Containers on Comet, XSEDE Gateways, Jupyterhub

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Singularity on Comet

- Singularity 2.3.1
- Supports MPI through MVAPICH
- Supports CUDA 8 for GPU nodes
- User services provides containers instead of modules (e.g. Tensorflow)
- github.com/zonca/singularity-comet

Containers in XSEDE Gateways (1/2)

- NeuroScience Gateway (Kenneth Yoshimoto): Singularity containers to run applications on Comet
- DesignSafe, natural hazard engineering (Rion Dooley): Docker gateway setup, Docker applications on cloud, Singularity applications on HPC via Agave
- Galaxy, biomedical workflows (Enis Afgan): Docker for installation of Galaxy, packaging of tools, isolate interactive environments, portability across cloud services

Containers in XSEDE Gateways (2/2)

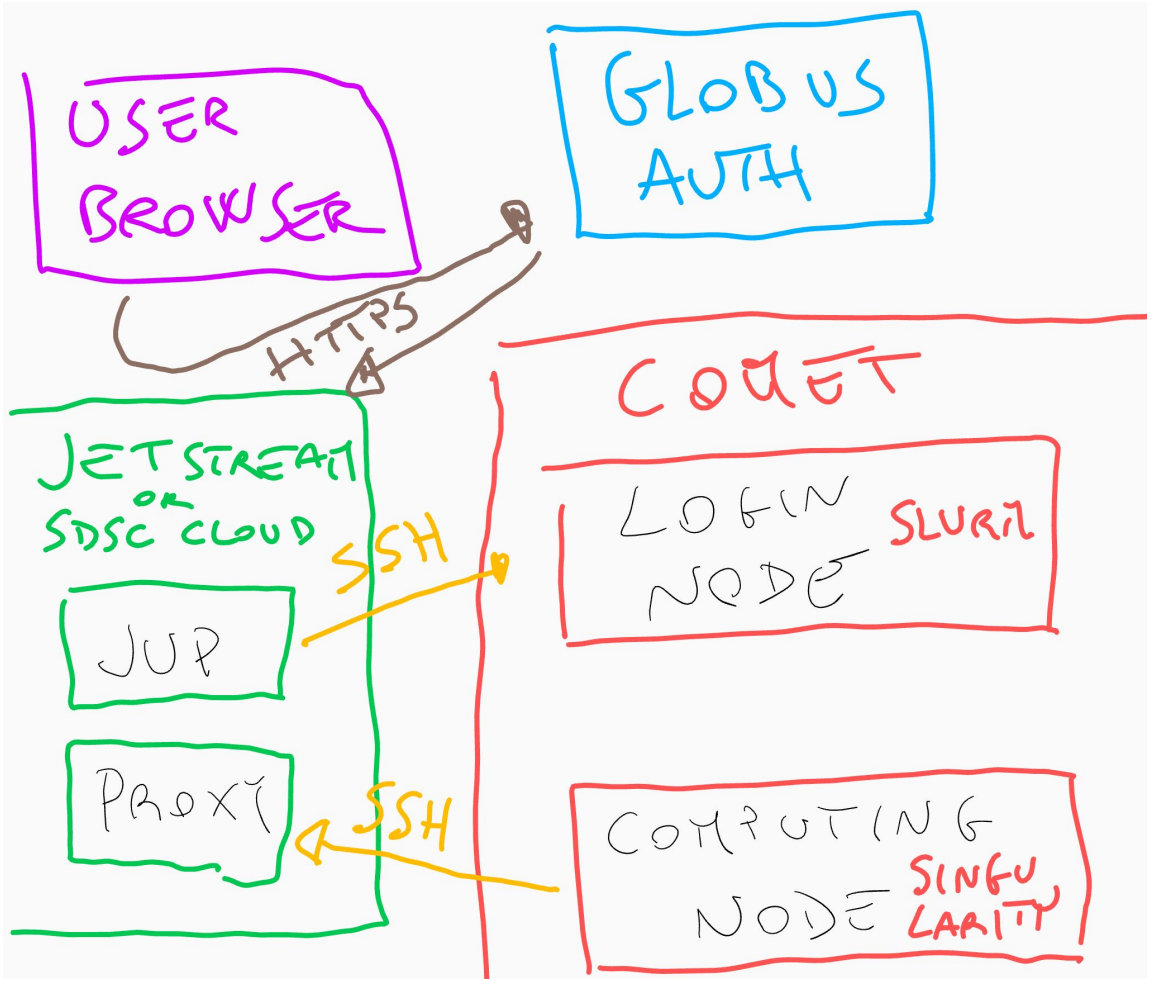
- OpenNeuro, open MRI datasets and analysis tools (Rion Dooley): Community provides Dockerfiles for applications, then converted to Singularity
- TGen, *omics problem at scale (Rion Dooley): Docker with extended storage API to make high speed networking native
- Unidata, Geoscience data and tools (Suresh Marru): Docker packaged software tools on Jetstream with Mesos + Jupyter

Jupyterhub on HPC

- Demo at http://bit.ly/jupyterhub_singularity
  - Jupyterhub
  - Batchspawner
  - Globus Auth

Jupyterhub on HPC

- Ease of access to HPC
  - Bring your own container
  - Default access for local HPC (e.g. Minnesota)
  - Centralized software stack
- Access jobs and data
  - Launch and monitor jobs
  - Analyze interactively large amount of data


USER
BROWSER
GLOBUS
AUTH
HTTPS
COMET
JETSTREAM
OR
SDSC CLOUD
SSH
LOGIN
NODE
SLURM
JUP
PROXY
SSH
COMPUTING
NODE
SINGU
LARITY

Jupyterhub in XSEDE Gateways

- Companion service for:
  - Interactive postprocessing
  - Custom pipeline
  - Call main gateway API
- Possible deployment:
  - Jetstream
  - Spawner for Kubernetes or Docker Swarm
  - Globus Auth to enable data transfer

Thanks

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