



Extreme Science and Engineering
Discovery Environment

Cyberinfrastructure Resource Integration

Bringing the pieces together

SC 18

11/14/2018

Eric Coulter
Senior XCRI Engineer

What are we trying to accomplish?

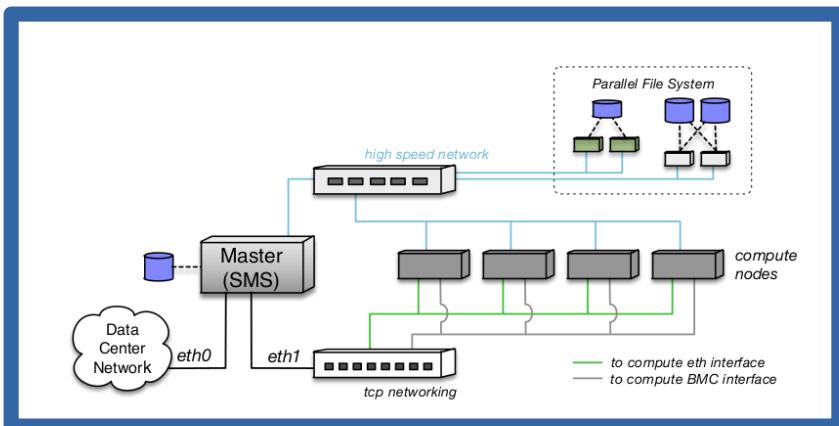
- The mission of the XSEDE Cyberinfrastructure Integration (XCI) team is to integrate, adapt, and disseminate software tools and related services across the national CI community enabling the US research community to do its work better and more easily than before – making it easier for administrators and users of campus-based cyberinfrastructure systems to make use of tools created by XSEDE for local benefit, and expand upon XSEDE's effort to enable the creation of an integrated national cyberinfrastructure...
- In other words, Make Science Easier by enabling ease-of-access to local and national CI!

What is XCRI? (XSEDE Cyberinfrastructure Resource Integration)

- Enable seamless transition between local and remote CI Resources
- Software toolkits for local or remote resources
- We also do site visits and remote consultation!
- Continually looking for feedback from XSEDE users, Campus Champions, and service providers



XCBC – XSEDE Compatible Basic Cluster



- Formerly Rocks, now based on the OpenHPC Project
- **Ansible Playbooks** – for compute node configuration and continued maintenance
- Intended for local, hardware-based HPC systems



XSEDE

The Site Visit Process

- ✓ Contact XCRI via:
 - help@xsede.org
 - Or talk to us in person!
- ✓ Discussion:
 - ✓ Desired toolkits
 - ✓ Hardware configuration
 - ✓ Scheduling and visit planning
- ✓ XCRI Staff will travel to the site, and spend a week to build/upgrade/repair the cluster

FREE FOR HOST INSTITUTIONS!



DOANE
UNIVERSITY



XSEDE

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Discovery Environment



SOUTH DAKOTA
STATE UNIVERSITY



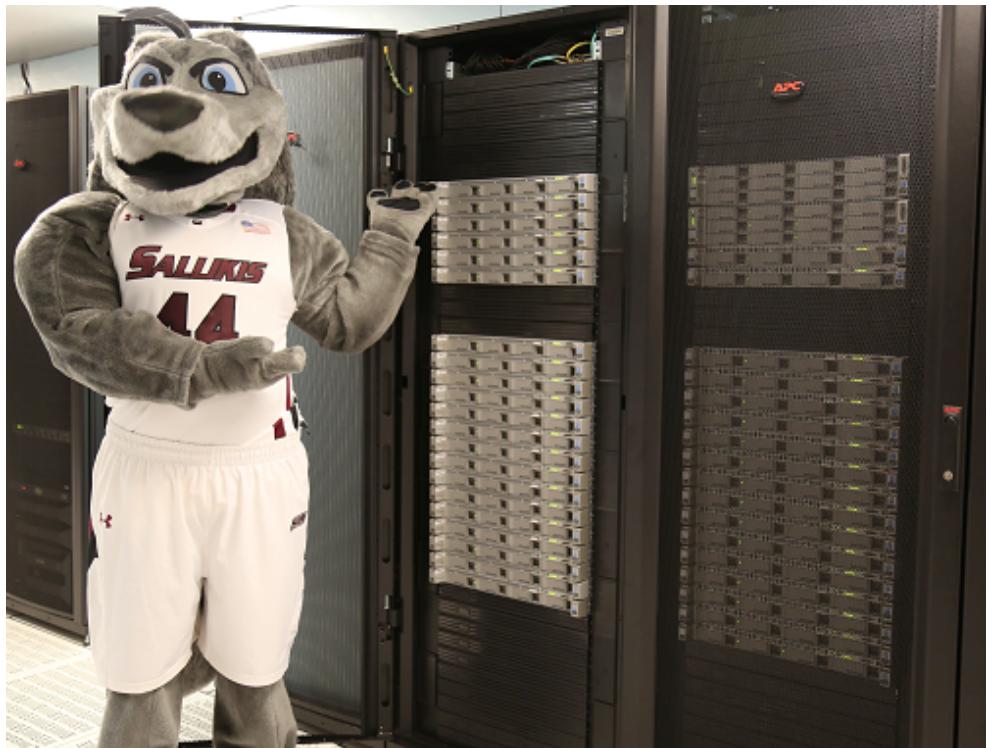
BENTLEY
UNIVERSITY



Southern Illinois University

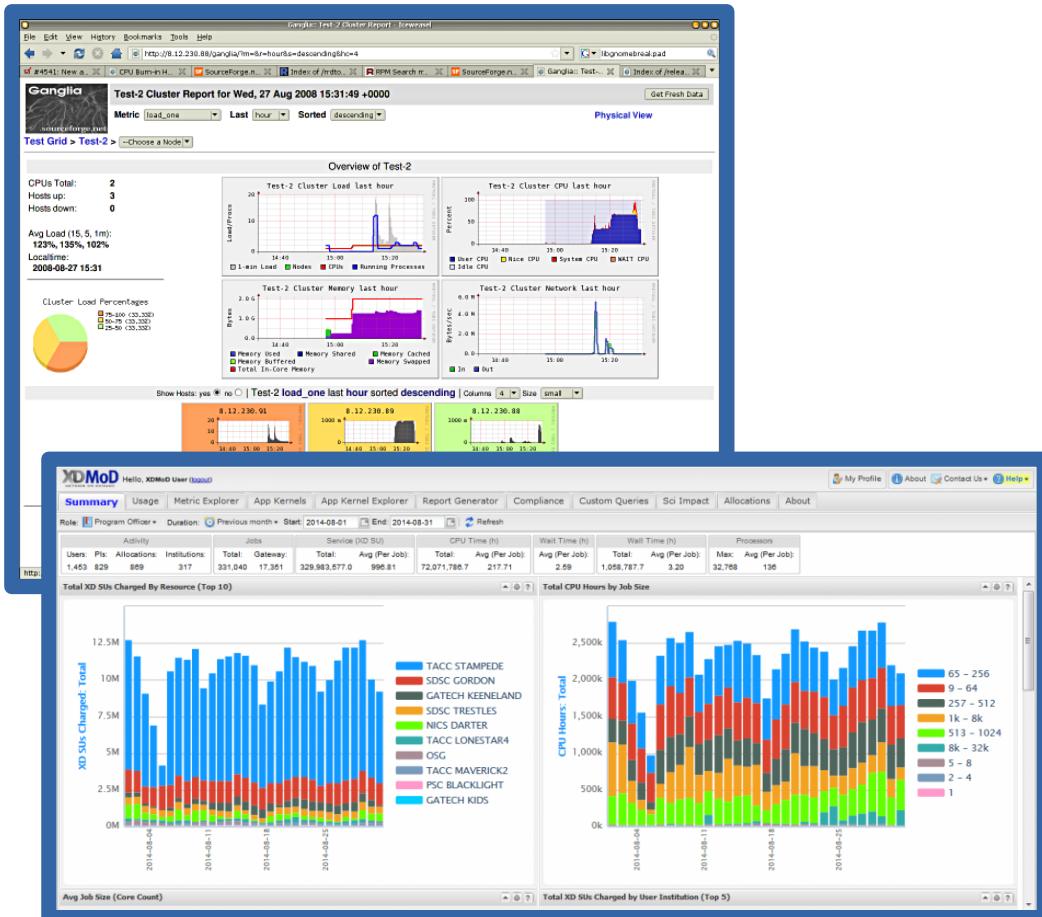
- First visit in Oct. 2015
- Rocks-based with GPU nodes and large storage
- Rebuilt to OpenHPC in early 2018 with remote support
- Enabled a variety of grad/undergrad projects, now an L3 SP!

BigDog:



Cluster Monitoring Toolkit

- Ganglia
 - For monitoring cluster state
- OpenXDMoD
 - XseDe Metrics on Demand
 - Job/user statistics and report generation



XSEDE

Doane University

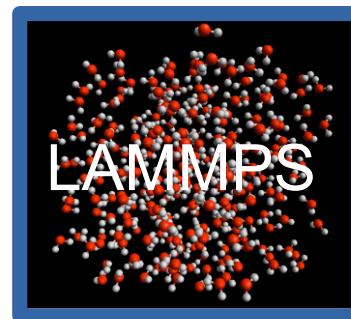
- Visited in Oct. 2018
- First HPC System at Doane!
- Turn donated hardware into a working system for research and training users in HPC skills
- Main computational resource available to the new Center for Computing in the Liberal Arts
- Carried out user training session as part of the visit

Onyx:



XNIT – XSEDE National Integration Toolkit

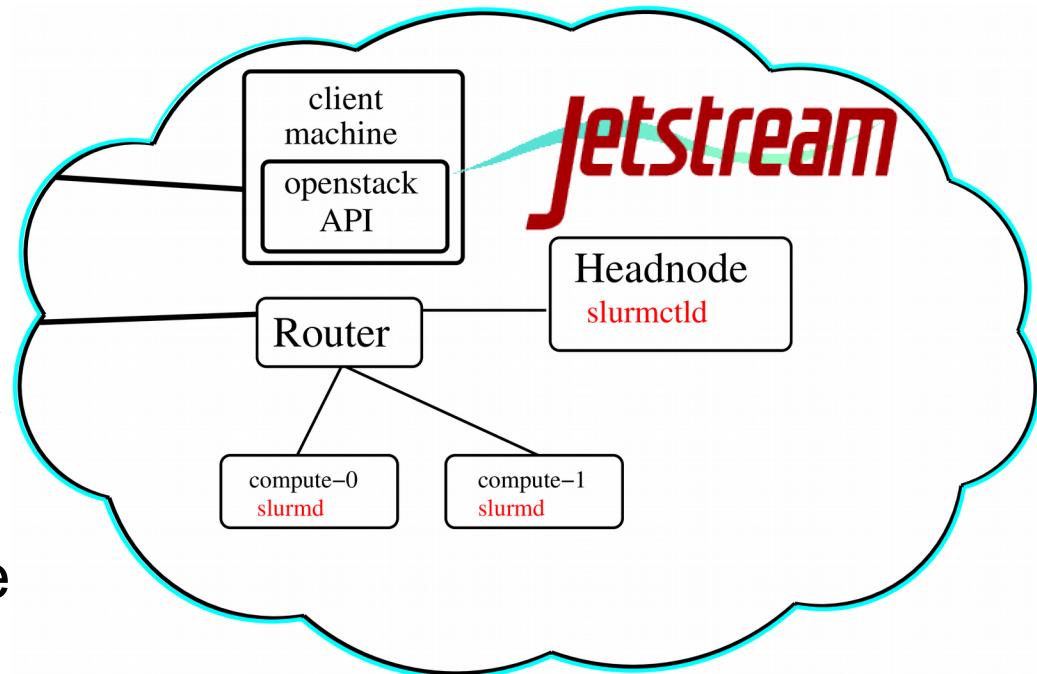
- Open source scientific software
- Originally available as a YUM repository
- Moving towards offering a container repository
- Always looking for suggestions!



XSEDE

Jetstream Virtual Clusters

- Inspired by a need for more resources on Science Gateways
- Two main use cases:
 - Additional resources for Gateway users
 - HPC system without the hardware hassle



Virtual Clusters in Reality: 3DQP Gateway

- With Dr. Murat Maga at Univ. Washington
- Enables processing, analysis, and visualization of 3D images
- Used as a Virtual HPC Environment, providing shell env and an interactive R/shiny server.

3D Quantitative Phenotyping Gateway (3DQPG)

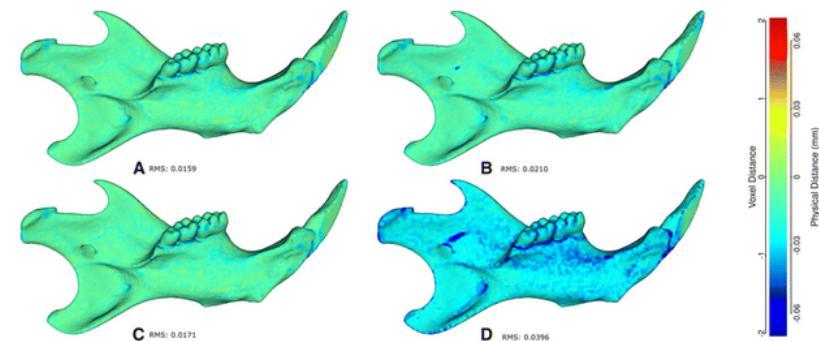


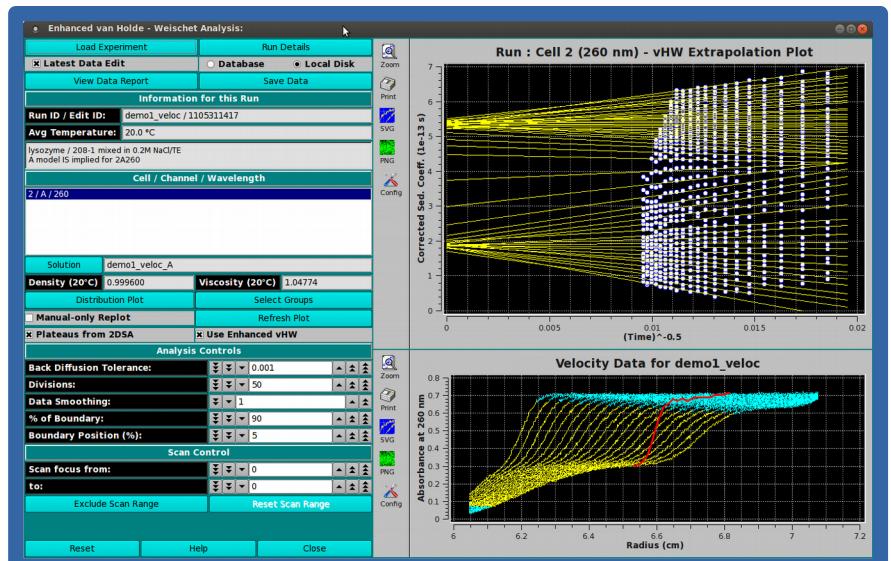
Fig. 1

Visualization of the distances between the atlas surface that was landmarked (p90) and four other surfaces constructed. **a** 50 % Probability surface (p50); **b** 70 % Probability surface (p70); **c** Surface thresholded at grayscale value of 35. **d** Surface thresholded at grayscale value of 55. RMS: Root mean square error

Ryan Young and A. Murat Maga
<https://doi.org/10.1186/s12983-015-0127-8>

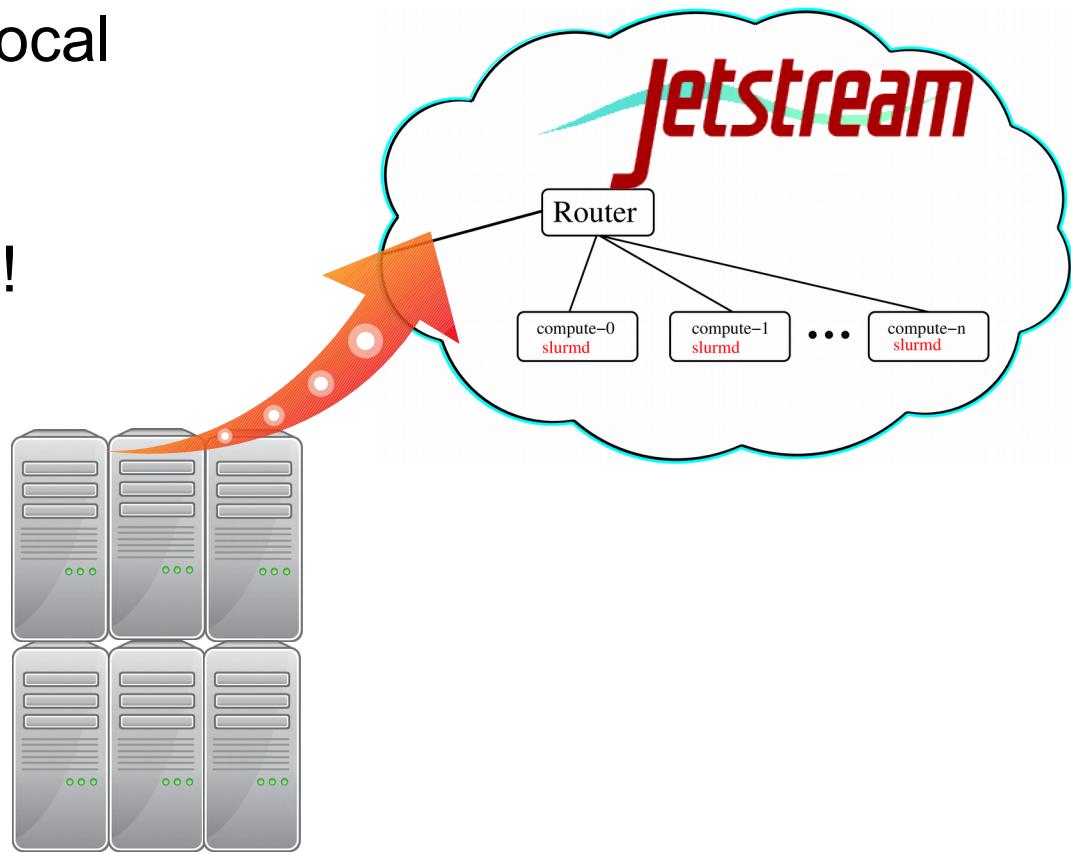
Virtual Clusters in Reality: Ultrascan Gateway

- With Dr. Borries Demeler at University of Lethbridge
- Users submit jobs via a web interface or desktop client
- Some 8,000 jobs to date with ~10,000 SUs used
- Early adopter of the VC toolkit, has helped shape the current iteration, making the experience easier for new users



Jetstream Remote Queue

- Enables bursting from local SLURM cluster to Jetstream.
- Project-specific queues!
- Lets researchers seamlessly use local and remote resources



Questions for you:

- Are you dealing with protected data?
 - Would you be interested in getting help from XCRI for this?
- What kind of software would you like available as a vetted container image?
- How can XCRI help you (or your campus) get more science done?
- Questions for me are also welcome! :)

Contact us or learn more:

- More Information: <https://www.xsede.org/ecosystem/xcri-mission>
- Documentation: <https://xcri-docs.readthedocs.io>
- Email: help@xsede.org with XCRI in the subject