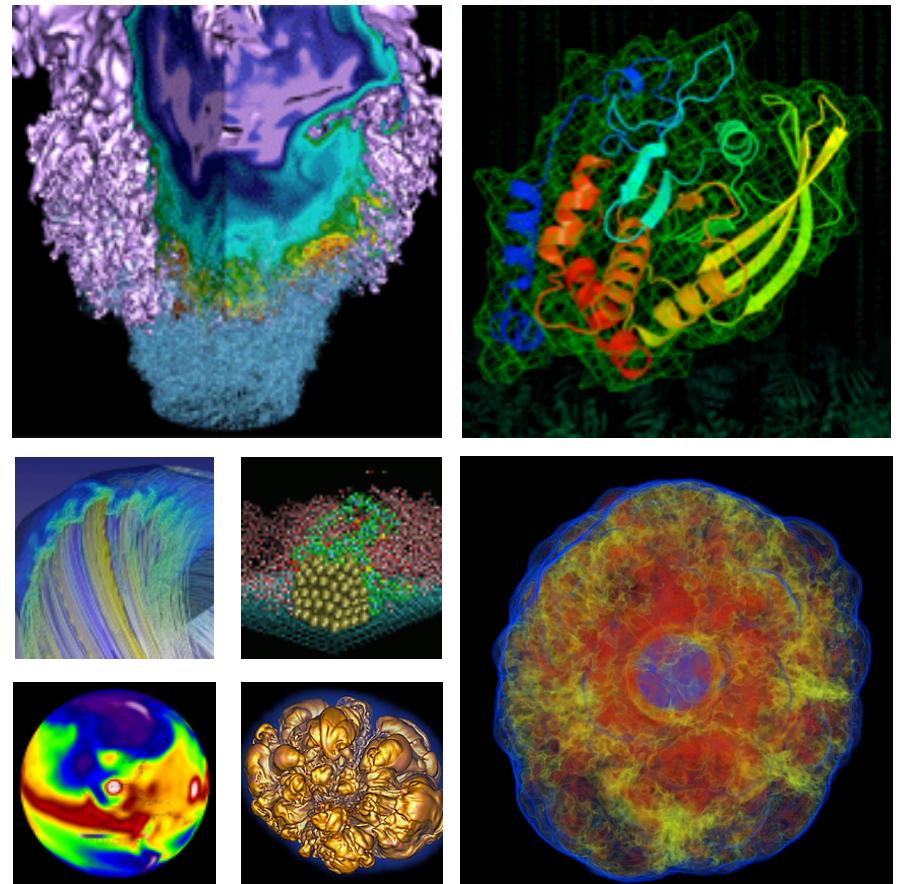


Driving Supercomputers With Jupyterhub: NERSC Experiences On Cori.



**Shreyas Cholia, Shane Canon,
Rollin Thomas**
NERSC Data & Analytics Services
Jupyterhub Mini-Workshop, July 22 2016

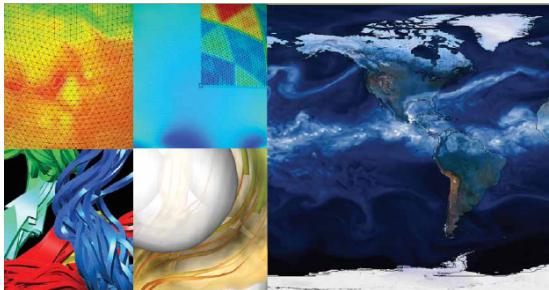
NERSC is the Production HPC & Data Facility for DOE Office of Science Research



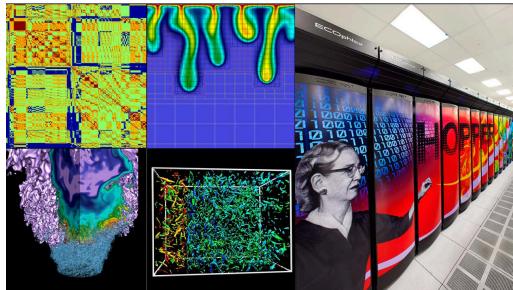
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ENERGY

Office of
Science

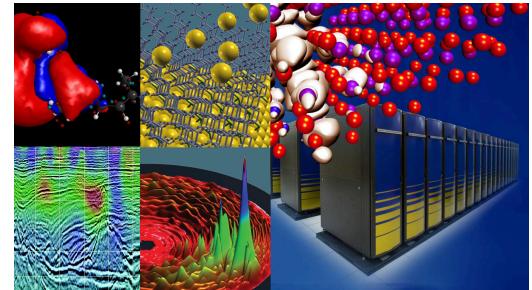
Largest funder of physical
science research in U.S.



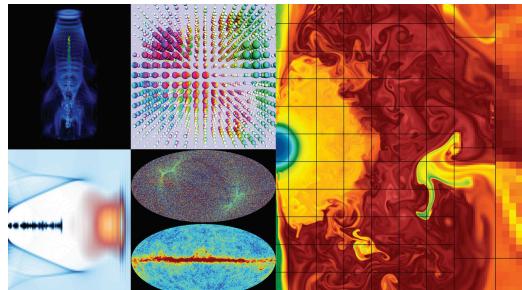
Bio Energy, Environment



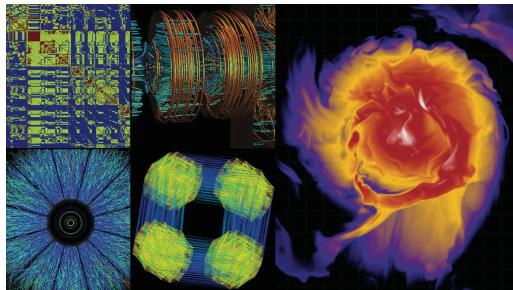
Computing



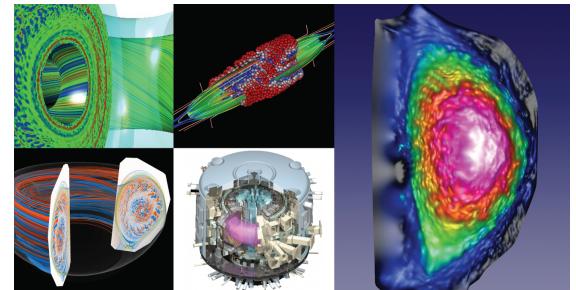
Materials, Chemistry,
Geophysics



Particle Physics,
Astrophysics



Nuclear Physics



Fusion Energy,
Plasma Physics



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The Cori System

Cori will transition HPC and data-centric workloads to energy efficient architectures

- Over 9,300 ‘Knights Landing’ compute nodes
 - Greater than 60 cores per node with four hardware threads each
 - High bandwidth on-package memory
- 1,600 ‘Haswell’ compute nodes as a data partition
- Big pool of large memory, login nodes for interactive analysis
- Aries Interconnect
- Lustre File system
 - 28 PB capacity, >700 GB/sec peak performance
- NVRAM “Burst Buffer” for I/O acceleration



Image source: Wikipedia

System named after Gerty Cori, Biochemist and first American woman to receive the Nobel prize in science.

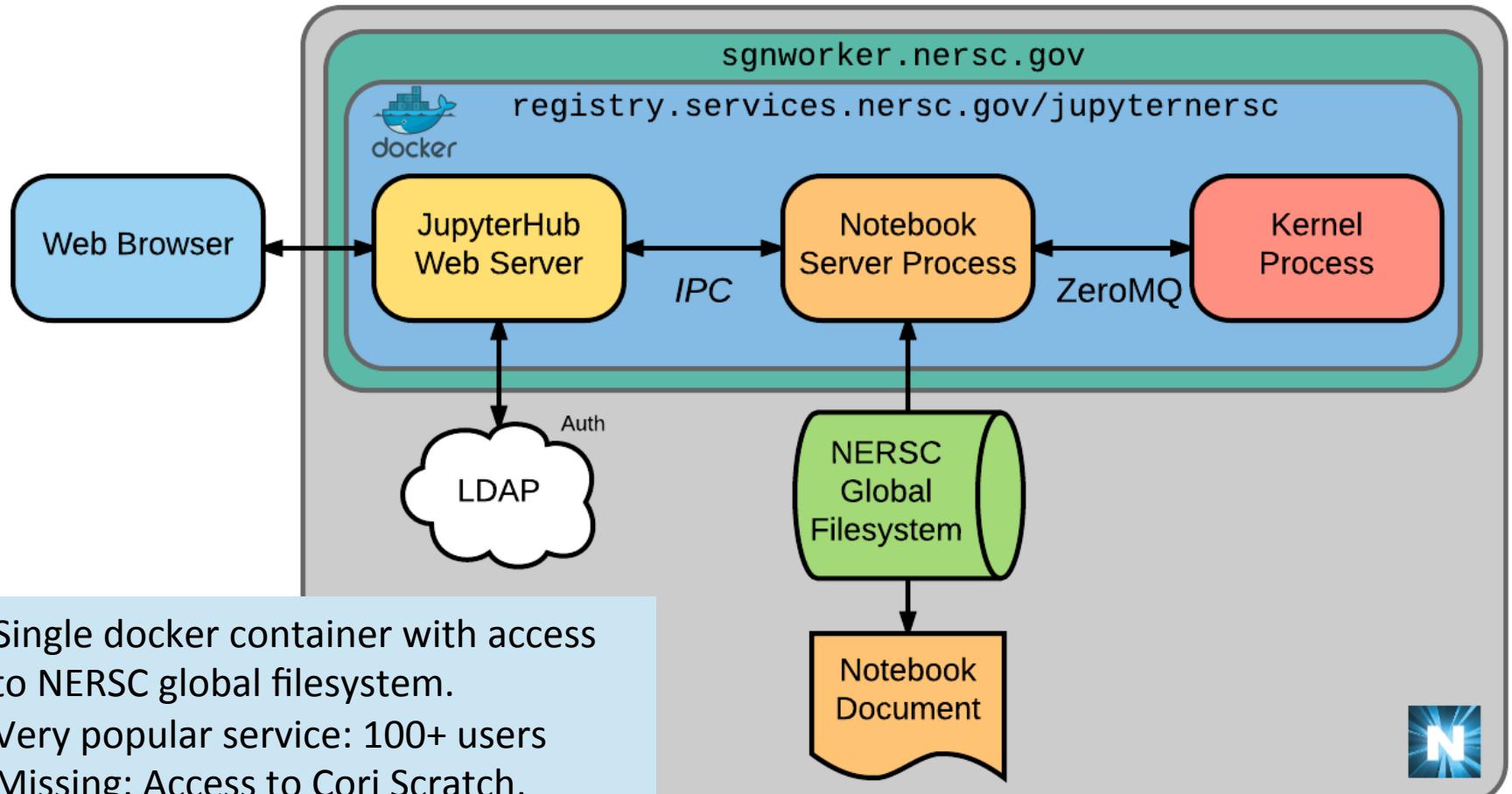


Motivating Use Cases

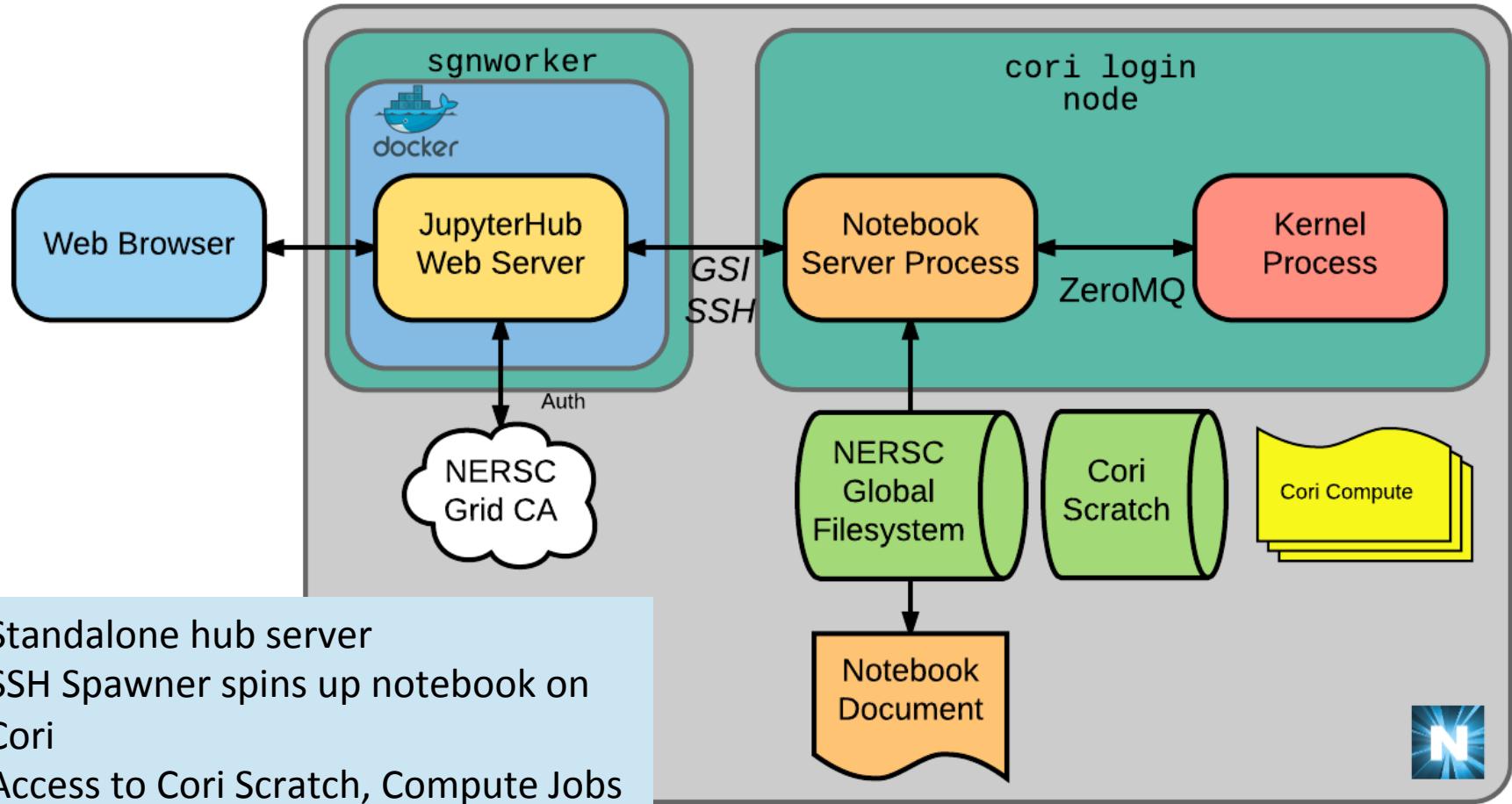
Python is the most popular language/tool at NERSC for scripting up workflows and analyzing scientific data

- Users want to be able to use Jupyter notebooks to drive their jobs, run post-job analyses etc.
- Access to NERSC resources (Filesystems, Batch Queue, Network, DBs) is key
- Add their own libraries to the notebook environment in a consistent manner
- Individual users to run their own notebook servers presents a potential security hole

Jupyterhub in a Single Container



New Jupyterhub Implementation For Cori



- Standalone hub server
- SSH Spawner spins up notebook on Cori
- Access to Cori Scratch, Compute Jobs via SLURM magic



Authentication

- Custom Authenticator uses myproxy to login to NERSC CA server with username/password and retrieves credentials (X509 certificate)
- Jupyterhub runs as a standalone service and doesn't need root access. In fact, no root access needed across this architecture.

Spawner: SSH

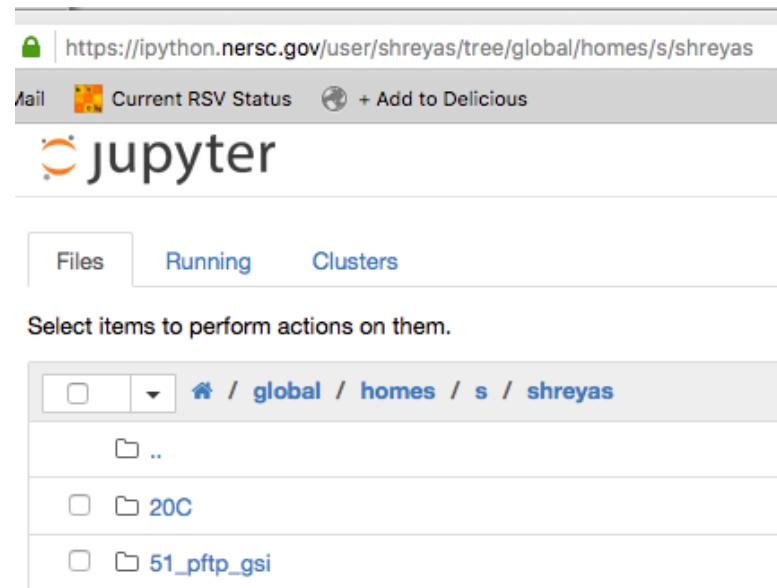
- We wrote an SSH Spawner that will will SSH into the Cori node with users credential
 - Uses GSISSH (but can also use regular SSH if you want to use SSH Keys instead of GSI Certificates)
- SSH Spawner starts up notebook server process and goes away; Notebook server communicates directly with hub
 - No tunnels or persistent connections needed
- Keep track of the PID for poll and shutdown functions (also via SSH)

Ipython Magic for SLURM

- Created some simple magics to facilitate interaction with SLURM batch queuing system
- Implemented %%sbatch and %squeue
- Pandas mode to slurp the results

Other Features

- Allow users to browse other filesystems while defaulting to homedir
- Users can drop in custom kernels in their .ipython dir

A screenshot of a web-based Jupyter interface. At the top, there is a header bar with a lock icon, the URL "https://ipython.nersc.gov/user/shreyas/tree/global/homes/s/shreyas", a mail icon, a "Current RSV Status" button, and a "+ Add to Delicious" link. The main title "jupyter" is displayed in a large orange font. Below the title, there are three tabs: "Files" (selected), "Running", and "Clusters". A message "Select items to perform actions on them." is shown above a file browser. The browser shows a directory structure under "/global/homes/s/shreyas": .., 20C, and 51_pftp_gsi. Each item has a checkbox to its left.

Future

- Driving a Spark job from a notebook on Cori
- Spawning notebooks on Cori compute nodes
- Tighter interaction with MPI jobs/HPC workflows

Users

OpenMSI

LUX

Cosmo

CMB

NGBI

Metatlas



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What Our Users Say

**“I’ll never have to leave a notebook again
that’s like the ultimate dream”**

More info

Contact us:

- scholia@lbl.gov
- scanon@lbl.gov
- rcthomas@lbl.gov

Repos will be posted on Github under

<https://github.com/NERSC>