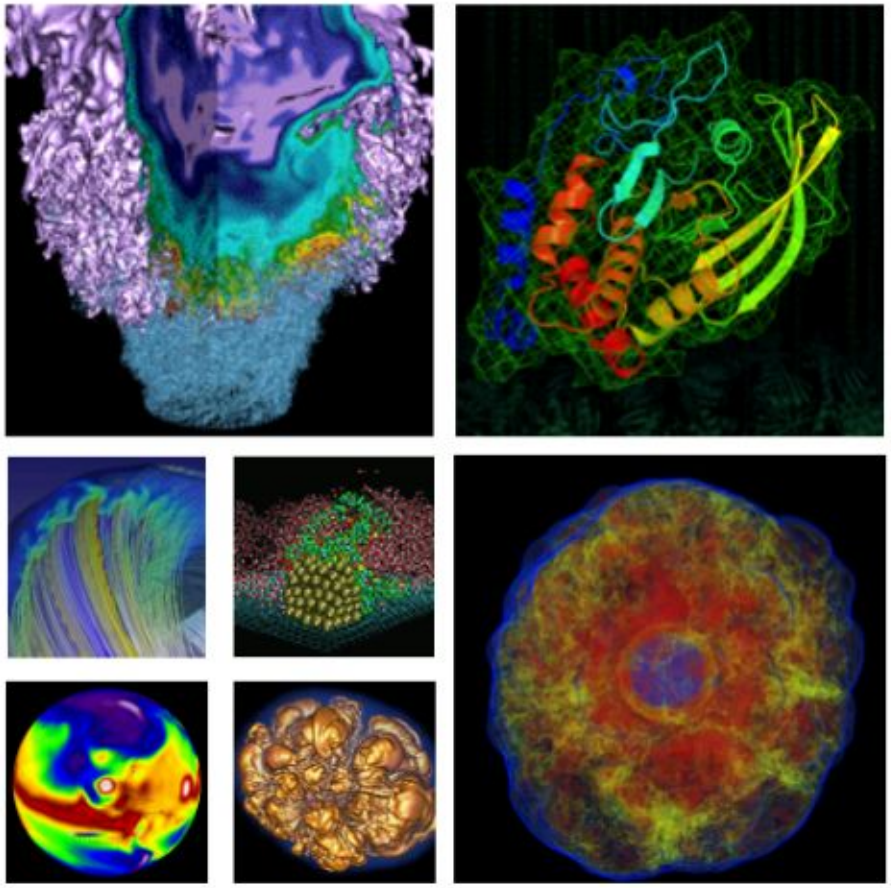
Toward Interactive Supercomputing at NERSC with Jupyter



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May 9 2017

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Data Science [Wikipedia Definition]

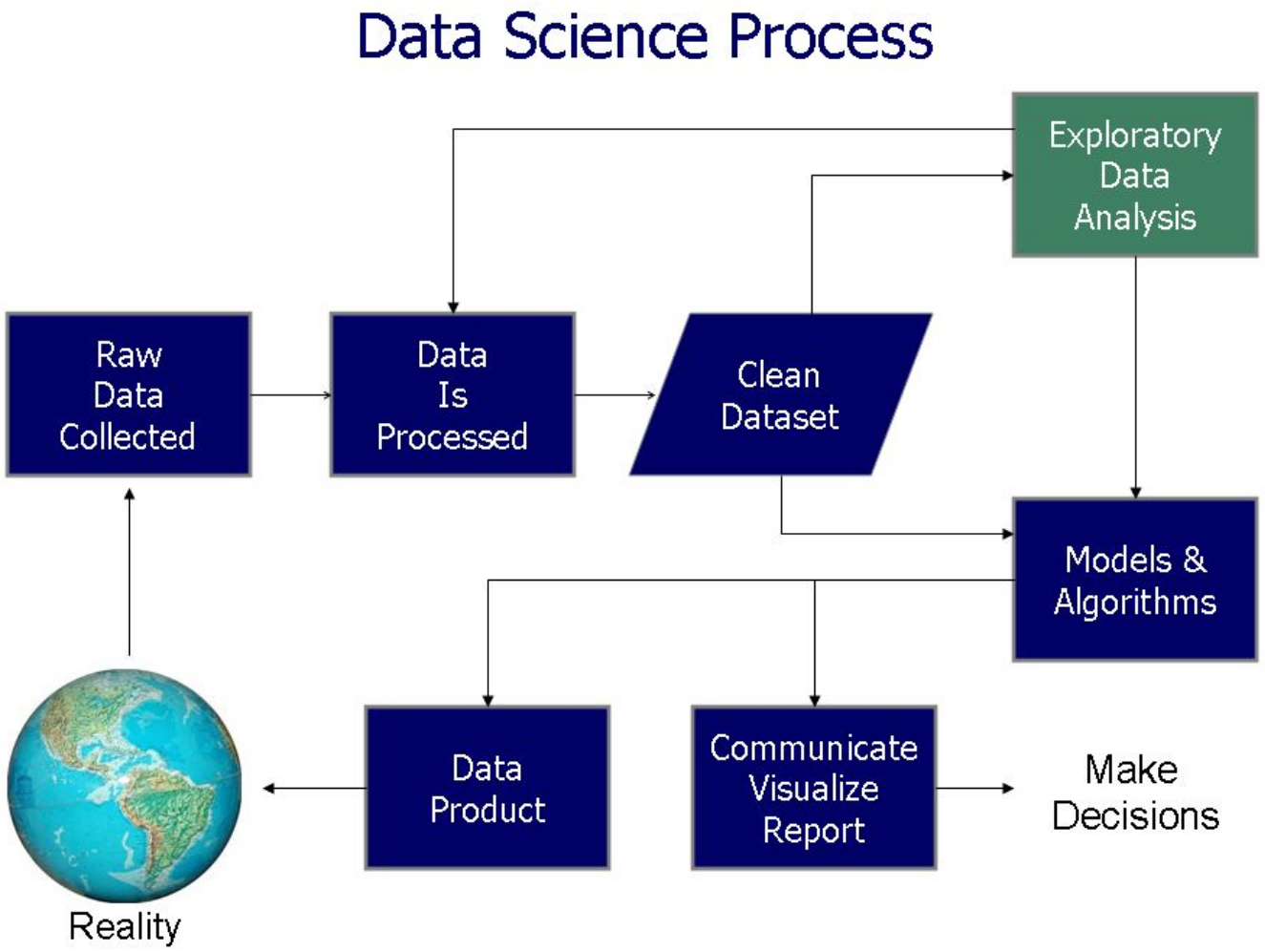
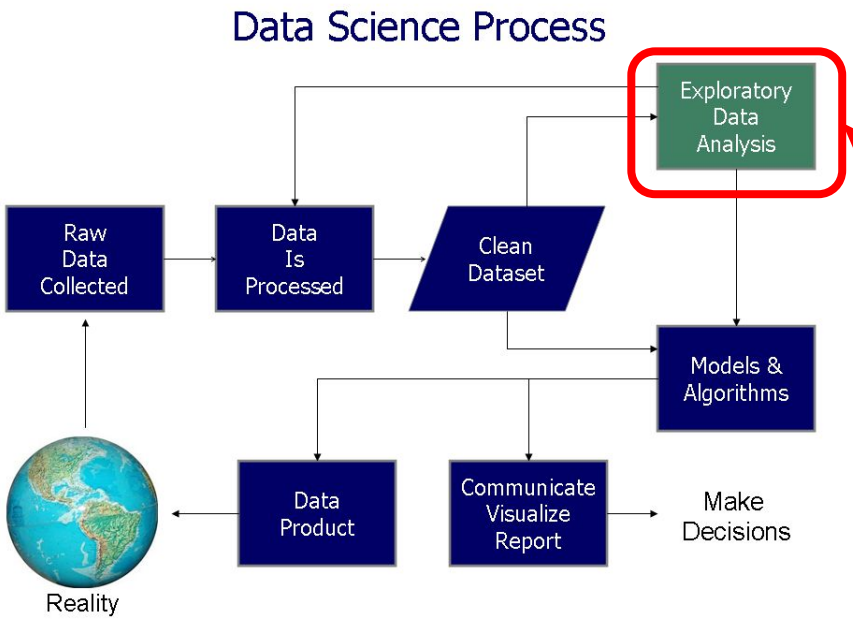
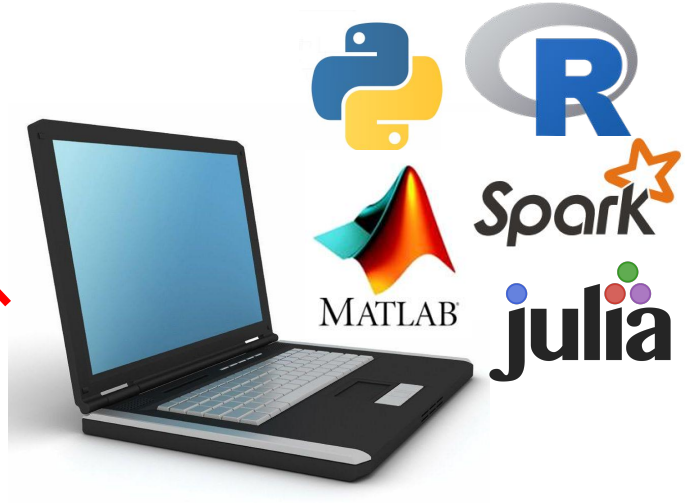


Diagram courtesy of "Farcaster" at English Wikipedia

Data Science [Wikipedia Definition]

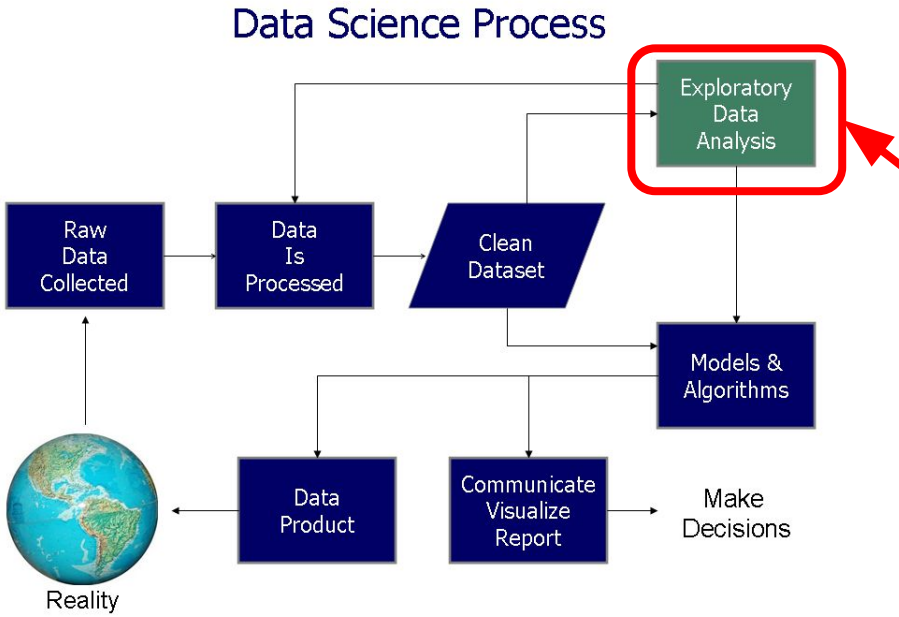


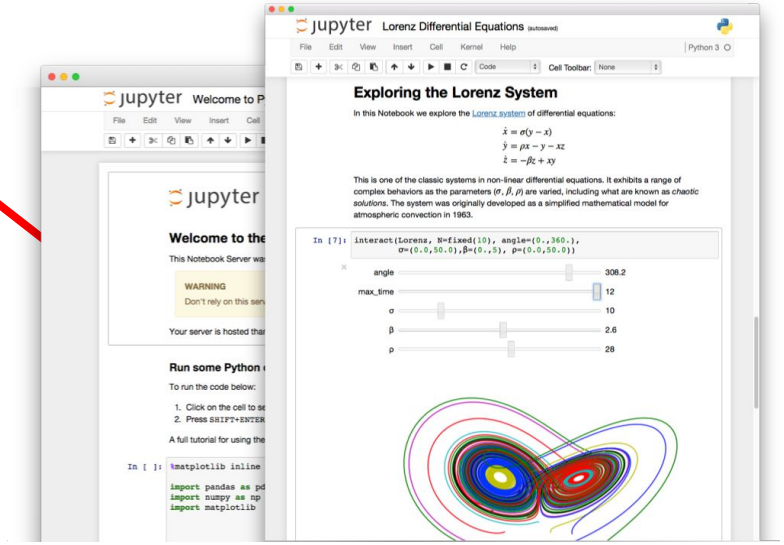


- **Get manageable chunk of data and copy it to your laptop/workstation**
- **Write code/scripts, make diagnostic plots, construct and test models**
- **Loop is very short between thinking up a query and executing it on data**
  - ***Real-time testing of models that explain the data***
  - ***Real-time feedback in the form of plots and results***
  - ***… hard to keep it all organized and explain what you did***

Diagram courtesy of "Farcaster" at English Wikipedia

Enter IPython and Jupyter





- **IPython: Side project that grew into a data analytics phenomenon.**
- **IPython Notebooks: *Literate Computing, "Narratives"***
  - **Code and comments: Reproducibility, show your work!**
  - ***But wait there's more:* Rich text, plots, equations, widgets, etc.**
- **Jupyter: Language agnostic "notebook" part of IPython**

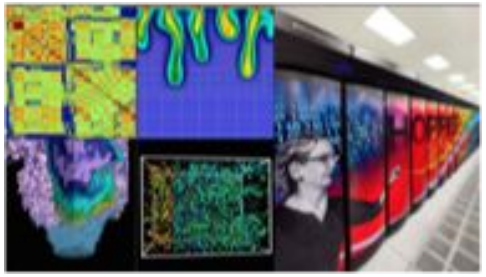
Why Jupyter@NERSC?

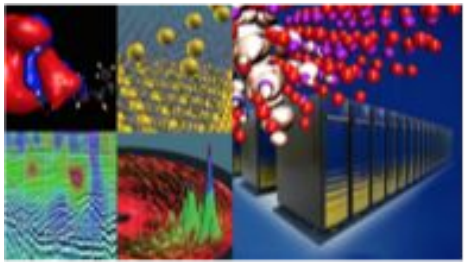
NERSC is the production HPC & Data Facility for Department of Energy Office of Science

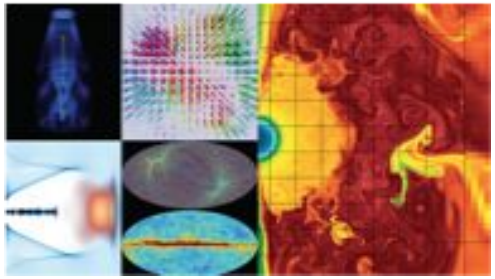
U.S. DEPARTMENT OF ENERGY | Office of Science

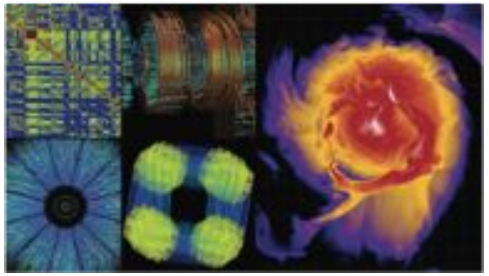
- Largest Federal sponsor of basic research in the physical sciences.
- Lead Federal agency supporting fundamental scientific research for our Nation's energy future.

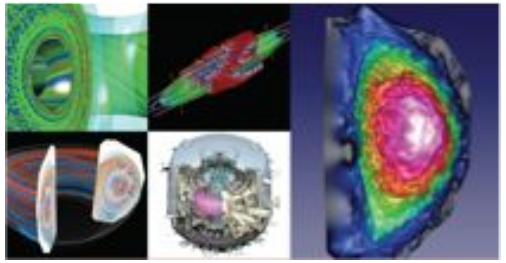

Bio Energy, Environment


Advanced Computing


Materials, Chemistry, Geophysics


High Energy Physics


Nuclear Sciences


Fusion, Plasma Physics

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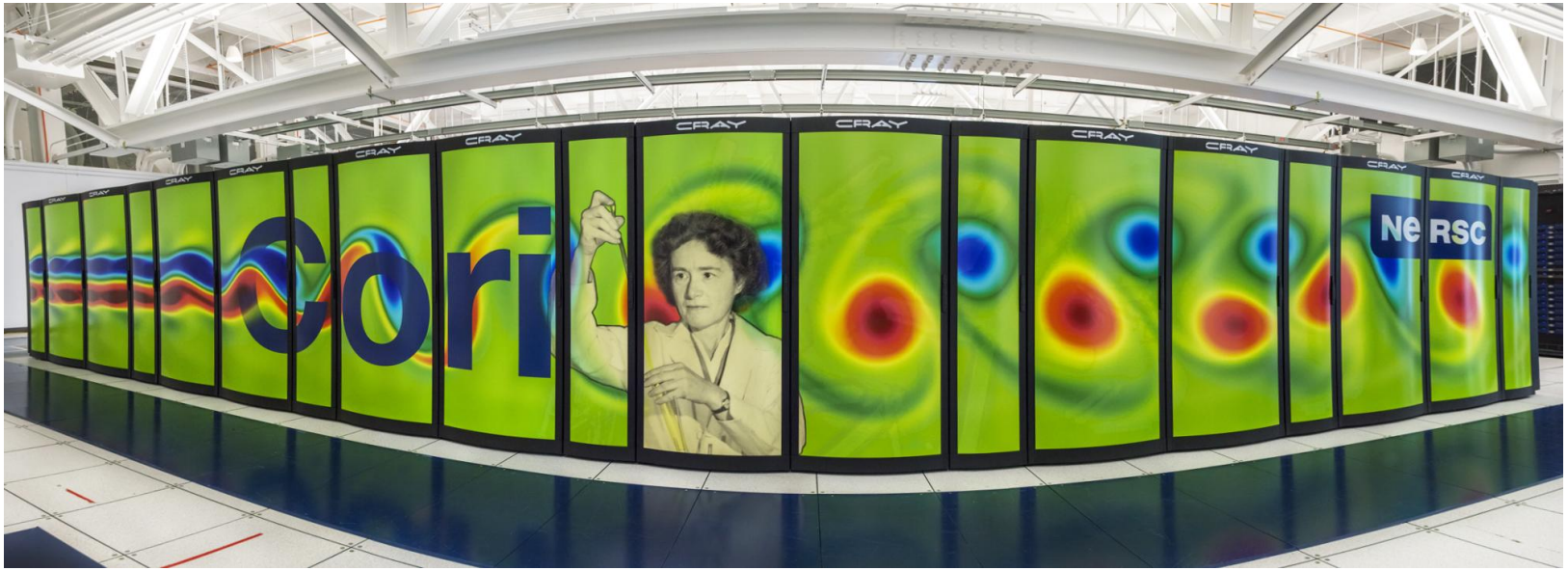
Cori: Friendly for "Data Users"



Gerty Cori: Biochemist and first American woman to win a Nobel Prize in science

- Two architectures in one system:
  - **Data** 2388 nodes 32-core Intel Xeon "Haswell" 128 GB DDR4
  - **HPC** 9688 nodes 68-core Intel Xeon Phi "KNL" 96 GB DDR4 + 16 GB MCDRAM
- Haswell login and **special-purpose large memory nodes** (512 & 768 GB)
- NVRAM Burst Buffer for IO acceleration
- Shared and real-time queues
- Shifter for containerized HPC

slurm workload manager

SHIFTER

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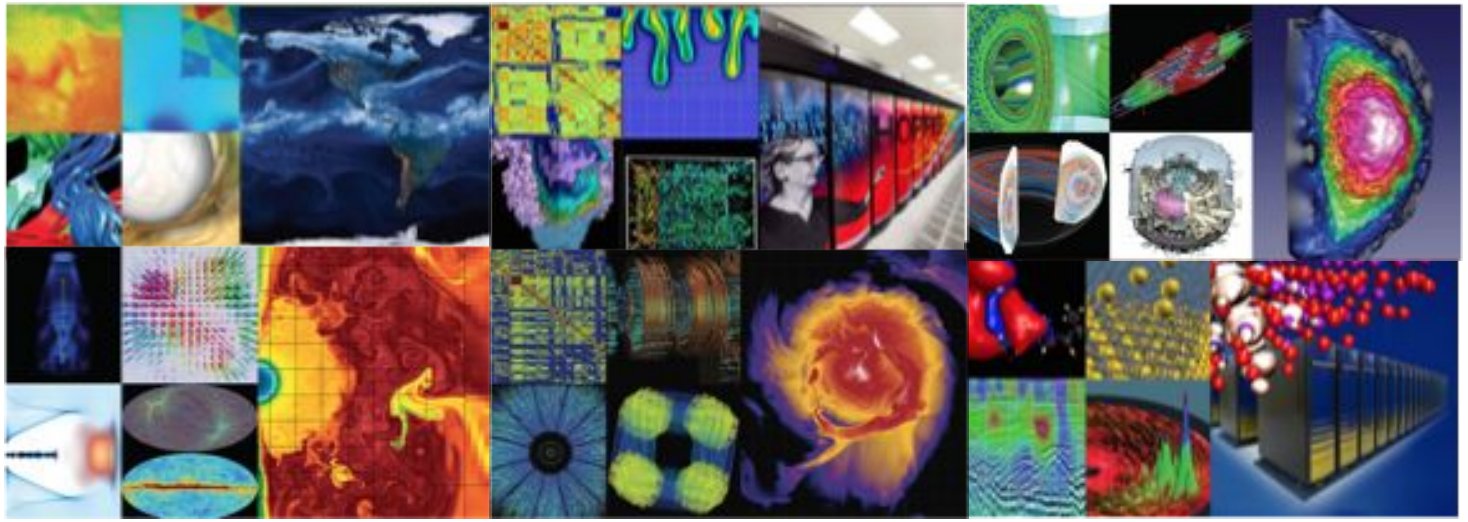
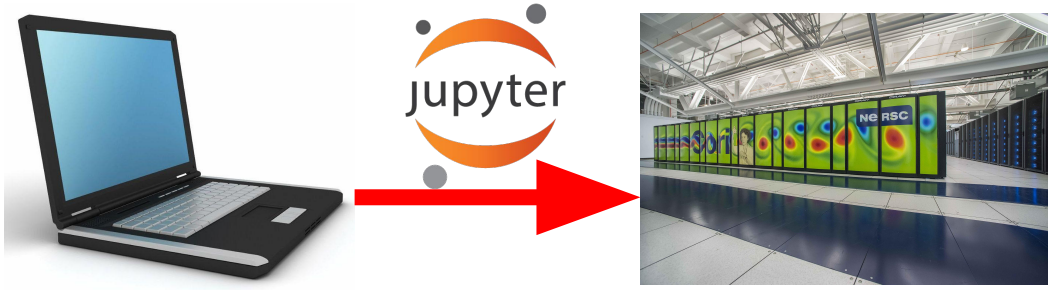
Why Jupyter@NERSC?



Deep Questions → **Expensive** Detector Technologies
Instruments/Facilities
High-bandwidth Networks
Simulations
→ **Insightful** Real time predictions?
Exploratory analysis?
Decision making?



Expose, Integrate NERSC Resources

submit, monitor, interact

Batch Queues
`sbatch squeue srun sacct`

query, analyze, visualize

NERSC Global File System
`/project` `$SCRATCH` `$HOME`

Database Servers
`mongodb01...` `scidb1...`

standardize, reproduce results

Software Environment Modules
`python/2.7-anaconda`
`python/3.5-anaconda`

Central Role of Python at NERSC

Python is the most popular language at NERSC used to:

- **Script workflows for both data analysis and simulations**
- **Perform exploratory data analysis**

Customizing Jupyter, Sane & Safe

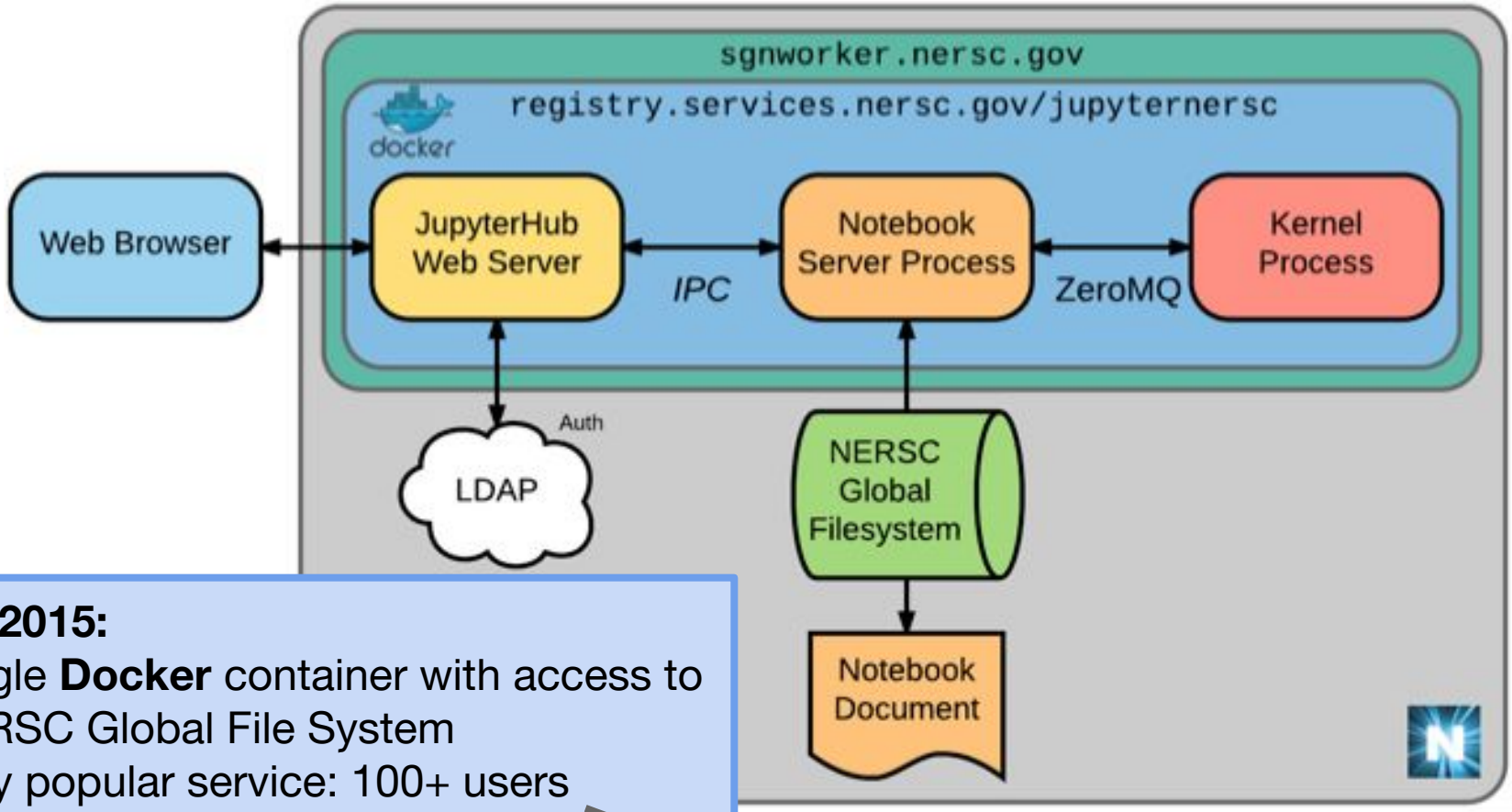
```
{
    "display_name": "HEP",
    "language": "python",
    "argv": [
        "/global/common/cori/software/python/2.7-anaconda/bin/python",
        "-m",
        "IPython.kernel",
        "-f",
        "{connection_file}"
    ],
    "env": {
        "LD_LIBRARY_PATH": "/usr/common/software/root/6.06.06/lib/root",
        "PYTHONPATH" : "/usr/common/software/root/6.06.06/lib/root"
    }
}
```

Example PyROOT Kernel Spec

- **Users customize their notebooks with libraries and APIs of their own design or from third parties.**
- **NERSC wants to offer Jupyter to users so they don't set it up themselves in an insecure way.**

Jupyter@NERSC
Evolution of Architecture

First Architecture: “Edge Service”

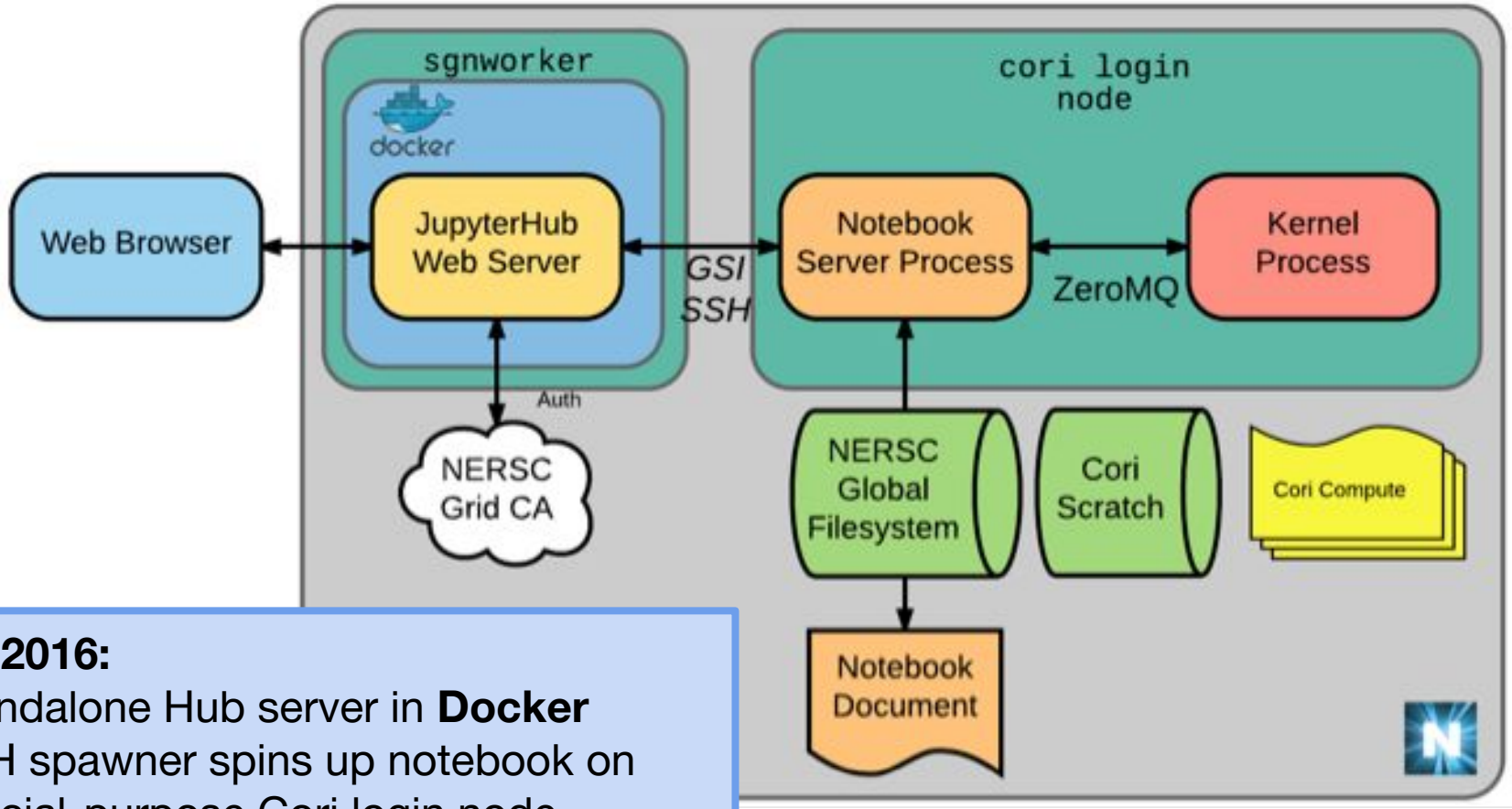


August 2015:

- Single **Docker** container with access to NERSC Global File System
- Very popular service: 100+ users
- Missing:
  - Access to Cori Lustre Scratch
  - Interactivity with Cori batch queues
  - Cori Python environment.

Projects:
OpenMSI
Metabolite Atlas
LUX

Second Architecture: Cori Login Node

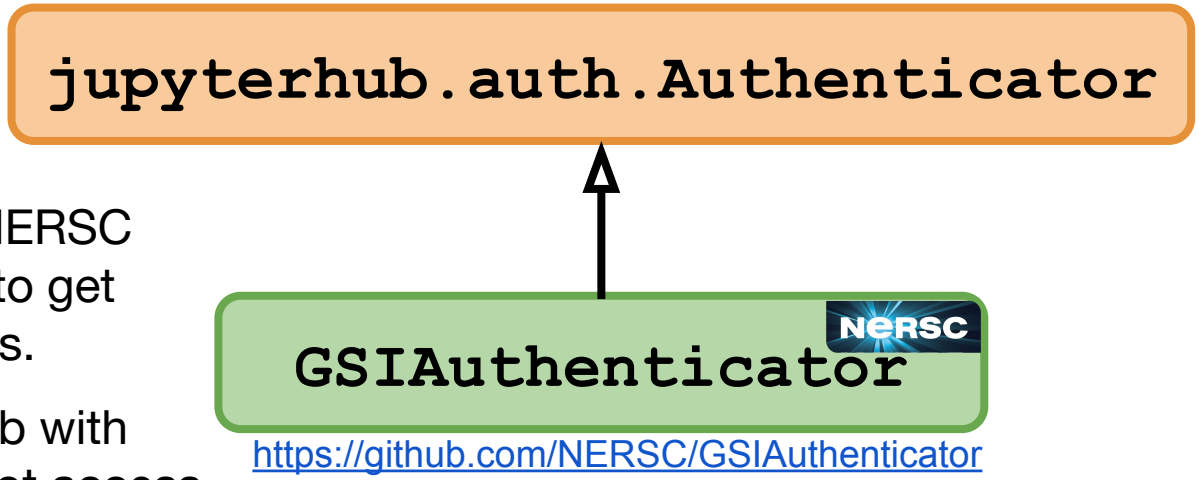


August 2016:

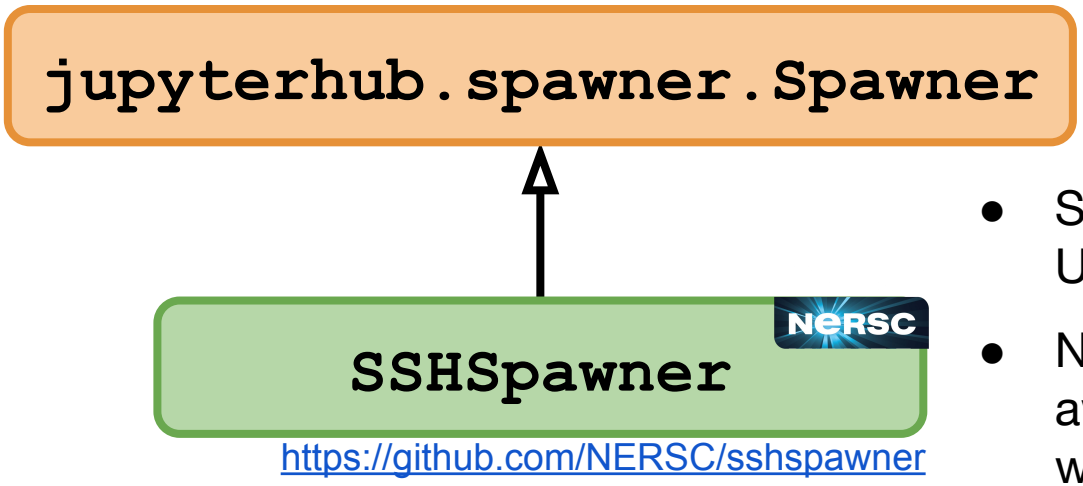
- Standalone Hub server in **Docker**
- SSH spawner spins up notebook on special-purpose Cori login node
- Access to Cori Lustre Scratch
- Same Python environment as Cori login
- Interactivity with batch queues

Projects:
LSST
Metabolite Atlas

Our Extensions to JupyterHub



- Use MyProxy to login to NERSC CA server with user/pass to get X509 certificate credentials.
- No need to run JupyterHub with additional privileges, or root access.



- SSH to Cori with user's credential. Uses GSISSH, but can use SSH.
- Notebook starts up, spawner goes away, Notebook communicates w/Hub, keep PID.

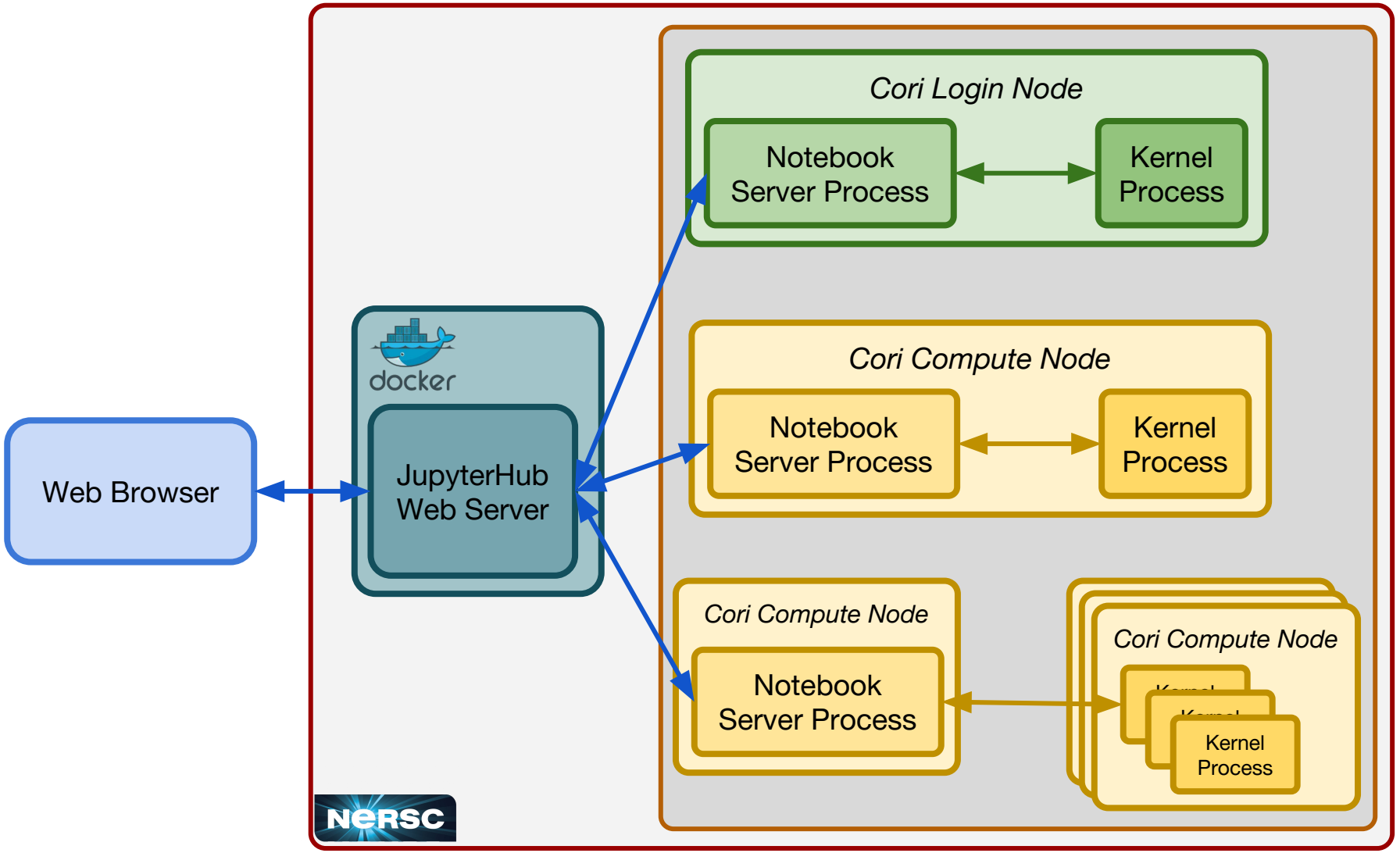
SLURM MAGIC

- Jupyter “%magic” commands:
  - Expose extra-language functionality
  - Outputs are first-class Notebook objects
- Developed wrappers around SLURM commands.
  https://github.com/NERSC/slurm-magic

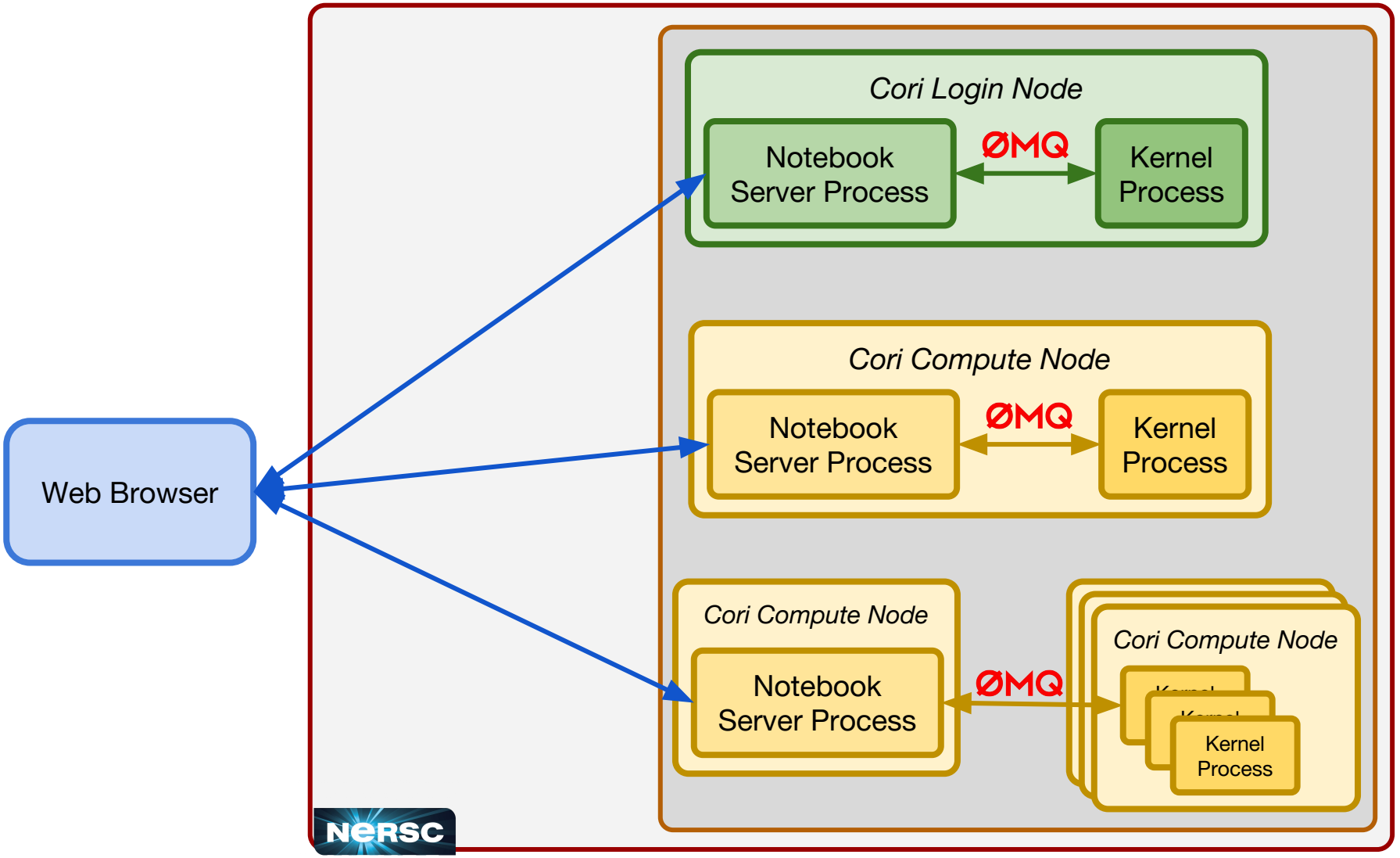
- `%squeue`
  ```
  %squeue -u rthomas
  ```
- `%sbatch`
  ```
  %sbatch script.sh
  ```
- `%%sbatch`
  ```
  %%sbatch -N 1 -p debug -t 30 -C haswell
  #!/bin/bash
  srun ...
  ```

LIVE DEMO: What Could Go Wrong!?

In Development: Cori Computes



Role of SDN after Authentication



The Ultimate Jupyter@NERSC

Software defined networking

Advertise IP of notebook server back to user.
Notebook on login node, kernel on compute.
Notebook+kernel on login, Spark job on computes.

Leveraging interactive QOS

Immediate access to compute up to four hours.

Shifter

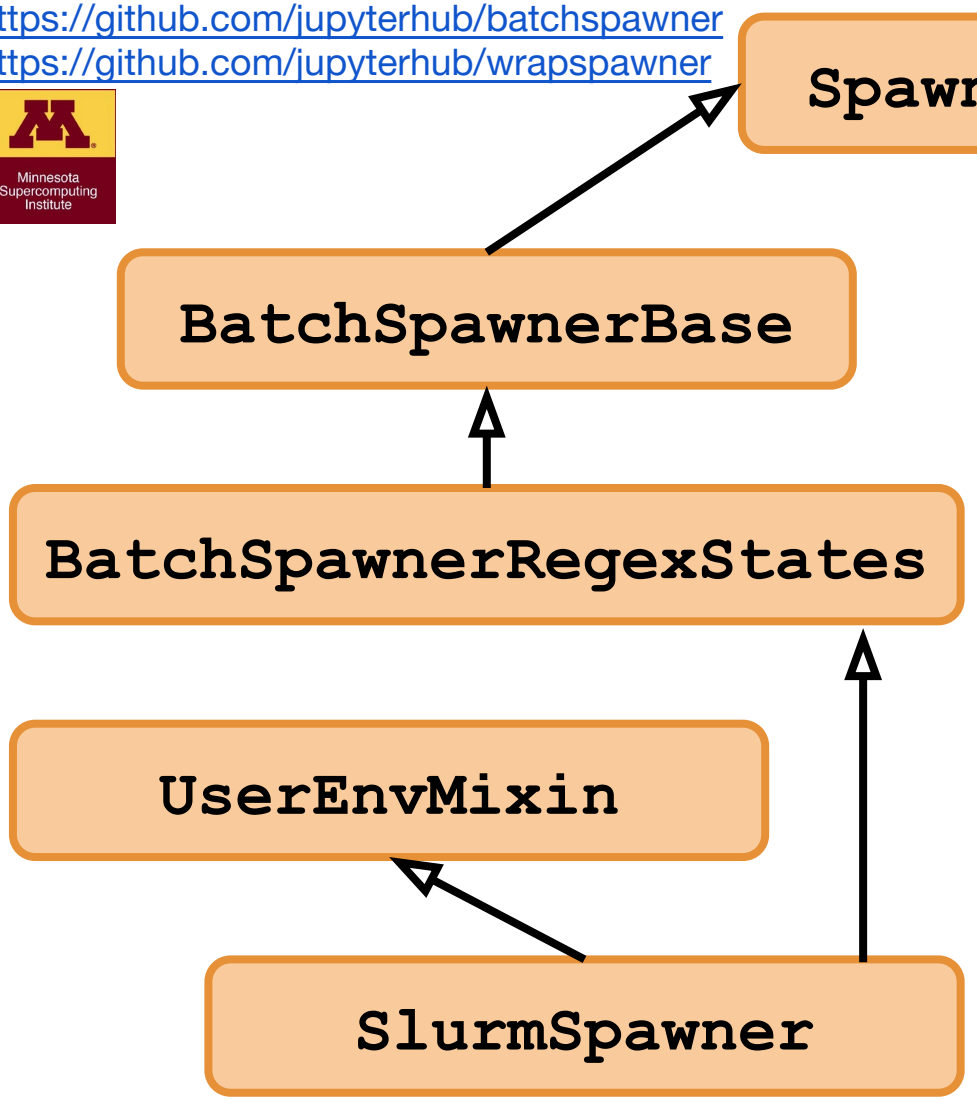
Customize notebook/kernel's environment.
Make larger-scale analytics apps actually start up.

Other possibilities

Notebook/scheduler on Haswell, kernels on KNL?

Customizations to Jupyter

https://github.com/jupyterhub/batchspawner
https://github.com/jupyterhub/wrapspawner



Customize Access

- Burst buffer for your job?
- Cori node or compute?

Customize NERSC UX

- "My Shifter images"
- "My favorite job templates"
- ...

Who is Responsible?

NERSC

- Data and Analytics Services Group
- Security and Networking Group
- Computational Systems Group
- Infrastructure Services Group

LBL Computational Research Division

- Usable Software Systems Group

Developer Community

- Jupyter Developers
- MSI, TACC, SDSC

Conclusion

- Jupyter is a powerful tool for exploratory data analysis that is increasingly popular with NERSC users.
- We anticipate that more users will be asking for tools like Jupyter, and for the data sets they analyze to be getting larger, requiring multi-node Jupyter jobs.
- We are working to find ways to scale Jupyter up to handle bigger data sets and interoperate with NERSC resources and environment.
- Thank you!

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