Blue Waters User Monthly Teleconference
Extreme Scaling Workshop 2013

• Successful workshop in Boulder.
• Presentations from 4 groups with allocations on Blue Waters. Industry representatives were present.
• We look forward to seeing more groups presenting at the next workshop.

https://www.xsede.org/web/xscale/
Agenda

Topics for this webconference:
• XK Upgrade Status
• Other changes.
• Friendly User Period
• July Programming Environment
• Job node shape specification
• Blue Waters Governance
• Request for publications, presentations, …
• Upcoming Maintenance Event
• Future Blue Waters Users telecons/webinars
  • Advanced Kepler features, NVIDIA, September 16th
XK Upgrade Status

Upgrade mostly complete

- 12 additional XK cabinets ups total to 4,224 XK nodes. Currently 3,840 XK nodes available.
- Increase of overall torus dimension to 24x24x24.
- Changes to XK node shape: from 8x8x24 to 15x6x24.
  - Improves aggregate bandwidth.
  - Relocation of IO blades into XK region.
• XE
• XK
• LNET (IO)
• MOM
• Other
Other changes

• Upgraded to Torque 4.2.4 and Moab 7.2.4.
  • Resolved many bugs.
  • Improved responsiveness under large job launch.
• CLE 4.2 UP01
  • Improvements in node health check (NHC).
  • Improvements in aprun usage reporting.
  • See documents at http://docs.cray.com/relnotes/ for more information.
Friendly User Period

- August 15\textsuperscript{th} – August 24\textsuperscript{th} (7 AM)
- Charging factor set to 1/10\textsuperscript{th} the production value for each queue.

- We have seen numerous congestion protection events. For some applications we have recommended setting APRUN\_BALANCED\_INJECTION to 64 while we analyze the system and the applications. Please see https://bluewaters.ncsa.illinois.edu/balanced-injection for more information.
July Programming Environment

- Will become default programming environment on August 28th.
- Statically linked applications should not require any changes.
- Dynamically linked applications (OpenACC and CUDA) require proper modules to maintain build environment or rebuild with new default environment.
- New MPICH features and functionality:
  - Merging of ANL MPICH 3.0.3
  - MPI-3 features: non-blocking collectives, RMA-3, Neighborhood Collectives, Mprobe and related functions.
  - MPI-2: "external32" data representation is now supported.
  - Improved MPI_Alltoall performance for 8 byte to 2K byte sized messages at large core counts.
  - cray-mpich module replaces cray-mpich2 module.
Known Issues

- Building a FORTRAN MPI application using MPT 6.0.1 under GNU 4.8 environment with static linking generates warning messages
  - `/usr/bin/ld: Warning: alignment 16 of symbol `mpifcmb8_' in /opt/cray/mpt/6.0.1/gni/mpich2-gnu/48/lib/libmpich-gnu_48.a(setbot.o) is smaller than 32 in /tmp/cc4vg3so.o`
List of latest releases up to July PE

• CCE 8.1.9
• atp 1.6.3
• lgdb 2.1.0
• stat 2.0.0.1
• cray-mpich 6.0.1
• cray-ga 5.1.0.2
• perftools 6.1.1
• papi 5.1.1
• papi-acc 5.1.1
• Apprentice2 for Windows 7 6.1.1
• Apprentice2 for Mac 6.1.1
• acml 5.3.0
• fftw 2.1.5.5
• fftw 3.3.0.3
• petsc 3.3.06
• trilinos 11.2.2.0
• cray-libsci 12.1.01

http://docs.cray.com/relnotes/

• tpsl 1.3.04
• libsci_acc 2.1.00
• ddt-4.0.0.0_31795
• GNU 4.8.1
• PGI 13.6.0
• cudatoolkit 5.0.35
• cray-gdb 7.5.1
• cray-hdf5 1.8.11
• cray-netcdf 4.3.0
• parallel-netcdf 1.3.1
• iobuf 2.0.4
• java jdk1.7.0_07
• libonesided-ntk 1.5.0
• cray-gcc-gmp 4.3.2
• cray-gcc-mpc 0.8.1
• cray-gcc-mpf 2.4.2
• cray-gcc 4.8.1
Job node shape specification

- To improve application consistency and performance, we are working to provide by request node allocations in two defined shapes: XZ sheets and XYZ cubes, at common node counts.
- The resource handler finds the appropriate shape or shapes to satisfy the node count requested. Charged for node count requested. Excess nodes available for users.
- Most performance tests to date favor XZ sheets over cubes.
- This is an interim solution while our work with Adaptive on topology aware node allocation.
Blue Waters Governance

- We are looking for participation in the Blue Waters User Executive Advisory Committee (UEAC).
- We will send out details for the positions and a request for recommendations (including self-nomination) later.
- The GLCPC, Illinois and Education allocations will also be represented.
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), 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

• Maintenance Outage August 24 – 27.
  • Needed to complete the XK upgrade.
  • Logins, file systems and HPSS will be available.
• Next Blue Waters User webinar September 16th.
  • Presentation by NVIDIA on advanced Kepler features.
• Next Blue Waters Workshop early December.
Upcoming Events

  - Four Points Sheraton, Schiller Park, IL (near ORD)
  - Two tracks: User and Developer
  - Experiences with using PTP for developing large scientific applications
  - Tips and strategies for maximizing the productive use of PTP
  - Shortcomings with, and possible extensions to, the existing functionality
  - Using PTP for developing applications for hybrid heterogeneous or many-core systems
  - Using PTP for Python, Perl, or other interpreted language development
  - Static or dynamic analysis tools that could be integrated with PTP
  - Support for additional runtime systems or schedulers
  - Other tools that would benefit the PTP community
  - [http://www.ncsa.illinois.edu/Conferences/Eclipse](http://www.ncsa.illinois.edu/Conferences/Eclipse)
Future Topics?

• Please send us your suggestions on topics for future teleconferences / webinars