WVU RESEARCH COMPUTING INTRODUCTION

Introduction to WVU's Research Computing Services

WHO ARE WE?

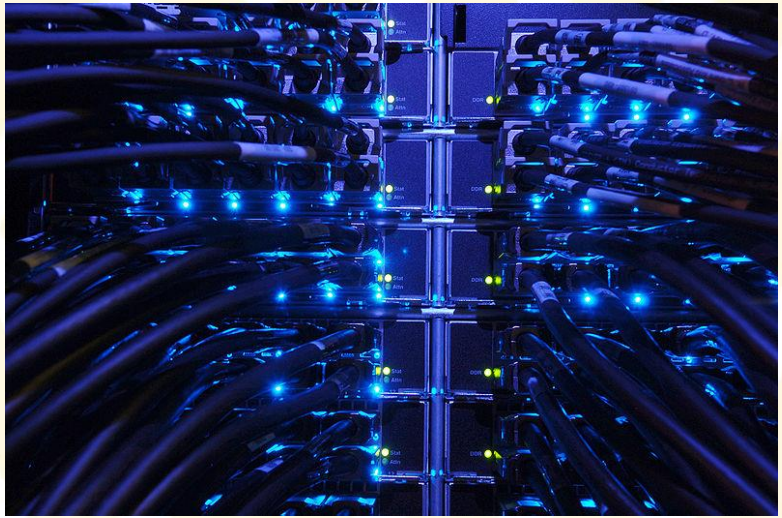
- Division of Information Technology Services
- Funded through WVU Research Corporation
- Provide centralized HPC systems and support staff to help researchers compute scientific data
- Support 30 individual research groups across campus and ~150 active users

MOUNTAINEER

- 32 Compute Nodes
  - Dual 6 core Intel Xeon (Westmere) processors (12 cores)
  - 48 Gbytes of memory (4 GB per core)
  - 10 Gbps Ethernet Interconnect
- 50 Terabytes of shared storage
- Open community access

SPRUCE KNOB

- 165 Compute Nodes/3,064 Cores
- Current node offerings
  - Small Memory Nodes
    (24 Intel Xeon Broadwell Cores/64 GB Ram)
  - Medium Memory Nodes
    (24 Intel Xeon Broadwell Cores/128 GB Ram)
  - Large Memory Modes
    (24 Intel Xeon Broadwell Cores/512 GB Ram)
  - GPU memory nodes
    (24 Intel Xeon Broadwell Cores/64 GB Ram/
    NVIDIA k20x GPU)
- 54 Gbps Infiniband Interconnect
- 17 GPU Accelerator cards



SPRUCE KNOB – HYBRID MODEL

Condo Model

- Faculty pay for any nodes that they want in the cluster
- Faculty investors (and their research teams) have priority access to their nodes
- Any Spruce HPC users can use idle faculty owned nodes for up to 4 hours (standby queue)

Community Model

- 51 Nodes/848 Cores are generally available to the HPC community (WV)
- Fair-share scheduling, not subject to owner preemption

HPC SOFTWARE

- MOAB Schedule Suite
- Intel Studio XE (Fortran, C, MPI, etc)
- Matlab
- Module avail command
- Discipline specific software
- Researchers self-installed software

LOCAL STORAGE

- DDN GRIDScaler System
- 1 PB Raw Storage
- ~ 400 TB scratch/transfer space
- Expandable from 2 PB to 8 PB
- GPFS Parallel Filesystem
- Direct Infiniband Connection

RESEARCH DATA DEPOT

Central Storage Repository

- Centrally Managed
- NSF/NIH Data Management Requirements
- Low cost storage solution for researchers
- Expandable Solution
- Multiple protocol support
  - CIFS (Windows Shares)
  - Globus Online
  - SFTP/SCP
- Connected to Science DMZ
- Coming Soon!

DDN GS7K System

ARCHIVING RESEARCH DATA

Google Drive for Education

- Unlimited Storage
- Max file size limit 5TB
- Easy file sharing
- But how do I get it there?
  - See shortly …

HOW DO I TRANSFER MY DATA?

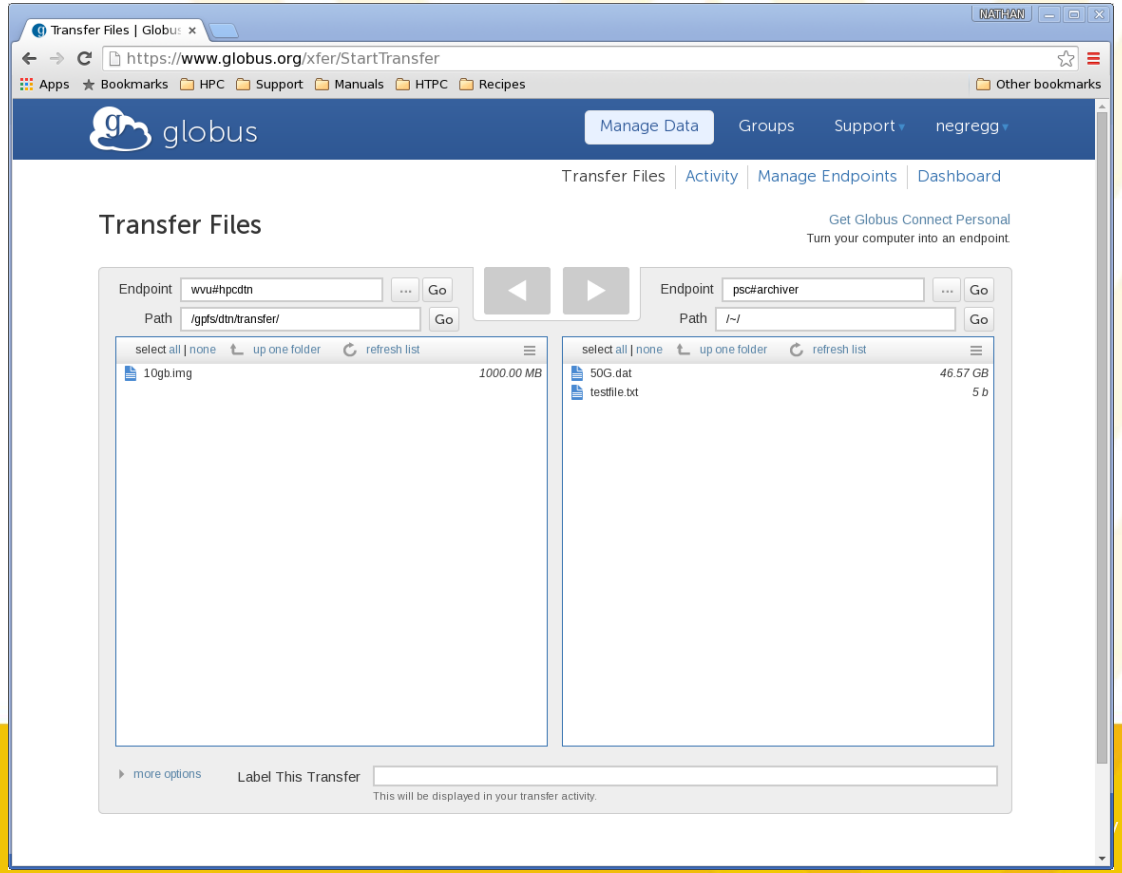
- Preferred Method: Globus Online
- Alternative Methods:
  - scp
  - rsync
  - sftp

GLOBUS ONLINE

- File Transfers
  - Fast, reliable, secure
  - Restartable
  - Google Drive Connector (Coming Soon!)
- File Sharing
  - Self-managed/no admins needed
  - Custom groups
- Data Publication
  - Publish datasets in searchable web-interface
  - Helps meet NSF/NIH Data Management Plans

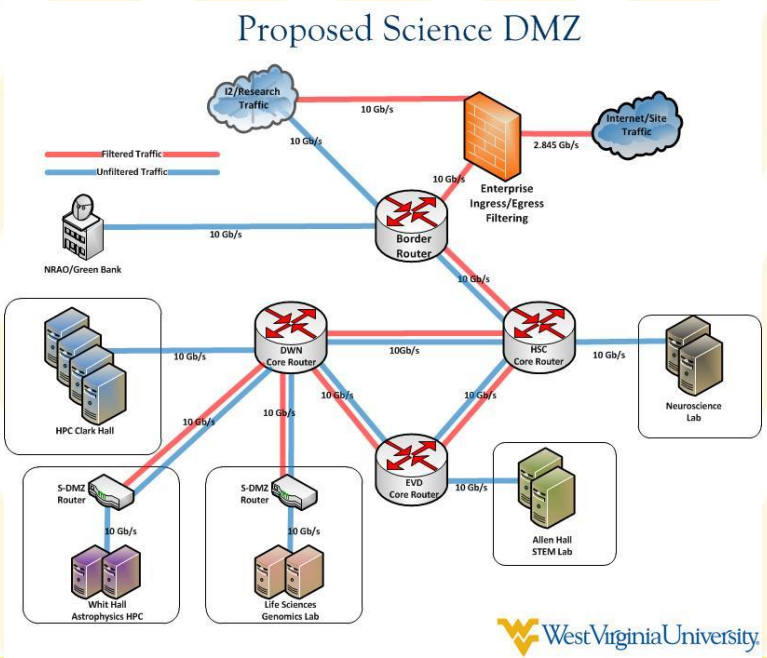
WHY GLOBUS ONLINE?

GLOBUS – INTUITIVE WEB INTERFACE



SCIENCE DMZ

- Science/Research Dedicated Dual 10 Gb Link
- Soon connected to:
  - HPC
  - Dr. Spirou Neuroscience Lab @ HSC
  - Astrophysics HPC @ White Hall
  - Genomics Core Lab @ LSB
  - College Education and Human Services
  - Greenbank
  - Outside endpoints
- Monitored with perfSONAR



RESEARCH NETWORKING

- WVU-Pittsburgh Internet2 connection = 10Gbps
- WVU research network to Pittsburgh shared with DOE - NETL
- WVU – member of Internet2
- Internet2 100 Gbps nationwide network
- 3ROX implemented a 100 Gbps connection to I2

ADDITIONAL INFORMATION

- Main Website
  - http://hpc.wvu.edu
- Wiki
  - http://wiki.hpc.wvu.edu

QUESTIONS?

- Main Contact: https://helpdesk.hpc.wvu.edu or helpdesk@hpc.wvu.edu
- Contact Nathan Gregg (Research Computing Manager/HPC Systems Administrator)
  - Email: nathan.gregg@mail.wvu.edu
  - Phone: 304-293-0963
- Contact Guillermo Franco (Research Computing Software Developer)
  - Email: gufranco@mail.wvu.edu
- Contact Brice Knotts (ITS Enterprise Infrastructure -- Executive Director)
  - Email: baknotts@mail.wvu.edu

February 14, 2017

Overview of XSEDE Resources and System

LCSEE Graduate Seminar – February 13, 2017

XSEDE

Extreme Science and Engineering Discovery Environment

First a little history

- A long history of supercomputing in scientific research
- In the “olden days”…
  - many supercomputers at different institutions
  - very siloed
  - independent, unique administrative procedure
  - little or no coordination
  - many supported by the National Science Foundation

First a little history

- In 2001 NSF recognized the need for a more coordinated approach to scientific computing in the U.S.
- Announced a competitive solitation to build a large scale, coordinated network of supercomputers and their respective organizations
- Awarded in 2004

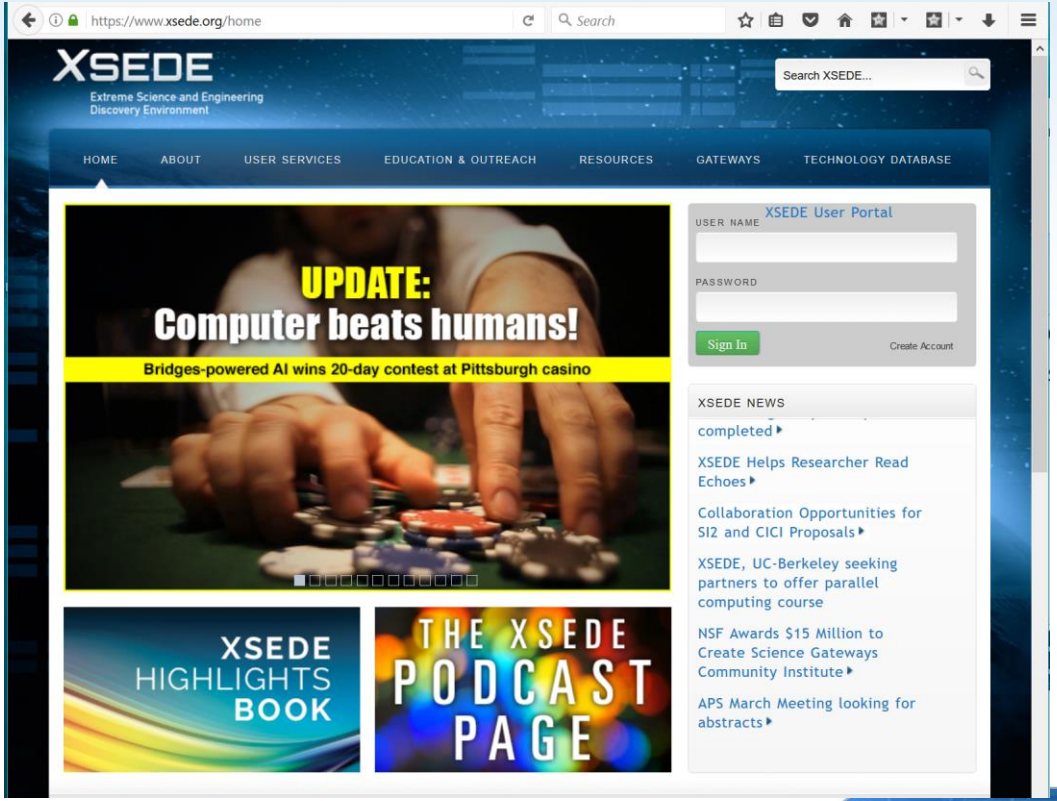
First a little history

- Awarded in 2004
- Became known as the Teragrid
- Teragrid was a coordinated consortium of scientific computing resources – including computational and storage resources
- Teragrid operated from 2004 to 2011

First a little history

- In July 2011 Teragrid “transitioned” to XSEDE
- A new consortium – many original members
- A new focus

www.xsede.org



What is XSEDE?

- A network of scientific computing resources…
  - with coordinated administration
- an organization

XSEDE

- A network of scientific computing resources…
  - High performance computing
  - High throughput computing
  - Visualization
  - Storage
  - ….

XSEDE

- High performance computing
- A collection of HPC systems at institutions across the country
- Including…
  - Stampede at TACC 9600 Pflops
  - Comet at SDSC 7000 Pflops
  - Bridges regular memory at PSC 895 Pflops
  - Bridges large memory at PSC
- ….

XSEDE

- High performance computing
  - Stampede at TACC
    - Dell Poweredge cluster with Intel Xeon Phi coprocessors
    - OS: Linux – CentOS
    - Cores: 102400
    - Nodes: 14336
    - Storage: 14 PB
    - SLURM job management system
    - Nvidia Kepler2 GPUs

XSEDE

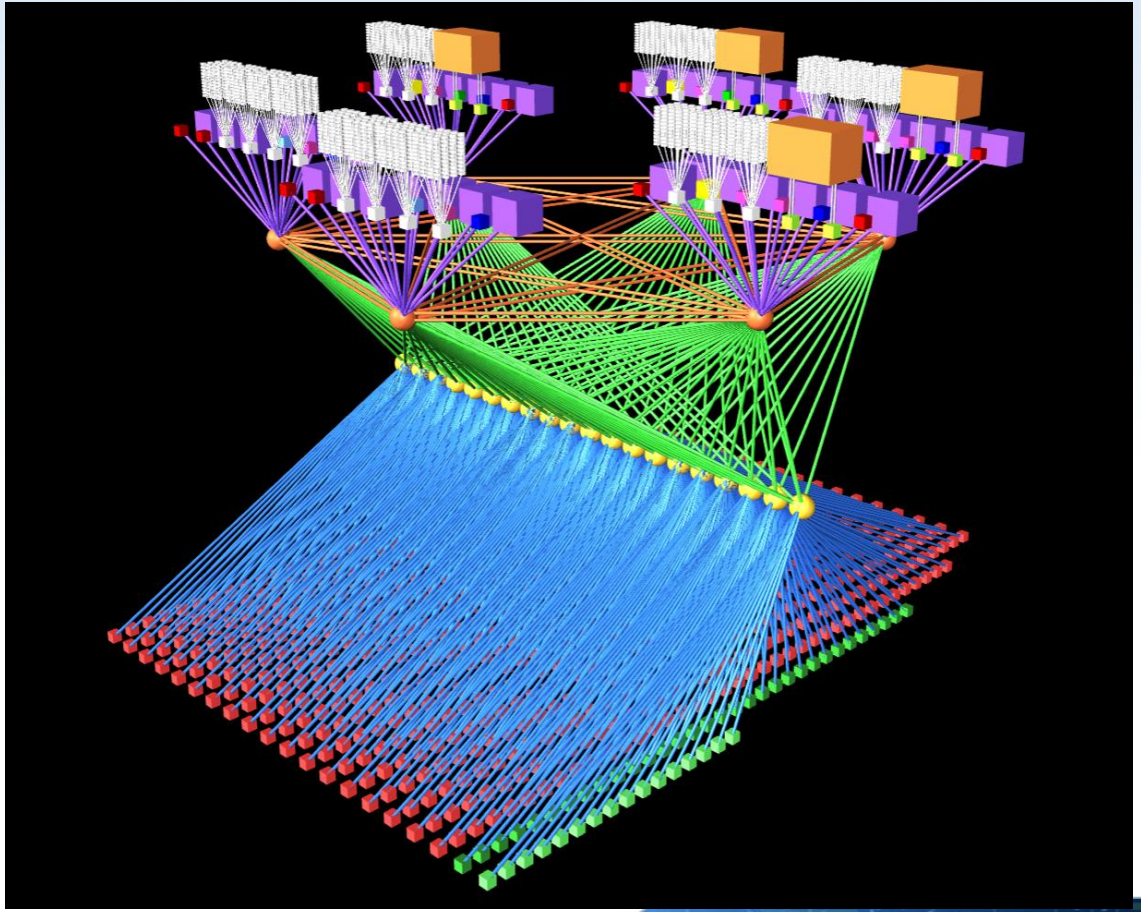
- High performance computing
  - Bridges – Regular memory at PSC
    - HP cluster with Intel Xeon processors
    - 128 GB Memory per node
    - OS: Linux – CentOS
    - Cores: 21056
    - Nodes: 752
    - Intel Omnipath Interconnect
    - Shared storage system + 8 GB storage per node
    - Many unique features

XSEDE

- High performance computing
  - Bridges – Large memory at PSC
    - HP nodes – 4 with 12 TB memory, 42 with 3 TB memory each
    - OS: Linux – CentOS
    - Cores: 160
    - Intel Omnipath Interconnect
    - Pylon - Shared storage system + 8 GB storage per node
    - Many unique features

XSEDE HPC – Bridges

https://www.psc.edu/index.php/bridges-virtual-tour



XSEDE

- High throughput computing
  - Open Science Grid
    - 60,000 compute nodes (distributed)
- ….

XSEDE

- Visualization
  - Maverick – 2640 cores
  - 20 Pbytes of storage
  - designed specifically to do scientific data visualization
  - does visualization remotely

- ….

XSEDE

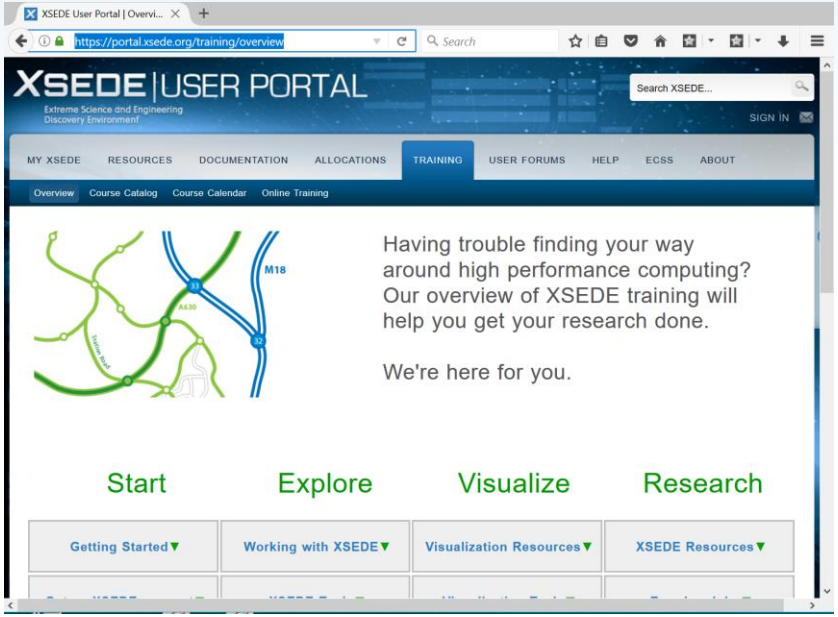
- Storage
  - DATA OASIS @ San Diego Supercomputing Center
    - Default/max storage per XRAC: **500GB/50TB**
  - PYLON @ the Pittsburgh Supercomputing Center
    - Default/max storage per XRAC: **500 GB/none**
  - RANCH @ the Texas Advanced Computing Center
    - Default/max per XRAC: **none/1 PB**
  - Wrangler @ the Texas Advanced Computing Center
    - Default/max per XRAC: **TBD**

Software

- Too much to tell - too little time
- See –
  - https://www.xsede.org/software

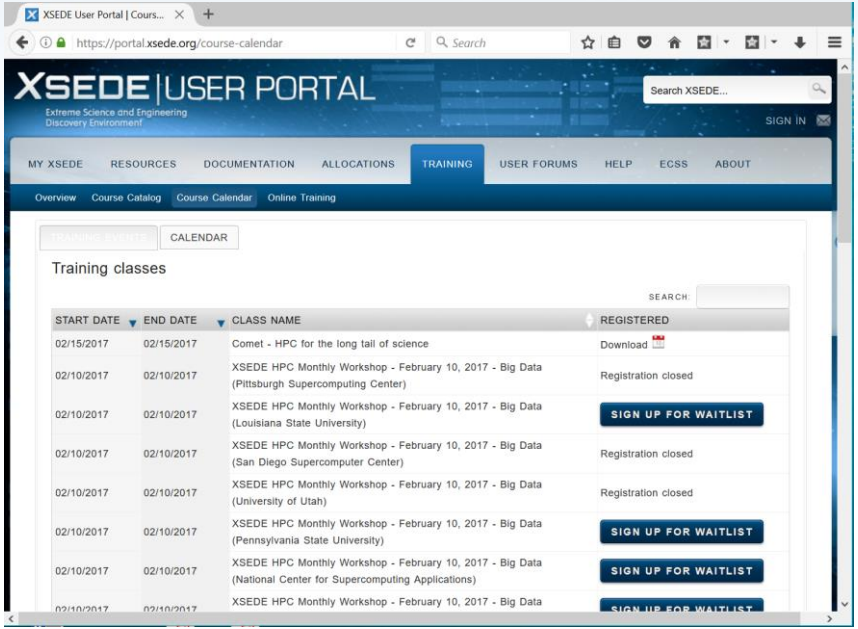
Training

- https://portal.xsede.org/training/overview



Training

- https://portal.xsede.org/course-calendar



Resource Allocations – how do you get to use these resources?

- Resources Types –
  - Computational Resources
  - Visualization Resources
  - Storage Resources

- https://portal.xsede.org/allocations-overview

Resource Allocations

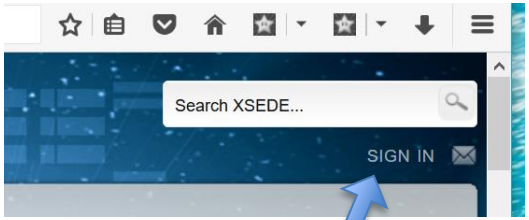
- Allocation Types
  - **Trial** – very limited 1000 SUs, 6 months, COMET
  - **Startup** – limited, getting started, benchmarks, available to faculty/post-doc & K-12 teachers
  - **Educational** – for training, workshops, classroom instruction and classroom projects, limited
  - **Research** – large scale resources, awarded based on research proposals, scientific merit+, competitive, proposal submissions quarterly, awarded quarterly, good for one year

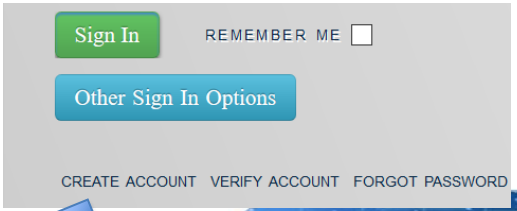
Campus Champions

- Support and assistance in using XSEDE resources, getting accounts, etc.
- Liaison between you and XSEDE
- @ WVU
  - Nathan Gregg
    - Nathan.Gregg@mail.wvu.edu
  - Don McLaughlin
    - Don.McLaughlin@mail.wvu.edu

Final comments

- XSEDE Resource Allocations are available to
  - Faculty and Post-docs
  - not graduate students and undergraduate students
  - However, students can be on project teams and be given access to faculty project allocations
  - But, **everyone** must have a portal account





Thank you

Any Questions?


Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
XSEDE
Extreme Science and Engineering
Discovery Environment