BLUE WATERS

SUSTAINED PETASCALE COMPUTING

February 11, 2015

Getting Started on Blue Waters

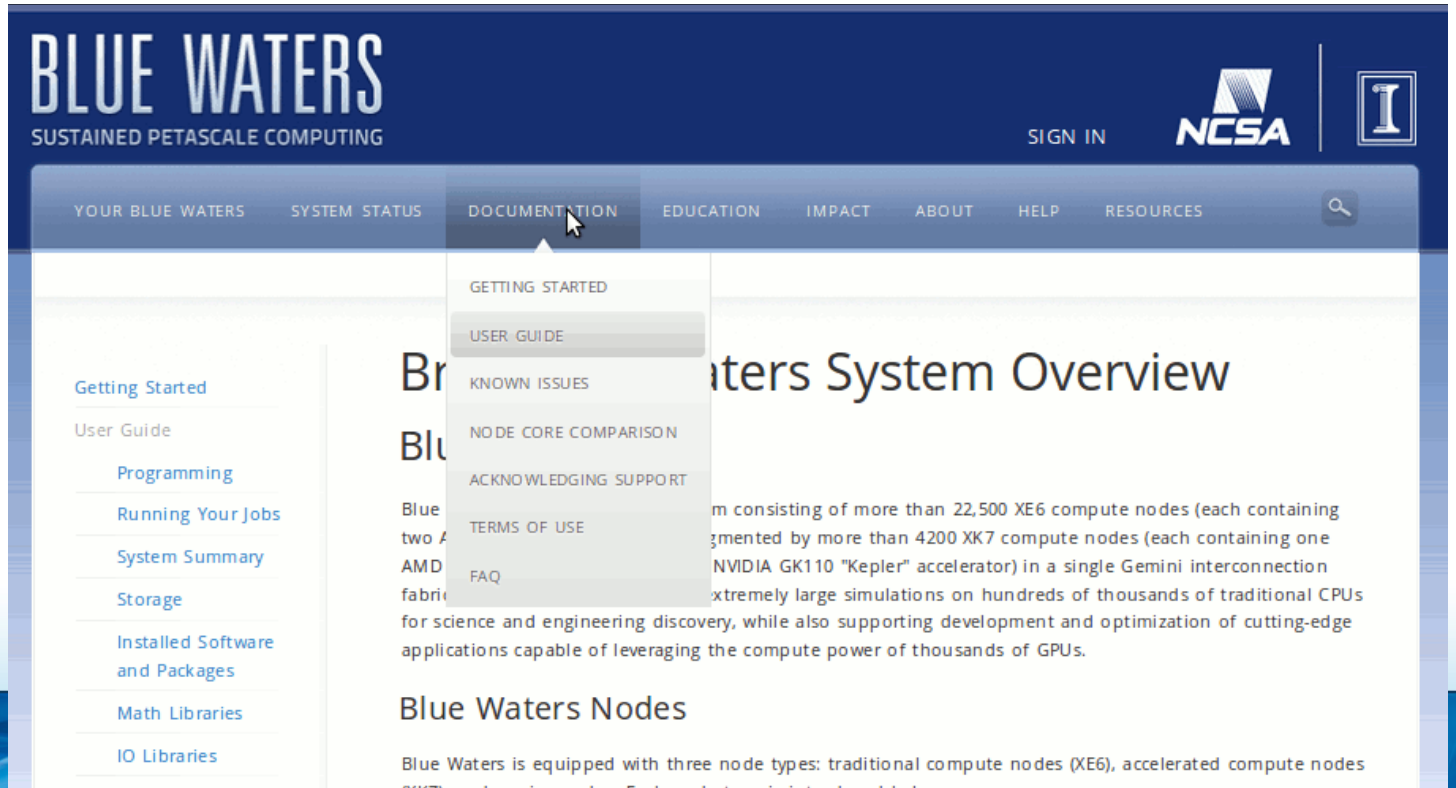
GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

Blue Waters Web Portal

- bluewaters.ncsa.illinois.edu
  - contains:
    - system status
    - documentation
    - help links
    - user management tools for PIs
    - Globus Online for moving data

Blue Waters User Documentation On Portal

- bluewaters.ncsa.illinois.edu
  - Documentation tab → User Guide



Blue Waters Portal: Your First Source For Info

- Everything in today's presentations is from information in the portal or about the portal itself
- Portal has a search function
- Help link on portal goes to help sources

Baseline Level Of Knowledge

- unix file systems
  - especially including file permissions (support staff does NOT have root privileges)
- editing files using emacs or vi or …
- using and configuring unix shells
  - bash
  - tcshrc
  - …

Baseline Level of Knowledge

- compiling and running programs in unix environment
  - (you should know what this means:)

```
gcc -I ../include_dir -c mysource1.c

gcc –L ../lib_dir –lmylib –o my_program
mysource1.o mysource2.o
```

PBS job submission

- job files:
  - #PBS –l nodes=1
  - #PBS –l walltime=2:00:00
- Queue management
  - qsub
  - qstat
  - qdel

Blue Waters Login Shells

- bash (vast majority of users)
- csh
- tcsh
- zsh

(changing user shell requires a ticket; no “chsh”)

Cray Environment Differences

~~gcc~~ → cc

~~mpicc~~ → cc

~~mpirun~~ → aprun

(see Programming Environment and Running Jobs talks for more details)

Blue Waters Status Information

Blue Waters: Heterogeneous System

- 22,640 XE ("traditional" compute) nodes
- 4224 XK GPU compute nodes
- 3 user login nodes
  - compiling
  - editing files
  - submit jobs
  - execution closely monitored
  - very limited use of rsync/scp (see Globus later)

Logging In

- ssh username@bw.ncsa.Illinois.edu
  - round-robins the three login nodes
- ssh username@h2ologin1.ncsa.Illinois.edu
  - or h2ologin2 or h2ologin3
  - for specific login node
    - why?
    - specific files in /tmp
    - slowness

Logging in for Training Accounts

- ssh -X trainXZY@bwbay.ncsa.illinois.edu
- Uses a VM with certificates to pass you on to Blue Waters login node.
- No scp via bwbay into Blue Waters.

RSYNC or SCP

- Not forbidden, but please, be smart
- Sends all data traffic through login node, rather than data movement infrastructure
- Large data movement/rsync *seriously* impacts other users on the same login
- Do NOT synchronize large data stores
- Golden Rule

XE/XK node summary

- XE node:
  - 1 OS image
  - 64 GB RAM
  - 4 NUMA domains
  - 16 Bulldozer modules
  - 32 integer (execution) cores
- XK node:
  - 1 OS image
  - 32 GB RAM
  - 2 NUMA domains
  - 8 Bulldozer modules
  - 16 integer (execution) cores
  - 1 Kepler GPU

Storage on Blue Waters

- Online (mounted) storage (accessible from BW)
  - /u/sciteam/* (“/home”)
  - /projects
  - /scratch
- Nearline (tape) storage (NOT accessible from BW)
  - /~/ (“/home”)
  - /projects
- Globus Online
  - (how do I get to non-mounted storage?)

Storage Summary Table (also on portal)

Storage System Type+Name	Default Quota	Quota Type	Purge Policy?	Sample Path	Globus Endpoint
Lustre home	1 TB	user	no	/u/sciteam/me	ncsa#BlueWaters
Lustre projects	5 TB	group	no	/projects/sciteam/jxx	ncsa#BlueWaters
Lustre scratch	500 TB	group	YES (30 days)	/scratch/sciteam/me	ncsa#BlueWaters
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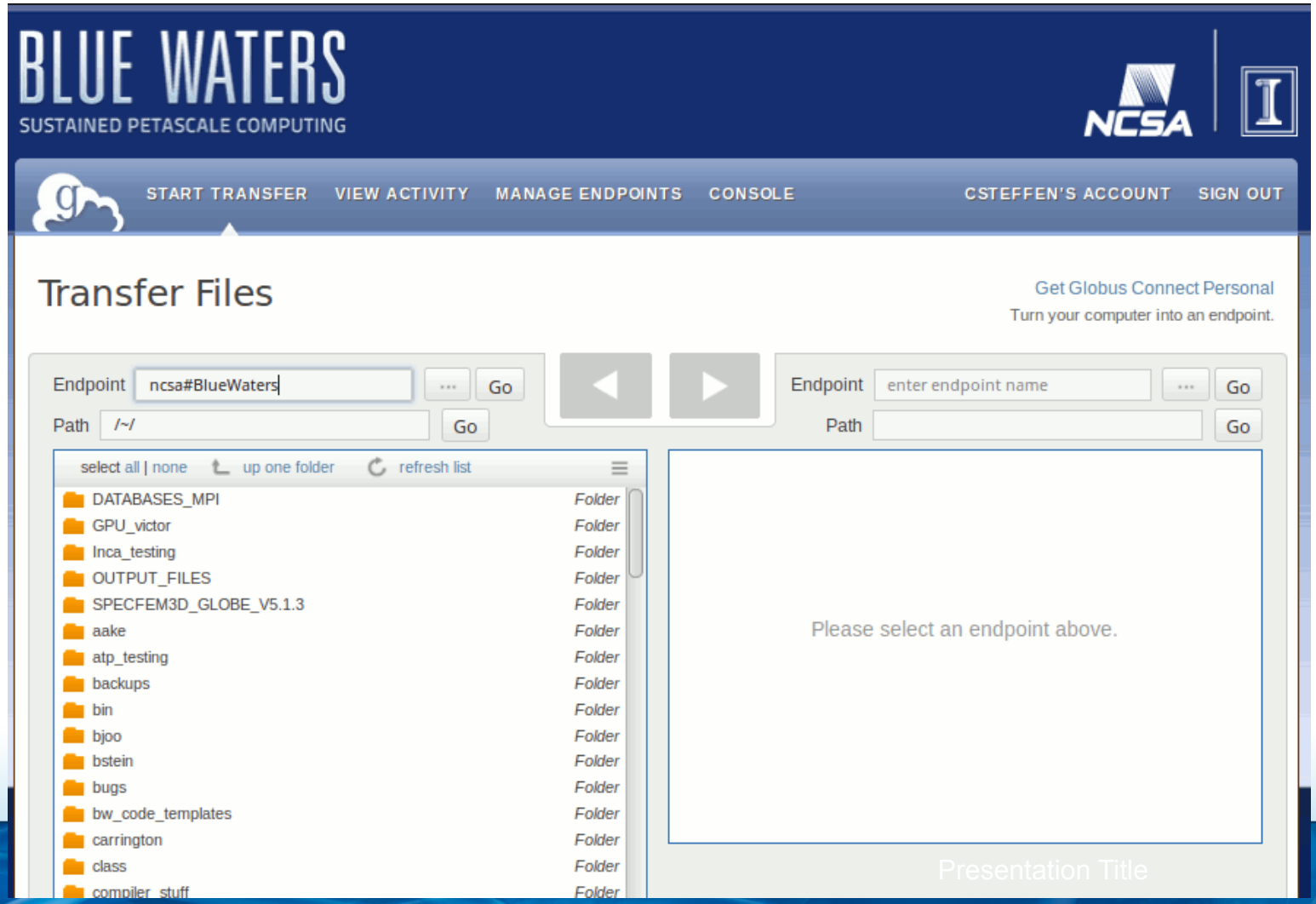
Nearline home	5 TB	user	no	/~/ (only from Globus)	ncsa#Nearline
Nearline Projects	50 TB	group	no	/projects/sciteam/jxx (only from Globus)	ncsa#Nearline

GridFTP / Globus Online (GO)

- GridFTP client on Import/Export nodes and Nearline storage nodes
  - Must be used to access Nearline
- GO interface
  - Blue Waters Portal (https://go-bluewaters.ncsa.illinois.edu)
  - globus-url-copy
  - Globus Command-Line Interface (CLI)
  - Create your own endpoint with Globus Connect
- GO also recommended for transferring large files between Lustre filesystems (*within* Blue Waters)

Globus Online Screenshot



Globus Online Characteristics

- Very high bandwidth
- Asynchronous
- Very parallel
- Uses dedicated resources
  - (avoids file I/O bottlenecks that make rsync/scp not tenable for files of significant size),

File Size/Number Considerations

- Globus Online designed for fewer, larger files
- Transferring enormous numbers (100,000+) of small files bogs down transfers
- Packaging up small files into larger before transferring to nearline is better

File Transfers for Training Accounts

- Need to pull on to Blue Waters from *local* site.
- rsync, scp, wget, curl for smaller files on hosting services like box.com (sftp) and SeedMe (wget or curl).
- For large files we recommend using Globus Online by way of Globus Connect Personal client.
- See Blue Waters portal page Data Transfer for Education and Training Allocations for more information.

Important Help Topics:

- If you forget your PIN:
  - https://bluewaters.ncsa.illinois.edu/forgot-pin
  - go to https://otp.ncsa.illinois.edu/
  - authenticate using your security questions, then reset your PIN

Important System Commands

- quota
  - individual and group amounts and quotas
- usage
  - your system compute-time allocation
- man (contains *official* Cray documentation)
  - example: man crayftn

Blue Waters Support

- Documentation
  - BW Portal (https://bluewaters.ncsa.illinois.edu/)
    - Documentation => User Guide
- System status
  - Portal
  - MOTD (Message Of The Day)
  - Broadcast e-mails from admins
- Help – SEAS team
  - Phone, chat, e-mail
    - JIRA

Blue Waters Support (continued)

- SEAS team (Science and Engineering Applications Support)
  - Phone*: (217) 244-6689
  - Chat (portal)*: Your Blue Waters => Live Chat
  - JIRA ticket system
    - Portal: Your Blue Waters => Your Tickets
    - E-mail: help+bw@ncsa.illinois.edu
  - One support tier for all problems
    - Basic (logging in) to advanced (software debugging and optimization)

* Monitored M-F 9am – 5pm Central Time

Please Submit Tickets If:

- Documentation on something is
  - wrong
  - missing
- Something doesn't work right
- Something doesn't work the way you expected
- Something doesn't work the way it used to
- You're not sure how to proceed and you want to do it right the first time

- Don't be afraid to submit tickets; it helps us self-evaluate
- The same people triage tickets as monitor the phone and chat

Help Information on Portal