

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

February 11, 2015

Getting Started on Blue Waters



GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY®

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

SUSTAINED PETASCALE COMPUTING

[SIGN IN](#)

[YOUR BLUE WATERS](#)
[SYSTEM STATUS](#)
[DOCUMENTATION](#)
[EDUCATION](#)
[IMPACT](#)
[ABOUT](#)
[HELP](#)
[RESOURCES](#)

Current views of job placement and activity

Machine Status

SUB-SYSTEM	STATUS
Login Nodes	Up
Scheduler	Up
Compute Nodes	Up
Network	Up
Storage	Up
Nearline Storage	Up

USAGE

The current usage of the Blue Waters compute nodes is presented below in a table on the left, as a sum of both XE and XK nodes in the first pie chart, and by individual node types below. The state of the compute nodes can be one of: "In Use" - nodes allocated to jobs; "Idle" - nodes not allocated or reserved to a job; "Draining" - nodes reserved for a job but could be used by a backfilled job; and "Down" - nodes not available for running jobs.

Nodes:

- 1892 XK Nodes In Use
- 14543 XE Nodes In Use
- 359 XK Nodes Idle
- 3517 XE Nodes Idle
- 1957 XK Nodes Draining
- 4560 XE Nodes Draining
- 16 XK Nodes Down
- 20 XE Nodes Down

Total Node usage

- XK In Use
- XE In Use
- XK Draining
- XE Draining
- XK Idle
- XE Idle
- Other

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)

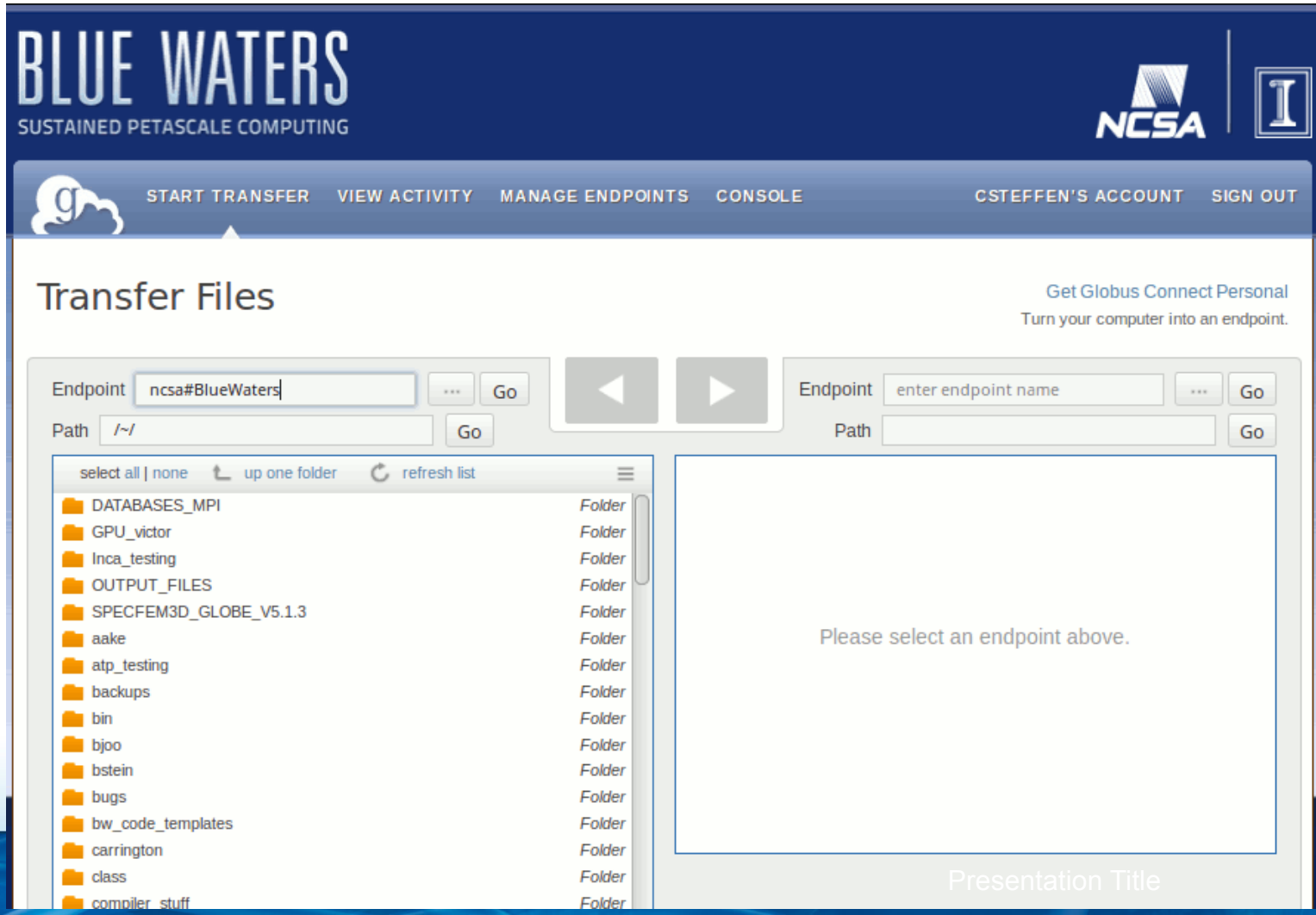
Storage System Type+Name	Default Quota	Quota Type	Purge Policy?	Sample Path	Globus Endpoint
Lustre home	1 TB	user	no	/u/sciteam/me	ncsa#BlueWaters
Lustre projects	5 TB	group	no	/projects/sciteam/jxx	ncsa#BlueWaters
Lustre scratch	500 TB	group	YES (30 days)	/scratch/sciteam/me	ncsa#BlueWaters

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



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NCSA

START TRANSFER VIEW ACTIVITY MANAGE ENDPOINTS CONSOLE CSTEFFEN'S ACCOUNT SIGN OUT

Transfer Files

[Get Globus Connect Personal](#)
Turn your computer into an endpoint.

Endpoint ... Go

Path Go

select all | none up one folder refresh list

- DATABASES_MPI Folder
- GPU_victor Folder
- Inca_testing Folder
- OUTPUT_FILES Folder
- SPECFEM3D_GLOBE_V5.1.3 Folder
- aake Folder
- atp_testing Folder
- backups Folder
- bin Folder
- bjoo Folder
- bstein Folder
- bugs Folder
- bw_code_templates Folder
- carrington Folder
- class Folder
- compiler_stuff Folder

Endpoint ... Go

Path Go

Please select an endpoint above.

Presentation Title

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)

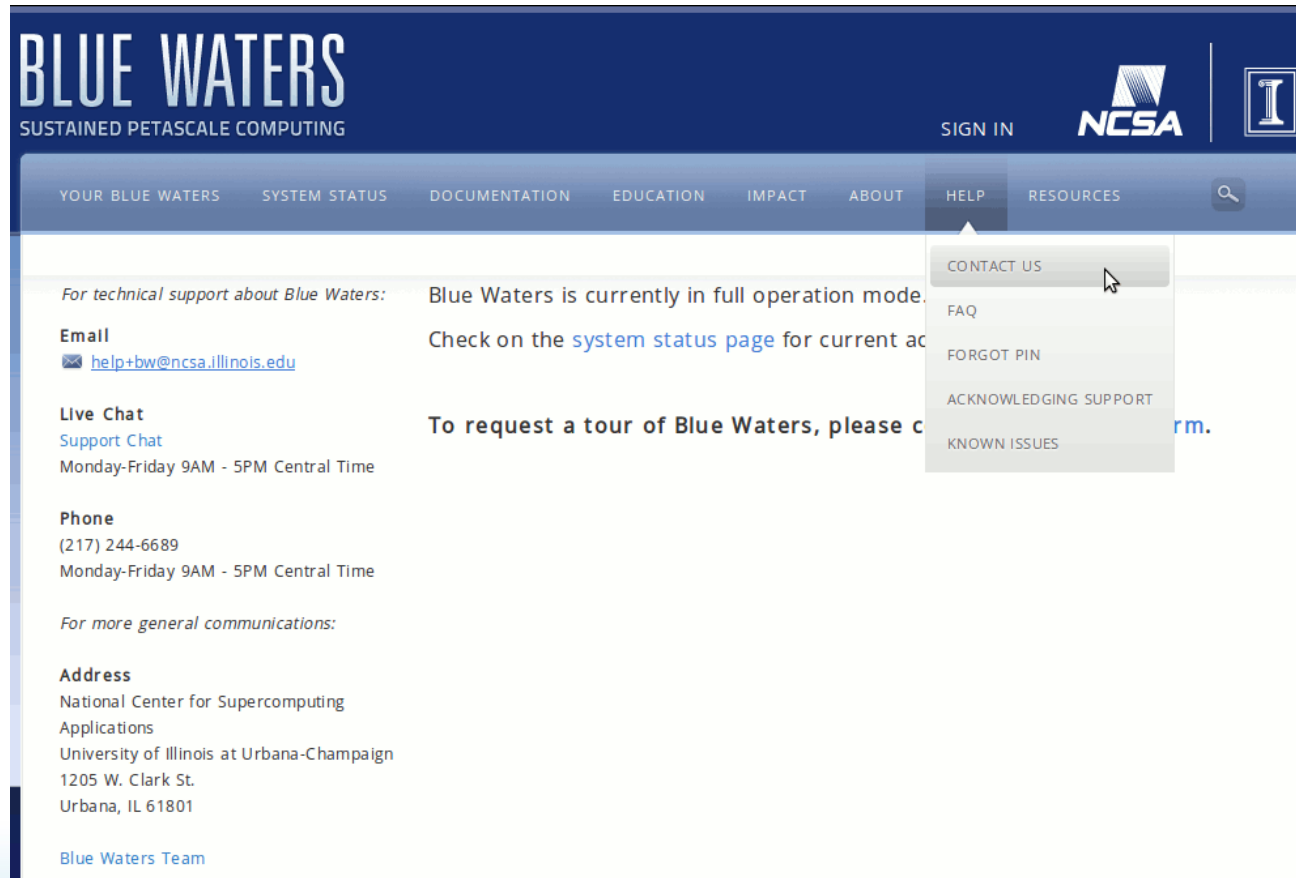
- SEAS team (Science and Engineering Applications Support)
 - Phone*: (217) 244-6689
 - Chat (portal)*: Your Blue Waters => Live Chat
 - JIRA ticket system
 - Portal: Your Blue Waters => Your Tickets
 - E-mail: help+bw@ncsa.illinois.edu
 - One support tier for all problems
 - Basic (logging in) to advanced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



The screenshot shows the Blue Waters portal's help page. The header includes the Blue Waters logo, navigation links (YOUR BLUE WATERS, SYSTEM STATUS, DOCUMENTATION, EDUCATION, IMPACT, ABOUT, HELP, RESOURCES), and a search icon. The 'HELP' menu is open, showing options: CONTACT US, FAQ, FORGOT PIN, ACKNOWLEDGING SUPPORT, and KNOWN ISSUES. The main content area provides contact information for technical support, including email, live chat, and phone, along with the physical address of the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign.

BLUE WATERS
SUSTAINED PETASCALE COMPUTING

SIGN IN  

YOUR BLUE WATERS SYSTEM STATUS DOCUMENTATION EDUCATION IMPACT ABOUT **HELP** RESOURCES

For technical support about Blue Waters:

Email
✉ help+bw@ncsa.illinois.edu

Live Chat
[Support Chat](#)
Monday-Friday 9AM - 5PM Central Time

Phone
(217) 244-6689
Monday-Friday 9AM - 5PM Central Time

For more general communications:

Address
National Center for Supercomputing
Applications
University of Illinois at Urbana-Champaign
1205 W. Clark St.
Urbana, IL 61801

Blue Waters Team

Blue Waters is currently in full operation mode.
Check on the [system status page](#) for current ac

To request a tour of Blue Waters, please c

CONTACT US
FAQ
FORGOT PIN
ACKNOWLEDGING SUPPORT
KNOWN ISSUES