

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

5/20/13

Blue Waters User Monthly Teleconference



GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY®

Agenda

Topics for this webconference:

- XK Upgrade Update.
- Resource Management and Job Scheduling
- Allocation usage monitoring.
- Storage matters.
- April Programming Environment.
- Other Updates.
- Executive Advisory Committee Involvement
- Request for publications, presentations, ...
- Upcoming Events
- Topics for future Blue Waters Users telecons/webinars.
- Open Discussion

XK Upgrade Status

- Reminder of upgrade specifics
 - 12 more XK cabinets moves total to 4,224 XK nodes.
 - Increase of overall torus dimension to 24x24x24.
 - XK region of torus improves aggregate bandwidth.
- The start date of the compute system outage has been moved back by 4 weeks.
- New outage to begin June 24th.
- Please contact us if this outage conflicts with your ability to meet deadlines.

Resource Management and Job Scheduling

- Upgraded to Torque 4.2.x and Moab 7.2.x
 - Some new issues: torque responsiveness.
 - Job suffix will change again.
- Job scheduling priorities (in progress)
 - Change from QOS-based to queue-based scheme.

QUEUES	Priority (1 highest)	Charge Factor	Preemptible
Debug	1	1	No
High	2	2	No
Normal	3	1	No
Low	4	.5	Yes

Allocation monitoring

- Usage monitoring from portal being enhanced.
 - Improved hierarchical view in progress.
- usage command now available on login nodes.

```
> usage -h
```

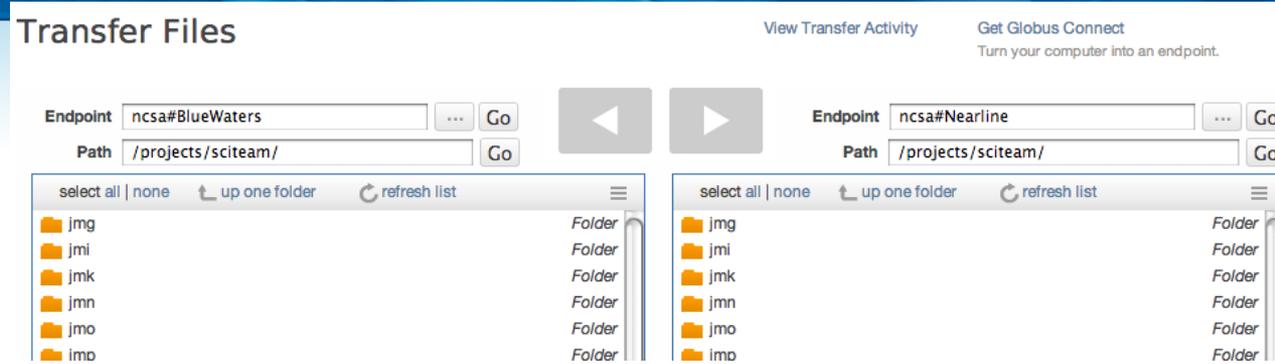
```
usage [ -p proj ] [ -u login ] [ -m mach ] [ -t [ pmu ] ] [ -s start-date ] [ -e  
end-date ] [ -l period ] [ -r ] [ -a ] [ -i ] [ -h ]
```

- date – m/d/y (e.g. 05/20/13)
- period – 1d (one day) , 2w (two weeks), 3m ...
- Shows multiple projects that you belong to.
- Provides total project usage.
- Handles queue charging.

Speaking of Usage

- Utilization of the XE portion of the system has been at times low since charging started.
- Blue Waters is fully allocated.
- Need to avoid end of allocation period congestion.
- Proceeding with queue charging to encourage use of available cycles.
 - “low” queue category with lower charge factor.
- Continue to refine quarterly “return” concept to promote steady usage.
- We are working to provide “usage rate” tools on the portal and notification via email. This will include some projected usage including possible return.

Storage



- HPSS
 - Note the presence of Lustre and Nearline /projects
- Quotas
- Purging
 - Enabled with file last access and file last modified greater than 30 days. More the 220 million files were eligible.
- Data Movement
 - Limitations to Globus Online (GO).
 - Analyzing options for additional features.

	HOME	SCRATCH	PROJECTS
LUSTRE FILESYSTEM	1 TB (user)	500 TB (grp)	5 TB (grp)
HPSS NCSA#NEARLINE	5 TB (user)	N/A	50 TB (grp)

April Programming Environment (PE)

- Defaults for some modules changed to newer versions in line with the April PE release.
- New features
 - cray-mpich2 – (5.6.4) MPICH_G2G_PIPELINE - larger buffers of pipelining GPU-to-GPU messages (wait for CLE upgrade), (5.6.3) MPICH_RDMA_ENABLED_CUDA - MPI application to pass GPU pointers directly to point-to-point and collective communication functions.
 - CrayPAT and PAPI - Support for gemini network counters.
 - PGI 13.3 - Support for CUDA5.
- Bug fixes
 - CCE 8.1.7 – Numerous issues fixed.
- Future PE changes
 - Likely will involve recompilation/linking. Several months away.

Other Updates

- Removal of old packages.
- On the [Portal](https://bluewaters.ncsa.illinois.edu) (<https://bluewaters.ncsa.illinois.edu>)
 - About > [Science Teams](#)
 - Information about teams from different allocation categories
- CUDA 5.5 in October possibly.

Executive Advisory Committee

- We are forming an Executive Advisory Committee composed of NSF PRAC members, and other allocated user groups.
- We are looking for nominations or self-nominations.
- Quarterly Meeting requirements: one meeting in-person, three by videoconference.

Request for publications, presentations, ...

- We need to be current on products that result from time on Blue Waters such as:
 - Publications, Preprints (e.g. [arXiv.org](https://arxiv.org) ), Presentations.
- Appreciate updates sooner than annual reports.
- NSF PRAC teams send information to PoCs.
- See the [Share Results](#) section of the portal as well.

Upcoming Events

- Next Blue Waters User webinar June 17th.
- Blue Waters PRAC Symposium May 21 – 22.
- New User Workshop May 22 – 23.
- See the [Workshops](#) portal page for more information.

- Topics for future teleconferences / webinars
- Open Discussion