June 2014 Programming Environments Release Announcement for Cray XE and Cray XK Systems

The following product/versions are released:

**Product/Version**

Cray Compiling Environment 8.3.0
CCE 8.3.0

Cray Message Passing Toolkit 7.0.0
MPT 7.0.0
PMI 5.0.4
Global Arrays 5.1.0.5
cray-mpich-compat 1.0.0

Cray Performance Measurement & Analysis Tools 6.2.0
Perftools 6.2.0
Papi 5.3.1
Apprentice2 for Windows7 6.2.0
Apprentice2 for Mac 6.2.0

Cray Scientific and math libraries 7.3.0
LibSci 13.0.0
LibSci_acc 3.0.2
PETSc 3.4.4.0
Trilinos 11.8.1.0
TPSL 1.4.1
FFTW 3.3.4.0
FFTW 2.1.5.7
ACML 5.3.1 (XE/XK only)

Cray Environment Setup and Compiling support 5.42
Craype 2.1.2
Xt-asyncpe 5.27

Cray debugger Support Tools 2.3.0
ATP 1.7.3
LGDB 2.3.1
STAT 2.1.0.1
dwarf 14.2.0

Cray Third party products 5.41
GCC 4.8.1 and 4.8.2 rerelease
GCC 4.9.0
HDF5 1.8.13
NetCDF 4.3.2
Parallel-NetCDF 1.4.1

PGI
PGI 14.4.0

DDT
DDT 4.2.2.1.36484

Cray Application Developer's Environment 6.32
CADE 6.32

These products are available for download from CrayPort at:
NOTE: MPT 7.0 ABI compatibility change in this release.
An ABI change in the MPT 7.0 release requires all MPI user code to be recompiled. Scientific libraries, Performance Tools, Cray Compiling Environment and third party libraries compatible with the new ABI are included in this PE release.

NOTE: CLE versions supported by PE change.
Beginning in June 2014 the PE releases will no longer support CLE 4.0, 4.1 and 5.0 releases. CLE 4.0, CLE 4.1 and CLE 5.0 operating systems can continue to run PE products released prior to June 2014. Problems found with PE products on CLE 4.0, 4.1 and 5.0 systems will be addressed in releases for CLE 4.2 and CLE 5.1 and later releases only. Upgrading to a later release will be required to get these fixes.

NOTE: Craype required with CLE 5.2 on Cray XE/XK systems.
CLE 5.2.UP00 requires the March 2014 (CDT 1.14) or later Programming Environment release. CLE 5.2 requires the Craype 2.1.0 or later. On Cray XE and XK systems, Craype replaces xt-asyncpe which is deprecated and not compatible with CLE 5.2.

NOTE: New craypkg-gen product for generating module files for third party products.
The craypkg-gen feature allows users to create modulefiles for third party products such as Intel Composer and PGI compiler. The Intelsup and pgisup packages will no longer be released.

NOTE: Cray PE monthly releases changing to first Thursday of the month.
The PE updates were previously targeted for the third Thursday of each month. Beginning in June 2014, the PE updates will be targeted for the first Thursday of the month.

General Installation Instructions:
For general installations on Cray XE and XK systems, please see Cray Programming Environments Installation Guide S-2372-113. S-2372-113 is available at http://docs.cray.com/

Test Platforms:
These products were tested on:
Cray XE and XK systems running CLE 4.2 UP02 and CLE 5.2 UP00.

Compilers for Cray Libraries:
Libraries in this announcement require these minimum compiler versions:
Note: Because these compilers are used to build the libraries, the libraries may not be compatible with object files built with older compilers.
- CCE 8.3.0
- Intel 14.0.1
- GNU 4.8 and GNU 4.9
- PGI 14.1.0
- PathScale 4.0.9 (CLE 4.2 only)
  For the PathScale compiler, Cray only provides MPT libraries.

Please see specific product release announcements for additional library and compiler dependencies.
Cray Compiling Environment 8.3.0
CCE 8.3.0

Purpose:
CCE 8.3.0 provides Fortran, C, and C++ compilers for Cray XE, Cray XK, Cray XC and Cray CS300 systems.
NOTE: A new FlexNET license key is required for CCE 8.3.0.

The CCE 8.3.0 release provides the following key enhancements:
- To provide the basis for future C++11 support, a critical interface change requires a complete rebuild of all C++ libraries and applications when you move to CCE 8.3.
- The new option -h develop selects compiler optimization levels to balance compile time against application execution time. This option is intended for use during application development, when quick turnaround is desired. It minimizes compile time at the cost of some execution time performance.
- The new option -h flex_mp=strict is introduced to provide a level between -h flex_mp=conservative and -h flex_mp=intolerant. Other general improvements have also been made for -h flex_mp.
- The new option -h concurrent is equivalent to adding a CONCURRENT directive (pragma) before every loop in the file, including loops created from array syntax. This option may provide significant performance improvements for some codes. Care must be taken as improper usage may result in application errors.
- Support for Intel Haswell processors
- General performance improvements for Cray XE, Cray XK, and Cray XC30 systems.

Cray accelerator systems:
- The craype-accel-host module supports building OpenACC applications to be targeted to run on the X86 host processor. This provides source code portability between systems with and without an accelerator.
- The -Wx,arg and the -Wc,arg options can be used to pass command line arguments to the PTX assembler and the CUDA linker, respectively.
- The -h acc_model=fast_addr performance option is now safe for all OpenACC applications and is enabled by default.
- Limited use of Fortran character strings in OpenACC constructs is now supported.
- Multiple GPUs per node are now supported for OpenACC applications on Cray CS300 systems. Each host MPI rank can be mapped to a single GPU device for the duration of the application.

Library and programming model features:
- For applications using UPC, the new cray_upc_sheap_info() call provides symmetric heap usage information, and the new cray_upc_shared_cast() call creates a pointer-to-shared from a pointer-to-local.
- For Fortran applications, a string identifying MPI rank and OpenMP thread ID begins each line written to stdout and stderr.

Additional details can be found in the "Cray Compiling Environment 8.3 Release Overview and Installation Guide", S-5212-83.
Bugs Closed with CCE 8.3.0 release:
- 789247 Inlining bug in NEK5000 code
- 790921 Program termination when copying derived data types with allocatable components
- 802615 llvm abort
- 802618 Max record length for Fortran unformatted I/O
- 803045 Can we prepend each line of stdout and stderr with the thread that generated it?
- 803050 Can we prepend each line of stdout and stderr with the PE that generated it?
- 806236 Zero-sized arrays cause -Rb to issue incorrect warnings
- 806708 Cray compiler fails with an OpenACC code
- 807313 segmentation fault in optimizer
- 807422 Improve compiler behavior if TMPDIR does not exist
- 807997 Internal compiler error (ftn-7991) for no reason
- 808139 incorrect behavior with -G2
- 808592 ICON code not working with cce/8.2.1
- 808988 can't encode register '%ah' in an instruction requiring REX prefix.
- 809644 Internal error 'Function Pass Manager' on Optimization -O2 or higher
- 809742 Internal compiler error
- 809781 ICE when using program library and large character length
- 810106 Fortran Compiler possible vectorisation BUG with IFS
- 810365 Ktrap does not work with dynamically linked executables
- 810416 Compiler optimisation gives incorrect results
- 810675 Slow compilation optcg COALESCE_ANALYSIS
- 810761 INTERNAL COMPILER ERROR: "found dereference of host pointer on accelerator"
- 811007 SPEC ACCEL V1.0 suite: simple source gives "Unshaped C pointer" error.
- 811175 Ramses3d gives collapse errors at higher optimization levels
- 811333 Internal compilation error with cray ftnc
- 811502 Ramses3d gives internal diagnostics with NAN at runtime at -O3
- 811606 nvlink error : Undefined reference

Notes and Limitations:
Shared objects (binaries or shared libraries) built with CCE 8.2 (or earlier) are incompatible with those built with CCE 8.3. Mixing shared objects built with CCE 8.2 (or earlier) with those built with CCE 8.3 may encounter missing symbols at runtime.

Dependencies:
The CCE 8.3.0 release is supported on
- Cray XE and XK systems with the CLE 4.2 and CLE 5.2.
- Cray XC systems with the CLE 5.1 and CLE 5.2
- Cray CS300 systems running CentOS 6.2/6.3/6.4 and Redhat 6.2/6.3/6.4.

For Cray XE and XK systems the following products are required:
- Cray Compiler Drivers
  - xt-asynccpe 5.27 or later for systems with CLE 4.2
  - CrayPE 2.1.2 or later for systems with CLE 5.2
- GNU GCC 4.8.1 must be installed but does not need to be the default GCC
- Cray Scientific Libraries (LibSci) 13.0.0 or later
- PMI 4.0.0 or later
For Cray XC30 systems the following products are required:
  o  Cray Compiler Drivers (CrayPE) 2.1.2 or later
  o  GNU GCC 4.8.1 must be installed but does not need to be the default GCC
  o  Cray Scientific Libraries (LibSci) 13.0.0 or later
  o  PMI 4.0.0 or later

For Cray CS300 systems the following products are required:
  o  Cray Compiler Drivers (CrayPE) 2.1.2 or later
  o  GNU GCC 4.8.1 must be installed.
  o  Cray Scientific Libraries (LibSci) 13.0.0 or later

The CCE 8.3 release requires the following minimum versions if these products are used:
  o  HDF5 1.8.13
  o  NETcdf 4.3.2
  o  parallel-NETcdf 1.4.1
  o  MPT 7.0.0
  o  GA 5.1.0.5
  o  LibSci_acc 3.0.2
  o  TPSL 1.4.1
  o  PETSc 3.4.4.0
  o  Trilinos 11.8.1.0
  o  fftw3 3.3.4.0
  o  fftw2 2.1.5.7
  o  Perftools 6.2.0
  o  Reveal 1.4

Installation instructions:
To install the CCE, programming environment:
   rpm -ivh cce-8.3.0-188.x86_64.rpm

To make CCE 8.3.0 the default version of CCE, execute:
   /opt/cray/admin-pe/set_default_files/set_default_cce_8.3.0

License:
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Attribution notices for open source licensed software contained in this package are detailed in the file:
   /opt/cray/cce/8.3.0/ATTRIBUTIONS_8.3.txt

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Cray Message Passing Toolkit 7.0.0
MPT 7.0.0
Purpose:
The following feature was added to MPT 7.0.0 over MPT "6.3.1":

NOTE: MPI USERS WILL NEED TO RECOMPILE and RELINK!!!

The MPT 7.0.0 release adheres to the “MPICH ABI Compatibility Initiative” formed last year by Cray, ANL, Intel and IBM for MPICH ABI compatibility. See [https://www.mpich.org/abi/](https://www.mpich.org/abi/) for more information about this initiative. Cray believe this initiative will reduce the number of ABI incompatibilities in the future. The MPICH ABI Compatibility Initiative will allow moving dynamically linked applications between MPICH compatible versions on similar supported processors without recompiling in the near future. In addition, Cray will be creating documentation to assist users in future releases as more of the involved vendors release compatible versions.

The MPT 7.0.0 is based on MPICH 3.1 from ANL. Because the MPI API has not changed in MPT 7.0.0, no source changes are needed from code written for MPT 6.x.x versions. Cray supported libraries with dependencies on MPI are also being released and must be used with MPT 7.0.0 libraries. Below is a complete list of compatible libraries/products. To assist users in moving between sets of compatible libraries and products see the notes below concerning the cray-mpich-compat modules.

- Cray libraries/modules that are to be used together:
  - cray-mpich/7.0.0 or newer
  - cray-libsci/13.0.0 or newer
  - cray-libsci_acc 3.0.2 or newer
  - fftw/2.1.5.7 or newer
  - fftw/3.3.4.0 or newer
  - cray-tpsl/1.4.1 or newer
  - PETSc 3.4.4.0 or newer
  - Trilinos 11.8.1.0 or newer
  - cce/8.3.0 or newer
  - cray-hdf5-parallel/1.8.13 or newer
  - cray-netcdf-hdf5parallel/4.3.2 or newer
  - cray-parallel-netcdf/1.4.1 or newer
  - cray-ga/5.1.0.5 or newer
  - perftools/6.2.0 or newer
  - chapel 1.9.0.1 or newer

- To assist users changing between MPT 7.x.x and MPT 6.x.x. compatible libraries, two new modules are provided:
  cray-mpich-compat/v7
  cray-mpich-compat/v6

Assuming the scenario where modules are loaded to run an application using MPT 6.x.x libraries. If a "module load cray-mpich-compat/v7" is performed, the latest version of MPT 7.x.x and compatible libraries and products will be swapped based on the module list that were previously loaded. If any compatible libraries or products are not available, a message will be displayed and no additional modules will be swapped. To go back to the latest version of the MPT 6.x.x and the latest compatible versions of the libraries, a user can module swap back to cray-mpich-compat/v6. Note: The modulefile does not remember the specific previous library and product versions, rather it uses the latest installed versions that are compatible. Type “module help cray-mpich-compat/v7” for more information.
o Support for Intel Haswell processors

o MPI_Bcast performance improvement. A generic K-ary tree algorithm for MPI_Bcast has been implemented. Initial results show around 20% improvement for small and large messages and up to 40% improvement in the 8K-64K message range. See the MPICH_BCAST_INTERNODE_RADIX and MPICH_BCAST_INTRANODE_RADIX env variables for more info. Setting MPICH_COLL_OPT_OFF=MPI_Bcast disables this optimization.

o The MPI_Alltoallv throttle env variable default has been changed for XC systems. The MPICH_ALLTOALLV_THROTTLE env variable sets the per-process maximum number of outstanding Isends and Irecvs that can be posted concurrently and the new default is now 8 on XC systems instead of 1 for XE/XK systems. This can substantially improve (3-4x on Haswell) the performance of small-medium sized MPI_Alltoallv transfers. For very large transfers, the higher throttle value has shown a performance degradation over the previous default of 1, but the performance gain for all other message sizes outweigh this. The user is still free to set the throttle to any value they desire by setting the MPICH_ALLTOALLV_THROTTLE env variable.

o Support for the GCC 4.9.0 compiler

Incompatibilities/Differences:
- Binary incompatible with MPT 6.x.x or older
- Dropping support for GCC 4.7
- Maximum tag reduced from 4194303 to 2097151

The following bugs were fixed since MPT "6.3.1":
- 795128 - MPI I/O Seg Faults when using MPI_Type_hindexed
- 809147 - MPICH_USE_DMAPP_COLL and MPICH_RMA_OVER_DMAPP used together assert at termination

Product and OS Dependencies:
The Cray MPT 7.0.0 release is supported on the following Cray systems:
- Cray XE and XK systems running CLE 4.2
- Cray XC systems with CLE version 5.1 or later

Product and OS Dependencies by network type:

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<thead>
<tr>
<th></th>
<th>Gemini(XE)</th>
<th>Aries(XC)</th>
</tr>
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<tbody>
<tr>
<td>xt-asyncpe</td>
<td>&gt;=5.27</td>
<td>N/A</td>
</tr>
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<td>&gt;=2.1.2</td>
<td>&gt;=2.1.2</td>
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<tr>
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<tr>
<td>cray-libxpmem-devel</td>
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### cray-libdmapp

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<tbody>
<tr>
<td>cray-libdmapp</td>
<td></td>
<td></td>
</tr>
<tr>
<td>cray-libdmapp-devel</td>
<td>&gt;=4.0.1</td>
<td>&gt;=7.0.1</td>
</tr>
<tr>
<td>alps</td>
<td>default</td>
<td>default</td>
</tr>
</tbody>
</table>

### Documentation:
For more information see the intro_mpi and intro_shmem man pages.

### Modulefile:

**module load cray-mpich/7.0.0**

> The cray-mpich2 modulefile has been deprecated with this release. Please update any site configurations to load the cray-mpich instead of the cray-mpich2 modulefile.

### Installation:

```
rpm -ivh cray-mpich-*-7.0.0-gni1_10180.x86_64.rpm
```

The "*" in the install command represents compiler version combinations.

To make this the default version, execute:

```
/opt/cray/admin-pe/set_default_files/set_default_mpt_7.0.0
```

### PMI 5.0.4

**Purpose:**
The Cray Process Manager Interface Library provides the interface between the application launching facility (ALPS) and other communication libraries such as MPICH and SHMEM.

**Installation:**

```
rpm -ivh cray-libpmi0-5.0.4-* cray-libpmi-devel-5.0.4-*
```

### Global Arrays 5.1.0.5

**Purpose:**
This release fixes

- an assertion failure observed in GA's registration cache
**Dependencies:**
The Global Arrays 5.1.0.5 release is supported on Cray systems running Cray Linux Environment (CLE) operating system
- Cray XE and XK systems with CLE version 4.1 UP01 or later
- Cray XC systems with CLE version 5.0 or later

The Global Arrays 5.1.0.5 release requires the following software products:

For Cray XE and XK systems:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later
- cray-libdmapp 4.0.1 (gem) or higher
- cray-mpich 7.0.0 or higher

For Cray XC systems:
- craype 2.1.2 or higher
- cray-libdmapp 7.0.1 (ari) or higher
- cray-mpich 7.0.0 or higher

One or more compilers:
- pgi 14.1 or higher
- gcc 4.8.0 or higher
- intel 14.0.1 or higher
- cce 8.3.0 or higher

One of the craype-hugepages* modules must be loaded.

**Documentation:**
See the man page: man globalarrays

For more information see Global Arrays home page:
http://www.emsl.pnl.gov/docs/global/

**Modulefile:**
module load cray-ga

**Installation Instructions:**
Global Arrays is now packaged into separate compiler specific RPMs to allow rpmbuild to correctly include compiler dependencies.

    rpm -ivh cray-ga-*-5.1.0.5-05.x86_64.rpm

The "*" in the install command represents compiler version combinations.

To make this the default version, execute:
    /opt/cray/admin-pe/set_default_files/set_default_ga_5.1.0.5
**cray-mpich-compa1t 1.0.0**

**Purpose:**
The cray-mpich-comapt modules facilitate switching between the MPT 7.0 and MPT 6.3 environments.

The cray-mpich-comapt/v7 module ensures that the currently loaded modules, at the time of loading it, are compatible with mpich 7.x.x

The following modules on this system are compatible:
cray-mpich/7.0.0
cray-shmem/7.0.0
cray-ga/5.1.0.5
cray-libsci/13.0.0
cray-libsci_acc/3.0.2
cray-tpsl/1.4.1
cray-petsc/3.4.4.0
cray-hdf5-parallel/1.8.13
cray-netcdf-hdf5parallel/4.3.2
cray-parallel-netcdf/1.4.1
cray-trilinos/11.8.1.0
cce/8.3.0

The cray-mpich-comapt/v6 module ensures that the currently loaded modules, at the time of loading it, are compatible with mpich 6.x.x

The following modules on this system are compatible:
cray-mpich/6.3.1
cray-shmem/6.3.1
cray-ga/5.1.0.4
cray-libsci/12.2.0
cray-libsci_acc/3.0.1
cray-tpsl/1.4.0
cray-petsc/3.4.3.1
cray-hdf5-parallel/1.8.12
cray-netcdf-hdf5parallel/4.3.1
cray-parallel-netcdf/1.4.0
cray-trilinos/11.6.1.0
cce/8.2.6

**Installation Instructions:**

```
rpm –ivh cray-mpich-comapt-1.0.0-4.x86_64.rpm
```

Cray Performance Measurement & Analysis Tools 6.2.0
Perftools 6.2.0

Purpose:
Provide performance measurement, analysis and porting tools support for Cray XC, Cray CS300, Cray XE and Cray XK systems.
NOTE: A new FlexNET license key is required for Perftools 6.2.0.

Key enhancements or changes from the previous release:
- perftools/6.2.0 is part of PE compatibility release with cray-mpich/7.0.0, cce/8.3.0 and libsci/13.0.0 (see "Dependencies" section below)
- Reveal 2.0 release
- Upgrade to PAPI 5.3.1
- Support Aries network counters with native slurm on XC systems
- Improved predefined HWPC group support on Cray CS300 systems
- Improved CrayPat-lite functionality on CS300 systems
- Support Cray XC systems with Xeon Phi codenamed Knights Corner in offload mode
- HTML output can now be generated from pat_report

Reveal 2.0
- Programs must be built with CCE 8.3 or later
- Improved scoping capability
- Loop instance and backtrace information in navigation panel
- "Scoping Tool" also available from "View" menu to scope loops (same view when right-clicking on individual loop in navigation panel to scope loop)
- More control for "scope all loops" feature (see "Edit List" button in Scoping Tool window)
- Threshold for scoping loops available in Scoping Tool (replaces need for top 10 loops in navigation panel)
- Feedback on inlined variables (where they came from) in scoping results window

craypat-lite
- functionality improvements for CS300 systems

pat_build
- Better instrumentation of user functions with GNU compiler
- DWARF processing has been improved to increase the number of entry points that are eligible for tracing
- PGAS trace group has been updated to support version CCE 8.3.0

pat_report
- pat_report html output option (see -f option on pat_report man page)
- I/O statistics available in default reports

PAPI
- Network performance counters for Gemini now only support event names that reside on network tiles in the form of "GM_<row>_<col>_*". All other forms are considered an invalid event name.
Miscellaneous improvements in the CPU performance counter events for Sandy Bridge and Ivy Bridge processors.

**Bugs Fixed:**
- 809127 - pat_build generates userWrapFunctions.c that cannot be compiled
- 809763 - perftools/6.1.4: IFS code hangs with instrumentation when run on multiple nodes
- 810145 - code segfault when instrumented with pat_build
- 810355 - perftools/6.1.4(93):ERROR:102: Tcl command execution failed: if { $knc_module }
- 810693 - pat_report - xf_next: Number of bytes (0) too small in record nnn of type 0
- 812494 -201405210923 - modules craype-accel-nvidia35 + papi cause pkg-config error at compile

**Known Problems:**
- 812411 - app2/6.2.0 calltree shows numerous repeated call sites incorrectly for GPU codes
- 812642 - Intermittent seg faults during exit with OpenMP programs built with Intel compiler

**Notes and Limitations:**
**Cray CS300 systems**
- perftools is only supported with the Cray Compiling Environment (CCE). The PrgEnv-cray must be loaded prior to using perftools.
- perftools only works with the MVAPICH implementation of MPI
- Programs must be dynamically linked.
- A subset of the predefined trace groups available on Cray XC and XE systems is supported. pat_build will issue a message if unsupported groups are requested.
- Run 'module help PrgEnv-cray' for information on how to access and use Cray software on a CS300 system.

**All systems**
This release is part of the Cray PE compatibility release. Please review minimum versions of cce, MPI and libsci needed for perftools/6.2.0 use under "Dependencies".

This release no longer supports the following on Cray XE, XK and XC systems:
- CLE 4.0
- CLE 4.1
- CLE 5.0

**Dependencies:**
This release depends on the following minimum product versions.
- Cray XE and XK systems with CLE 4.2 and CLE 5.2
- Cray XC systems with CLE 5.1 and CLE 5.2
- Cray CS300 systems running CentOS 6.2

**Cray systems excluding Cray CS300:**
- papi/5.3.1
- One or more compilers running these minimum versions:
  CCE 8.3.0
  GCC 4.8.0
Intel 13.1
PGI 14.1.0
  o Cray Compiler Drivers
xt-asyncpe 5.27 (CLE 4.2)
CrayPE 2.1.2 (CLE 5.2 and all XC systems)
  o cray-mpich/7.0.0
  o PMI 5.0.1
  o CUDA 5.5 (including cudatoolkit)
  o Cray Scientific Libraries (LibSci) 13.0.0
  o Chapel 1.8.0

Cray CS300 systems:
  o Cray Compiler Drivers (CrayPE) 2.1.0
  o CCE 8.3.0 (only supported compiler with perftools on CS300)
  o MVAPICH 1.9
  o CUDA 5.5 (including cudatoolkit)
  o LibSci 13.0.0
  o Libsci_acc 3.0.2

Non-Cray systems:
Apprentice2 is supported on non-Cray systems running
  o Windows 7 (for the desktop version of Cray Apprentice2)
  o Mac OSX 10.7.5 or later

Documentation:
See the intro_craypat, craypat-lite and associated man pages or the
Performance Analysis documents available at http://docs.cray.com/
  o Using the Cray Gemini Hardware Counters
  o Using the Aries Hardware Counters
  o Using the PAPI Cray NPU Component
  o Cray Performance Measurement and Analysis Tools Release Overview and Installation Guide
  o Using Cray Performance Measurement and Analysis Tools

Installation instructions:

Installation of PAPI on non-Cray CS300 systems:
    rpm -ivh cray-papi-5.3.1-4.x86_64.rpm

    To make PAPI 5.3.1 the default version of PAPI, execute:
    /opt/cray/admin-pe/set_default_files/set_default_papi_5.3.1

Installation of perftools on non-Cray CS300 systems:
    rpm -ivh perftools-clients-6.2.0-2.x86_64.rpm
    rpm -ivh perftools-6.2.0-2.x86_64.rpm

    To make perftools/6.2.0 the default version of perftools, execute:
    /opt/cray/admin-pe/set_default_files/set_default_perftools_6.2.0
Installation of perftools on CS300 systems:
See "Installing the Cray Programming Environment for CS300", S-2800-08 for installation instructions.

Installation of app2 remote client (+ server) on Mac systems:
Apprentice2Installer_6.2.0.dmg

The Cray Apprentice2 installer for Mac is included in the Perftools package. Download the Cray Apprentice2 installer onto a desktop or laptop running Mac OS. Double click on installer to begin installation. The installer will walk you through the process for your system.

Installation of app2 remote client on Linux desktops/laptops:
tar -xvzf perftools-remote-clients-6.2.0.tar.gz
cd perftools-remote-clients-6.2.0
./Install
Type 'yes' to agree to software license prior to rpm install.
If you're using modules software, load the perftools module to access the software.
module load perftools

Installation of app2 remote client (+ server) on Windows 7 systems:
Apprentice2Installer_6.2.0.exe

The Cray Apprentice2 installer for Windows is included in the Perftools/6.2.0 package. Download the Cray Apprentice2 installer onto a desktop or laptop running Windows 7. Double click on installer to begin installation. The installer will walk you through the process for your system.

PAPI 5.3.1
Purpose:
Bug fixes and support for Perftools 6.2.0

Documentation:
Visit the PAPI Reference pages for more information at:
http://icl.cs.utk.edu/projects/papi/wiki/Main_Page
And visit the PAPI website for the latest updates:
http://icl.cs.utk.edu/papi/

Cray Scientific and Math Libraries 7.3.0
LibSci 13.0.0
Purpose:
Cray LibSci 13.0.0 provides scientific libraries for Cray XE, XK, XC, and CS300 Systems. Cray LibSci is supported on the host CPU but not on the accelerator of Cray XK, XC, or CS300 systems.

The Cray LibSci 13.0.0 release provides the following:
Compatibility with CrayPE 2.1.2. NOTE: The default linking behavior has changed for GNU and Intel so that the single threaded version of libsci is used unless the OpenMP compiler flag is specified.

- Compatibility with Cray MPT 7.0.0.
- Introduced CrayBLAS support with optimizations for Haswell Processors.
- Introduced LAPACK/ScalAPACK support with optimizations for Haswell Processors.
- Added CrayBLAS support to dynamically change the number of threads used in a parallel region.
- Improved performance of CrayBLAS DGEMM for medium square matrices where $N \approx 200$-$1000$.
- Improved performance of CrayBLAS ZGEMM for IvyBridge Processors.
- Added selection of alternate algorithm for LAPACK routine DSYEV with improved performance (LIBSCI_OPT_DSYEV=1).
- Added selection of alternate algorithm for LAPACK routine ZHEEV with improved performance (LIBSCI_OPT_ZHEEV=1).

Cray LibSci 13.0.0 includes the following versions of publicly available libraries:

- LAPACK 3.5.0 - For further information, see http://www.netlib.org/lapack
- ScalAPACK 2.0.2 - (Scalable LAPACK) For further information, see http://www.netlib.org/scalapack.

Product and OS Dependencies:
The Cray LibSci 13.0.0 release is supported on the following Cray systems:

- Cray XE and XK systems with CLE 4.2 and CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.
- Cray CS300 systems with CentOS 6.2/6.3/6.4 and Redhat 6.2/6.3/6.4.

The Cray LibSci 13.0.0 release requires the following software products:

For Cray XE and XK systems:

- xtasyncpe 5.27 or later / craype 2.1.2 or later
- MPT 7.0.0 or later

One or more compilers:

- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later
- PGI 14.1.0 or later

For Cray XC series systems:

- craype 2.1.2 or later
- MPT 7.0.0 or later

One or more compilers:

- CCE 8.3.0 or later
- GCC 4.8.0 or later
For Cray CS300 systems:
  o craype 2.1.2 or later
  o MVAPICH 1.9
  o CCE 8.3.0

Notes and Limitations:
The Cray LibSci 13.0.0 release is dependent on the new Cray MPI library (MPT 7.0.0) that is binary incompatible with previous Cray MPI libraries. Users will need to recompile with a supported compiler and relink their codes with MPT 7.0.0 and Cray LibSci 13.0.0 to take advantage of new features and benefit from performance optimizations.

The CrayPE 2.1.2 release adds supports for link line generation for the multi-threaded versions of the libsci library based on the OpenMP option the user specifies for each compiler:
  o CCE by default links to the OpenMP LibSci library. CrayPE will link in the serial version of LibSci when the CCE flag –hnoomp is used.
  o GNU by default links serial LibSci library. CrayPE will link in the OpenMP version of LibSci when the GNU flag -fopenmp is used.
  o INTEL by default links serial LibSci library. CrayPE will link in the OpenMP version of LibSci when the INTEL flag -openmp is used.

Starting with the release of Cray LibSci 12.2.0, FFTW3 is no longer a required dependency and the fftw module will no longer be automatically loaded with the cray-libsci module. Users should load the fftw module for applications requiring the Cray FFTW3 library.

Starting with the release of Cray LibSci 12.2.0 the CRay Adaptive FFT (CRAFFT) subroutine library for computing the discrete Fourier transform (DFT) is no longer supported. The Cray FFTW3 library can be used instead to compute Fourier transforms.

Documentation:
See the intro_libsci man page for additional information.

See the csmlversion man page for information to display version information on the currently loaded scientific libraries.

Modulefile:
module load cray-libsci

Installation instructions:
rpm -iv cray-libsci-*.-13.0.0-3.x86_64.rpm

The "*" in the install command represents compiler version combinations.

To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_libsci_13.0.0
The csmlversion RPM is now packaged with the LibSci distribution.

rpm -ihv csmlversion-1-0.x86_64.rpm

csmllversion does not have a module file so the last installed version is the only version available.

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LibSci_acc 3.0.2
Purpose:
Cray LibSci_ACC 3.0.2 provides accelerated versions of scientific libraries for Cray XK, XC30, and CS300 Systems.

The Cray LibSci_ACC 3.0.2 release provides the following:
- Compatibility with Cray MPT 7.0.0
- Compatibility with LibSci 13.0.0
- Improved performance for the hybrid version of PDGEMM on the accelerator
- Added multi-GPU support on CS300 systems for a subset of LAPACK routines
  See the intro_libsci_acc man page for more information on this functionality.
- Improved performance of [D,Z]GETRF on the accelerator
- Improved performance of [D,Z]POTRF on the accelerator

Bugs Closed with Cray LibSci_ACC 3.0.2 release:
- Bug 808723 Errors in the zgemm_cuda.c example code
- Bug 809198 PDGEMM crashes with CP2K and libsci_acc

Product and OS Dependencies:
The Cray LibSci_ACC 3.0.2 release is supported on the following Cray systems:
- Cray XK systems running CLE 4.2 UP02 and CLE 5.2
- Cray XC systems running CLE 5.1 UP00 and CLE 5.2
- Cray CS300 systems with CentOS 6.2/6.3/6.4 and Redhat 6.2/6.3/6.4.

The Cray LibSci_ACC 3.0.2 release requires the following software products:

For Cray XK and XC systems:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later
- cudatoolkit 5.5.20 or later
- cray-libsci 13.0.0 or later
- MPT 7.0.0 or later
One or more compilers:
  o CCE 8.3.0 or later
  o GCC 4.8.0 or later

**NOTE:** GCC 4.9.0 is not supported

For Cray CS300 systems:
  o craype 2.1.2 or later
  o cudatoolkit 5.5.20 or later
  o cray-libsci 13.0.0 or later
  o MVAPICH 1.9
  o CCE 8.3.0

**Notes and Limitations:**
The Cray LibSci_ACC 3.0.2 release is dependent on the new Cray MPI library (MPT 7.0.0) that is binary incompatible with previous Cray MPI libraries.
Users will need to recompile with a supported compiler and relink their codes with MPT 7.0.0 and Cray LibSci_ACC 3.0.2 to take advantage of new features and benefit from performance optimizations.

CudaToolkit 5.5 from NVIDIA does not support GCC 4.9.x and therefore Cray LibSci_ACC 3.0.2 does not support applications built with GCC 4.9.x.

Cray LibSci_ACC 3.0.2 supports NVIDIA Tesla K20 & K40 accelerators

Applications running PBLAS routines on the accelerator should set the environment variable 
`MPICH_NO_GPU_DIRECT=1` to ensure correctness.

Performance improvements can be achieved in programs calling libsci_acc subroutines by using pinned memory. See the intro_libsci_acc man page for details.

Use of the aprun option "-cc none" to disable core affinity is strongly suggested to improve performance.

This version and previous versions of LibSci_ACC are not thread-safe.

**Documentation:**
See the intro_libsci_acc man page for additional information.

**Modulefile:**
module load cray-libsci_acc

**Installation instructions:**
`rpm -ivh cray-libsci-acc-*-3.0.2-2.x86_64.rpm`

The "*" in the install command represents compiler version combinations.
To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_libsci_acc_3.0.2

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/opt/cray/libsci_acc/3.0.2/ATTRIBUTIONS_libsci_acc3.0.2.txt

PETSc 3.4.4.0
Purpose:
The Cray PETSc 3.4.4.0 release is supported on Cray XE, XC series, and XK Systems. Cray PETSc is supported on the host CPU but not on the accelerator of Cray XK systems.

The Cray PETSc 3.4.4.0 release is equivalent to the official patch release of PETSc 3.4.4 by Argonne National Laboratory. For further information about the PETSc 3.4.4 release, see http://www.mcs.anl.gov/petsc/documentation/changes/34.html

The Cray PETSc 3.4.4.0 release provides the following:
  o Compatibility with Cray MPT 7.0.0
  o Compatibility with Cray LibSci 13.0.0
  o PETSc 3.4.4 Update
    o Introduced CASK support with optimizations for Haswell Processors
    o Improved performance for PETSc applications using CCE or GCC compilers on XE systems with Interlagos processors and on XC systems.
    o Changed the PETSc default communication pattern to use MPI all to all communication for scatter (-vecscatter_alltoall)

Bugs Closed with Cray PETSc 3.4.4.0 release:
  o 811714 - XC30 degraded job performance due to bad communication interference from PETSc

Product and OS Dependencies:
The Cray PETSc 3.4.4.0 release is supported on the following Cray systems:
  o Cray XE and XK systems with CLE 4.2 and CLE 5.2.
  o Cray XC systems with CLE 5.1 and CLE 5.2.

The Cray PETSc 3.4.4.0 release requires the following software products:

For Cray XE and XK systems:
  o xt-asyncpe 5.27 or later / craype 2.1.2 or later
  o cray-libsci 13.0.0 or later
  o TPSL 1.4.1
  o MPT 7.0.0 or later
One or more compilers:
  o CCE 8.3.0 or later
  o GCC 4.8.0 or later
  o GCC 4.9.0 or later
  o Intel 14.0.1.106 or later
  o PGI 14.1.0 or later

For Cray XC series systems:
  o craype 2.1.2 or later
  o cray-libsci 13.0.0 or later
  o TPSL 1.4.1
  o MPT 7.0.0 or later

One or more compilers:
  o CCE 8.3.0 or later
  o GCC 4.8.0 or later
  o GCC 4.9.0 or later
  o Intel 14.0.1.106 or later

Notes and Limitations:
The Cray PETSc 3.4.4.0 release is dependent on the new Cray MPI library (MPT 7.0.0) that is binary incompatible with previous Cray MPI libraries. Users will need to recompile with a supported compiler and relink their codes with MPT 7.0.0 and Cray PETSc 3.4.4.0 to take advantage of new features and benefit from performance optimizations.

Documentation:

See the intro_petsc man page for additional information.

Modulefile:
module load cray-petsc

Installation instructions:
rpm -iv cray-petsc-*-3.4.4.0-3.x86_64.rpm

The "*" in the install command represents compiler version combinations.

To make this the default version, execute:
   /opt/cray/admin-pe/set_default_files/set_default_petsc_3.4.4.0

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Trilinos  11.8.1.0

Purpose:
The Cray Trilinos 11.8.1.0 is equivalent to the official patch release of Trilinos 11.8.1 by Sandia National Laboratories. For further information about the Trilinos 11.8.1 release, see http://trilinos.sandia.gov/release_notes-11.8.html

The Cray Trilinos 11.8.1.0 release provides the following:
- Compatibility with Cray MPT 7.0.0
- Compatibility with Cray LibSci 13.0.0
- Trilinos 11.8.1 Update
- Introduced CASK support with optimizations for Haswell Processors
- Introduced support for the Sundance package
- Improved Trilinos application performance at large PE counts
- Introduced support for OpenMP in the Epetra package (RFE 810370)

Bugs Closed with Cray Trilinos 11.8.1.0 release:
- 811420 - Trilinos cannot find -lciakrts at link time
- 811771 - Problems with the cmake file provided with Cray Trilinos 11.6.1.0

Product and OS Dependencies:
The Cray Trilinos 11.8.1.0 release is supported on the following Cray systems:
- Cray XE and XK systems with CLE 4.2 and CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.

The Cray Trilinos 11.8.1.0 release requires the following software products:

For Cray XE and XK systems:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later
- cray-libsci 13.0.0 or later
- TPSL 1.4.1
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later
- PGI 14.1.0 or later

For Cray XC series systems:
- craype 2.1.2 or later
- cray-libsci 13.0.0 or later
TPSL 1.4.1

Purpose:

One or more compilers:
  - CCE 8.3.0 or later
  - GCC 4.8.0 or later
  - GCC 4.9.0 or later
  - Intel 14.0.1.106 or later

Notes and Limitations:
The Cray Trilinos 11.8.1.0 release is dependent on the new Cray MPI library (MPT 7.0.0) that is binary incompatible with previous Cray MPI libraries.
Users will need to recompile with a supported compiler and relink their codes with MPT 7.0.0 and Cray Trilinos 11.8.1.0 to take advantage of new features and benefit from performance optimizations.

Documentation:
References and API guide are available at
To see descriptions of each individual Trilinos package, go to
http://trilinos.sandia.gov/capabilities.html
See the intro_trilinos man page for additional information.

Modulefile:
module load cray-trilinos

Installation instructions:
rpm -iv cray-trilinos-*-11.8.1.0-1.x86_64.rpm
The "*" in the install command represents compiler version combinations.
To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_trilinos_11.8.1.0

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/opt/cray/trilinos/11.8.1.0/ATTRIBUTIONS_trilinos11.8.1.0.txt

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TPSL  1.4.1
Purpose:
The TPSL 1.4.1 release is supported on Cray XE, XK, and XC series systems.
TPSL is supported on the host CPU but not on the accelerator of Cray XK systems.

The TPSL 1.4.1 release provides the following:
- Compatibility with Cray MPT 7.0.0
- Compatibility with Cray LibSci 13.0.0

TPSL (Third Party Scientific Libraries) contains a collection of outside mathematical libraries that can be used with PETSc and Trilinos. This module increases the flexibility of PETSc and Trilinos by providing users with multiple options for solving problems in dense and sparse linear algebra. The cray-tpsl module is automatically loaded when PETSc or Trilinos is loaded. The libraries included are MUMPs, SuperLU, SuperLU_dist, ParMetis, Hypre, Sundials, and Scotch.

- MUMPS 4.9.2. MUMPS (MUltifrontal Massively Parallel sparse direct Solver) is a package of parallel, sparse, direct linear-system solvers based on a multifrontal algorithm. MUMPS can now interface with SCOTCH as well. For further information, see http://graal.ens-lyon.fr/MUMPS/.

- SuperLU 4.3. SuperLU is a sequential version of SuperLU_dist and a sequential incomplete LU preconditioner that can accelerate the convergence of Krylov subspace iterative solvers. For further information, see http://crd.lbl.gov/~xiaoye/SuperLU/.

- SuperLU_dist 3.3. SuperLU_dist is a package of parallel, sparse, direct linear-system solvers (available in Cray LibSci). For further information, see http://crd.lbl.gov/~xiaoye/SuperLU/.

- ParMETIS 4.0.2. ParMETIS (Parallel Graph Partitioning and Fill-reducing Matrix Ordering) is a library of routines that partition unstructured graphs and meshes and compute fill-reducing orderings of sparse matrices. For further information, see http://glaros.dtc.umn.edu/gkhome/views/metis.

- HYPRE 2.9. HYPRE is a library of high-performance preconditioners that use parallel multigrid methods for both structured and unstructured grid problems (not included with petsc-complex). For further information, see http://www.llnl.gov/CASC/linear_solvers/.

- SUNDIALS 2.5.0 (SUite of Nonlinear and Differential/Algebraic equation Solvers) consists of 5 solvers: CVODE, CVODES, IDA, IDAS, and KINSOL. In addition, SUNDIALS provides a MATLAB interface to CVODES, IDAS, and KINSOL that is called sundialsTB. For further information, see https://computation.llnl.gov/casc/sundials/main.html.

- Scotch 6.0. Scotch is a software package and libraries for sequential and parallel graph partitioning, static mapping, sparse matrix block ordering, and sequential mesh and hypergraph partitioning. For further information, see http://www.labri.fr/perso/pelegrin/scotch.

**Product and OS Dependencies:**
The Cray TPSL 1.4.1 release is supported on the following Cray systems:
Cray XE and XK systems with CLE 4.2 and CLE 5.2.
Cray XC systems with CLE 5.1 and CLE 5.2.

The Cray TPSL 1.4.1 release requires the following software products:

For Cray XE and XK systems:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later
- cray-libsci 13.0.0 or later
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later
- PGI 14.1.0 or later

For Cray XC series systems:
- craype 2.1.2 or later
- cray-libsci 13.0.0 or later
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later

Notes and Limitations:
The Cray TPSL 1.4.1 release is dependent on the new Cray MPI library (MPT 7.0.0) that is binary incompatible with previous Cray MPI libraries. Users will need to recompile with a supported compiler and relink their codes with MPT 7.0.0 and Cray Trilinos 11.8.1.0 to take advantage of new features and benefit from performance optimizations.

Documentation:
http://graal.ens-lyon.fr/MUMPS/
http://crd.lbl.gov/~xiaoye/SuperLU/
http://glaros.dtc.umn.edu/gkhome/views/metis/
http://www.llnl.gov/CASC/linear_solvers/
https://computation.llnl.gov/casc/sundials/main.html
http://www.labri.fr/perso/pelegrin/scotch/

Modulefile:
module load cray-tpsl

Installation instructions:
rpm -iv cray-tpsl-*-1.4.1-3.x86_64.rpm
The "*" in the install command represents compiler version combinations.

To make this the default version, execute:

```
/opt/cray/admin-pe/set_default_files/set_default_tpsl_1.4.1
```

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```
/opt/cray/tpsl/1.4.1/ATTRIBUTIONS_tpsl1.4.1.txt
```

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**FFTW 3.3.4.0**

**Purpose:**
The Cray FFTW 3.3.4.0 release is supported on Cray XE, XK, and XC Systems.

FFTW is supported on the host CPU but not on the accelerator of Cray XK systems.

The Cray FFTW 3.3.4.0 release provides the following:
- FFTW 3.3.4 Update
- Compatibility with Cray MPT 7.0.0
- Introduced support with optimizations for Haswell Processors

For further information, see [http://www.fftw.org/release-notes.html](http://www.fftw.org/release-notes.html).

**Bugs Closed with Cray FFTW 3.3.4.0 release:**
- 810719  fftw module and undefined references to MPI
- 811412  errors with dynamic linking when using FFTW with PrgEnv-gnu or PrgEnv-intel
- 811488  Dynamic linking fails if the fftw/3.3.0.4 module is loaded on Cray XC30?

**Product and OS Dependencies:**
The FFTW 3.3.4.0 release is supported on the following Cray Systems running Cray Linux Environment (CLE) operating system

- Cray XE and XK systems with CLE 4.2 and CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.

The FFTW 3.3.4.0 release requires the following software products:

For Cray XE and XK systems:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
GCC 4.9.0 or later
- Intel 14.0.1.106 or later
- PGI 14.1.0 or later

For Cray XC series systems:
- craype 2.1.2 or later
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later

Notes and Limitations:
The Cray FFTW 3.3.4.0 release is dependent on the new Cray MPI library (MPT 7.0.0) that is binary incompatible with previous Cray MPI libraries.
Users will need to recompile with a supported compiler and relink their codes with MPT 7.0.0 and Cray FFTW 3.3.4.0 to take advantage of new features and benefit from performance optimizations.

Applications failed to link dynamically reporting undefined references to libfftw3f_mpi.so when the previous release of Cray FFTW 3.3.0.4 was loaded. This issue has been fixed in the Cray FFTW 3.3.4.0 release this month. The following workarounds enable you to continue using the previous Cray FFTW 3.3.0.4 version with MPT 6:
- each user can explicitly link to the mpich library:
  `~> cc -lmpich_gnu_48 -dynamic hello.c`
  `~> ldd a.o | grep libfftw3f_mpi`
  `libfftw3f_mpi.so.mpi30.3 => /opt/cray/lib64/libfftw3f_mpi.so.mpi30.3`
- on systems using CrayPE, a global correction can be made by adding "-lmpich" to the Libs line in the pkgconfig file
  `~/opt/fftw/3.3.0.4/*/lib/pkgconfig/fftw*_mpi.pc`

Documentation:
http://www.fftw.org/index.html#documentation

See the intro_fftw3 man page for additional information.

Modulefile:
module load fftw

Installation:
rpm -ivh fftw-3.3.4.0-2.x86_64.rpm

To make this the default version, execute:
FFTW 2.1.5.7

Purpose:
The Cray FFTW 2.1.5.7 release is supported on Cray XE, XK, and XC Systems. FFTW is supported on the host CPU but not on the accelerator of Cray XK systems.

The Cray FFTW 2.1.5.7 release provides the following:
- Compatibility with Cray MPT 7.0.0

Product and OS Dependencies:
The Cray FFTW 2.1.5.7 release is supported on the following Cray Systems:
- Cray XE and XK systems with CLE 4.2 and CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.

The FFTW 2.1.5.7 release requires the following software products:

For Cray XE and XK systems:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later
- PGI 14.1.0 or later

For Cray XC series systems:
- craype 2.1.2 or later
- MPT 7.0.0 or later

One or more compilers:
- CCE 8.3.0 or later
- GCC 4.8.0 or later
- GCC 4.9.0 or later
- Intel 14.0.1.106 or later

Documentation:
http://www.fftw.org/#documentation

Modulefile:
module load fftw/2.1.5.7

Installation:
rpm -ivh fftw-2.1.5.7-1.x86_64.rpm

To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_fftw_2.1.5.7

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ACML 5.3.1 (XE/XK only)
Purpose:
Rerelease of ACML 5.3.1 to address bug:
  o  809527 - acml on CLE 5.2-gem: "Package acml was not found in the pkg-config search path."

Product and OS Dependencies:
xt-asyncpe 5.04 or higher

Limitations:
ACML 5.3.1 is not compatible with:
  o  CCE 7.4.x or older
  o  GCC 4.5.x or older

Documentation:

Installation Instructions:
rpm -iv acml-5.3.1-3.x86_64.rpm

To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_acml_5.3.1

Environment Setup and Compiling support 5.42
CrayPE 2.1.2
Purpose:
This release includes enhanced link line generation for the CCE compiler.
CrayPE also supports link line generation for the multi-threaded versions of the libsci library based on the OpenMP option the user specifies for each compiler:
CCE by default links to the OpenMP LibSci library. CrayPE will link in the serial version of LibSci when the CCE flag –hnoomp is used.

GNU by default links serial LibSci library. CrayPE will link in the OpenMP version of LibSci when the GNU flag -fopenmp is used.

INTEL by default links serial LibSci library. CrayPE will link in the OpenMP version of LibSci when the INTEL flag -openmp is used.

The craype-haswell modulefile adds CPU targeting support for Haswell processor.

**Bugfixes:**

- 810742 - If dynamic library is created with compiler driver then ATP does not work.
- 806615 - Minimize list of dynamic libraries linked into an application

**Dependencies:**

The CrayPE 2.1.2 release is supported on the following Cray systems:

- Cray XE and XK systems with CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.
- Cray CS300 systems with CentOS 6.4 and Redhat 6.4.

The CrayPE 2.1.0 release is dependent on .pc files in the following software products:

- ATP 1.6.3 or later
- FFTW 3.3.0.4 or later
- FFTW 2.1.5.6 or later
- Global Arrays 5.1.0.2 or later
- HDF5 1.8.11 or later
- iobuf 2.0.5 or later
- LibSci 12.1.01 or later
- MPT 6.0.2 or later
- NetCDF 4.3.0 or later
- Parallel-NetCDF 1.3.1.1 or later
- PMI 4.0.1 or later
- PETSc 3.4.2.0 or later
- Trilinos 11.4.1.0 or later
- TPSL 1.3.04 or later
- TotalView 8.12-totalview-support-1.1.5 or later

**Documentation:**

See manpages for cc, CC, ftn, intro_hugepages and pkg-config

See section 2.6 Using Targeting Modules of the Cray Programming Environment User's Guide (S-2529-114)


**Installation:**
rpm -ivh craype-2.1.2-*-x86_64.rpm

To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_craype_2.1.2

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Xt-asyncpe 5.27
Purpose:
Bug fix release and update to support cray-libsci/13.0.0 and beyond.

Bugs closed with this release:
809455 - Cray Compiler fails with include error with certain headers when shared flags is used

Deprecated Features:
All targeting modules with prefix xtpe- are deprecated and replaced by ones with prefix craype-.
The xtpe- modules have been removed.

Product and OS Dependencies:
xt-asynpe 5.27 supports the following minimum compiler release versions. To compile and link using older compilers, use xt-asynpe 4.9 or older.
  o  CLE 4.2 UP02 and older
  o  pgii 10.9
  o  cce 7.3
  o  intel 12.0
  o  gnu 4.5.3
  o  pathscale 4.0.9 (xt-mpich2 only)

Documentation:
See manpages for cc, CC, ftn, csmlversion and intro_hugepages

Installation:
rpm -ivh xt-asynpe-5.27-*-x86_64.rpm

To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_xt-asynpe_5.27

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Cray debugger Support Tools 2.3.0
ATP 1.7.3
Purpose:
Added support for ALPS Suspend/Resume feature. This closes RFE:
  o  810894  ATP does not support the ALPS Suspend/resume feature

This does require one of OS levels:
Product and OS Dependencies:
The Cray ATP 1.7.3 release is supported on the following Cray systems running Cray Linux
Environment(CLE) operating system
  o Cray XE and XK systems running CLE 4.2
  o Cray XC systems with CLE version 5.1 or later

Product Dependencies:
  o xt-asyncpe 5.27 or later is required on XE/XK systems.
  o craype 2.1.2 or later is required on XC systems.
  o stat is recommended for viewing the merged stack backtrace tree.

ATP is supported on the host CPU but not on the accelerator on Cray XK systems.

Documentation:
For more information see the intro_atp man page.

Installation:
rpm -ivh atp-1.7.3-0_3473.x86_64.rpm

To change the product version to default after installation:
  /opt/cray/admin-pe/set_default_files/set_default_atp_1.7.3

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  /opt/cray/atp/1.7.3/ATTRIBUTIONS_atp1.7.3.txt

LGDB 2.3.1
Product Description:
l gdb is a GDB-based parallel debugger used to debug applications compiled with CCE, PGI, GNU, and Intel Fortran, C and C++ compilers. It allows programmers to either launch an application or attach to an already running application that was launched with aprun. Additionally, it provides comparative debugging technology that enables programmers to compare data structures between two executing applications. Comparative debugging should be used in conjunction with the CCDB GUI tool accessed by loading the cray-ccdb module.

Some features of l gdb include:
  o Command line parallel debugger allows for launching/attaching applications via aprun.
Utilizes process sets to operate on a subset of application ranks.
- gdb like feel, also implements a gdbmode to enable a true parallel gdb.
- OpenACC debugging support.
- Workload manager support.

Purpose:
This is a bugfix release.
- Fixed a bug where large group IDs caused lgdb to break. This was due to using an older ustar format. Switching to gnutar fixes the issue.
- Applied several patches to gdb binaries from upstream sources.

Bugs Closed with this release:
BUG 811393 - lgdb CTI error message: Numeric group ID too large

Product and OS Dependencies:
The Cray lgdb 2.3.1 release is supported on the following Cray systems running Cray Linux Environment (CLE) operating system
- Cray XE and XK systems running CLE 4.2 and CLE 5.2
- Cray XC series systems with CLE version 5.1 or later

Documentation:
Type `man lgdb` with the cray-lgdb module loaded to read the lgdb(1) man page.

Simple usage examples are provided at the end.

Also, type `help` at the lgdb command line for more information on commands.

Installation instructions:
To install the lgdb:
```
rpm -ivh cray-lgdb-2.3.1-0_3478.x86_64.rpm
```

To make lgdb 2.3.1 the default version of lgdb, execute:
```
/opt/cray/admin-pe/set_default_files/set_default_cray-lgdb_2.3.1
```

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STAT 2.1.0.1

Purpose:
Update STAT to version 2.1.0.

Product and OS Dependencies:
The STAT 2.1.0.0 release is supported on Cray systems running the CLE 4.2 CNL or later operating systems.
Documentation:
http://www.paradyn.org/STAT/STAT.html

Installation:
rpm -ivh cray-stat-2.1.0.1-1.x86_64.rpm

To make this the default version, execute:
   /opt/cray/admin-pe/set_default_files/set_default_stat_2.1.0.0

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dwarf 14.2.0
Purpose:
This release of dwarf 14.2.0 is intended for use by Cray products. This is NOT intended for user application or development use.

Product and OS Dependencies:
This dwarf release is required on Cray XC, XE and XK systems to satisfy PE product dependencies.

Documentation:
http://reality.sgiweb.org/davea/dwarf.html

Installation:
rpm -ivh cray-dwarf-14.2.0-0.x86_64.rpm

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Third Party Products 5.42
GCC 4.8.1 and 4.8.2
Purpose:
GCC 4.8.1 and GCC 4.8.2 are being rereleased to use the set-gcc-libs script that is being released this month.

Installation instructions:
rpm –ivh  cray-gcc-4.8.1-64.x86_64.rpm
rpm –ivh  cray-gcc-4.8.2-64.x86_64.rpm

To change the product version to default after installation:
   /opt/cray/admin-pe/set_default_files/set_default_gcc_4.8.2
GCC 4.9.0

Purpose:
The gcc 4.9.0 release.
The additional cray-set-gcc-libs rpm sets up the linking infrastructure for gnu shared libraries.

The following bug is fixed in the gcc 4.9.0 release.
  o 808706  NAMD GPU version segfaults when compiled with gcc/4.8.2 [GCC Bug 58800]

Product and OS Dependencies:
The gcc 4.9.0 release is supported on the following Cray systems:
  o Cray XE and XK systems with CLE 4.2 and CLE 5.2.
  o Cray XC systems with CLE 5.1 and CLE 5.2.

Limitations:
gcc 4.9.0 is not supported with Cuda 5.5.
The Cuda runtime header will show an error when compiling with nvcc.
It is recommended to only install gcc 4.9.0 as non-default on XK systems for this reason.

Documentation:
http://gcc.gnu.org/gcc-4.9

Modulefile:
module load gcc/4.9.0

This modulefile defines the system paths and environment variables needed to use gcc, gfortran and g++ on Cray systems. The gcc modulefile can be swapped for other gcc versions. This modulefile may be loaded as a standalone modulefile or as part of the GNU Programming Environment, PrgEnv-gnu. The CrayPE drivers, cc, CC, and gfortran, are recommended for use with PrgEnv-gnu to generate compilation and link lines.

The following modulefiles support the GNU 4.9.0 based Programming Environment:
For Cray XE and XK systems:
  o xt-asyncpe 5.27 or later / craype 2.1.2 or later
For Cray XC systems:
  o craype 2.1.2 or later
For Cray XE, XK, and XC systems:
  o cray-mpich 7.0.0 or later
  o cray-libsci 13.0.0 or later
  o libsci_acc 3.0.2 or later
  o cray-tpsl 1.4.1 or later
  o cray-petsc 3.4.4.0 or later
  o cray-trilinos 11.8.1.0 or later
HDF5 1.8.13

Purpose:
New version of HDF5 (1.8.13)
This version enables HDF5's Fortran 2003 interface.

Product and OS Dependencies:
The HDF5 release is supported on the following Cray systems:
  o  Cray XE and XK systems with CLE 4.2 and CLE 5.2.
  o  Cray XC systems with CLE 5.1 and CLE 5.2.

The HDF5 1.8.13 release requires the following software products:

One or more compilers:
  o  CCE 8.3.0 or later
  o  GCC 4.8
  o  GCC 4.9
  o  Intel 14.0 or later
  o  PGI 14.1 or later

For Cray XE and XK systems:
  o  xt-asyncpe 5.27 or later / craype 2.1.2 or later

For Cray XC systems:
  o  craype 2.1.2 or later

Notes and Limitations:
The HDF5 compiler scripts (h5cc, h5fc, h5c++) are not included in the release. The user should use the Cray compiler scripts (cc, ftn, CC) to include the HDF5 header files and link in the HDF5 libraries.

**Documentation:**

hdf5:

**Modulefile:**

module load cray-hdf5
OR
module load cray-hdf5-parallel

**Product description:**

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data. HDF5 is portable and is extensible, allowing applications to evolve in their use of HDF5. The HDF5 Technology suite includes tools and applications for managing, manipulating, viewing, and analyzing data in the HDF5 format.

**Installation:**

```
rpm -ivh cray-hdf5-*-1.8.13-2.x86_64.rpm
```

The "*" in the install command represents compiler version combinations.

To make this the default version, execute:
```
/opt/cray/admin-pe/set_default_files/set_default_hdf5_1.8.13
```

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**NetCDF 4.3.2**

**Purpose:**
A new version of NetCDF (4.3.2)

**Product and OS Dependencies:**
The NetCDF release is supported on the following Cray systems:
- Cray XE and XK systems with CLE 4.2 and CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.

The NetCDF 4.3.2 release requires the following software products:

One or more compilers:
- CCE 8.3 or later
- GCC 4.8
- GCC 4.9
- Intel 14.0 or later
- PGI 14.1 or later

For Cray XE and XK systems running CLE 4.2:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later

For Cray XC systems:
- CrayPE 2.1.2 or later

**Bugs Fixed:**
- 808634 - netcdf nf-config -flibs output is incorrect
- 792158 - netcdf 4.2.0 nf-config points to gnu and not pgi version

**Notes and Limitations:**
Unidata now packages Netcdf-4 and legacy netcdf-3 separately. Cray has decided not to continue supplying the legacy Netcdf-3 package. Due to CCE changes a version of netcdf built with "-sreal64" is neither needed nor provided.

NetCDF is supported on the host CPU but not on the accelerator on Cray XK systems.

**Documentation:**
http://www.unidata.ucar.edu/software/netcdf/docs

**Modulefile:**
module load cray-netcdf
OR
module load cray-netcdf-hdf5parallel

**Product description:**
NetCDF (network Common Data Form) is a set of interfaces for array-oriented data access and a freely-distributed collection of data access libraries for C, Fortran, C++, Java, and other languages. The netCDF libraries support a machine-independent format for representing scientific data. Together, the interfaces, libraries, and format support the creation, access, and sharing of scientific data.

**Installation instructions:**
rpm -ivh cray-netcdf-*-4.3.2-*_x86_64.rpm
The "*" in the install command represents compiler version combinations.

To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_netcdf_4.3.2

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Purpose:
New version of Parallel NetCDF 1.4.1

Product and OS Dependencies:
This Parallel NetCDF release is supported on the following Cray systems:
- Cray XE and XK systems with CLE 4.2 and CLE 5.2.
- Cray XC systems with CLE 5.1 and CLE 5.2.

The Parallel NetCDF 1.4.1 release requires the following software products:

One or more compilers:
- CCE 8.3 or later
- GCC 4.8
- GCC 4.9
- Intel 14.0 or later
- PGI 14.1 or later

For Cray XE and XK systems running CLE 4.2:
- xt-asyncpe 5.27 or later / craype 2.1.2 or later

For Cray XC systems:
- CrayPE 2.1.2 or later

Notes: Shared libraries are not provided as the Third Party software does not support shared libraries.

Documentation:

Modulefile:
module load cray-parallel-netcdf

Product Description:
Parallel NetCDF is a library providing high-performance I/O while still maintaining file-format compatibility with Unidata's NetCDF.

Installation:
parallel-netcdf is now packaged into separate compiler specific RPMs to allow rpmbuild to correctly include compiler dependencies.

```
rpm -ivh cray-parallel-netcdf-*-1.4.1-0.x86_64.rpm
```

The "*" in the install command represents compiler version combinations.

To make this the default version, execute:
```
/opt/cray/admin-pe/set_default_files/set_default_parallel-netcdf_1.4.1
```
PGI 14.4.0

**Purpose:**
Features of PGI 14.4.0 are documented at:

**Documentation:**
Documentation for PGI 14.4.0 is in /opt/pgi/14.4.0/linux86-64/14.4/doc/
PGI Fortran Reference, pgifortref.pdf
PGI CUDA Fortran Guide, pgicudaforug.pdf
PGI 14.4 Release Notes, pgirn144.pdf

**Installation Instructions:**
rpm –ivh pgi-14.4.0-02.x86_64.rpm
To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_pgi_14.4.0

DDT 4.2.1.1_36484

**Purpose:**
Release of Allinea DDT 4.2.1.1_36484

**Product and OS Dependencies:**
The Cray DDT 4.2.1.1_36484 release is supported on the following Cray systems running Cray Linux Environment(CLE) operating system
- Cray XE and XK systems running CLE 4.2
- Cray XC systems with CLE version 5.1 or later

**Documentation:**
http://www.allinea.com/products/ddt-support

/opt/cray/ddt/4.2.1.1_36484/doc/RELEASE-NOTES

**Installation:**
rpm -ivh ddt-4.2.1.1_36484-0.x86_64.rpm
To make this the default version, execute:
/opt/cray/admin-pe/set_default_files/set_default_ddt_4.2.1.1_36484
Cray Application Developer's Environment 6.32
CADE 6.32
CADE 6.32 supports Cray XE and Cray XK systems only.

Craype-installer 1.9.00 or later must be used to install with this release.

Purpose:
CADE is a collection of the latest basic programming environment for Cray XE and XK systems. CADE does not include licensed products (CCE, Cray Performance Measurement and Analysis Tools, Chapel, PGI, DDT, TV, etc.).
This package plus the licensed products (compilers, performance tools and debuggers) will update the system to the latest Programming Environment.
For more information see: Cray Programming Environments Installation Guide S-2372-113

Documentation:
S-2529-114: Cray Programming Environment User's Guide
S-2372-113: Cray Programming Environments Installation Guide

The contents of this CADE release package are:
CADE-6.32-17.iso
acml-5.3.1-3.x86_64.rpm
atp-1.7.3-0_3473.x86_64.rpm
cray-ccdb-1.0.2-0_3276.x86_64.rpm
cray-dwarf-14.2.0-0.x86_64.rpm
cray-ga-cray83-5.1.0.5-05.x86_64.rpm
cray-ga-gnu48-5.1.0.5-05.x86_64.rpm
cray-ga-gnu49-5.1.0.5-05.x86_64.rpm
cray-ga-intel140-5.1.0.5-05.x86_64.rpm
cray-ga-pgi141-5.1.0.5-05.x86_64.rpm
cray-gcc-4.8.0-52.x86_64.rpm
cray-gcc-4.8.1-64.x86_64.rpm
cray-gcc-4.8.2-64.x86_64.rpm
cray-gcc-4.9.0-09.x86_64.rpm
cray-gcc-gmp-4.3.2-2.x86_64.rpm
cray-gcc-mpc-0.8.1-2.x86_64.rpm
cray-gcc-mpfr-2.3.1-20.x86_64.rpm
cray-gcc-mpfr-2.4.2-2.x86_64.rpm
cray-hdf5-cray83-1.8.13-3.x86_64.rpm
cray-hdf5-gnu48-1.8.13-3.x86_64.rpm
cray-hdf5-gnu49-1.8.13-3.x86_64.rpm
cray-hdf5-intel140-1.8.13-3.x86_64.rpm
cray-hdf5-pgi141-1.8.13-3.x86_64.rpm
cray-libgdb-2.3.1-0_3478.x86_64.rpm
cray-tpsl-cr83-1.4.1-3.x86_64.rpm
cray-tpsl-gnu-48-1.4.1-3.x86_64.rpm
cray-tpsl-intel140-1.4.1-3.x86_64.rpm
cray-tpsl-pgi141-1.4.1-3.x86_64.rpm
cray-trilinos-cr83-haswell-11.8.1.0-1.x86_64.rpm
cray-trilinos-cr83-interlagos-11.8.1.0-1.x86_64.rpm
cray-trilinos-cr83-sandybridge-11.8.1.0-1.x86_64.rpm
cray-trilinos-cray-83-x86_64-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-48-haswell-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-48-interlagos-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-48-sandybridge-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-48-x86_64-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-49-haswell-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-49-interlagos-11.8.1.0-1.x86_64.rpm
cray-trilinos-gnu-49-sandybridge-11.8.1.0-1.x86_64.rpm
cray-trilinos-intel-140-haswell-11.8.1.0-1.x86_64.rpm
cray-trilinos-intel-140-interlagos-11.8.1.0-1.x86_64.rpm
cray-trilinos-intel-140-sandybridge-11.8.1.0-1.x86_64.rpm
cray-trilinos-intel-140-x86_64-11.8.1.0-1.x86_64.rpm
csmlversion-1.0.x86_64.rpm
fftw-2.1.5.7-1.x86_64.rpm
fftw-3.3.4.0-2.x86_64.rpm
iobuf-2.0.5-10.x86_64.rpm
java-jdk1.7.0_45-07.x86_64.rpm
libonesided-ntk-1.5.0-5.gem.x86_64.rpm
pgroupd-lin64-v1161.tar.gz
xt-asyncpe-5.27-06.x86_64.rpm
xt-gcc-4.4.4-12.sles11sp1.x86_64.rpm
xt-gcc-4.4.4-24.sles11sp3.x86_64.rpm
xt-gcc-4.6.1-13.sles11sp1.x86_64.rpm
xt-gcc-4.6.1-16.sles11sp3.x86_64.rpm
xt-pathscalesup-4.0.13-09.x86_64.rpm

Installation instructions:
For installations on a Cray XE or XK system, please see
S-2372-113 is available at http://docs.cray.com/.

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Latest PE Product Versions:
This list contains the latest version of all PE products.

Cray Compiling Environment
  CCE 8.3.0 (Supported on Cray XC, XE and XK systems)
  CCE 8.3.0

Cray Debugger Support Tools
  CDST 2.3.0 (Supported on Cray XC, XE and XK systems)
    atp 1.7.3
    CCDB 1.0.2
    lgdb 2.3.1
    stat 2.1.0
Cray Environment Setup and Compiling support
CENV  5.42
   craype-installer 1.9.00
   craypkg-gen 1.1.1
CENV  5.42 (Cray XE/XK systems with CLE 5.2 and all Cray XC systems)
   craype 2.1.2
CENV  5.42 (Cray XE and XK with CLE 4.2UP02)
   xt-asyncpe 5.27
   cray-modules-3.2.6.7-1.0400.6396.0.0.gem.x86_64.rpm (4.0 CLE)
   cray-modules-3.2.6.7-1.0401.6396.0.0.gem.x86_64.rpm (4.1 CLE)

Cray Message Passing Toolkit
CMPT 7.0.0 (Cray XC, XE and XK systems Support)
   cray-mpt 7.0.0
   cray-libpmi- 5.0.4
   cray-libpmi-devel- 5.0.4
   cray-ga 5.1.0.5
   cray-snplauncher 7.0.0 (Cray XC systems only)
   cray-mpich-compat 1.0.0

Cray Performance Measurement & Analysis Tools
CPMAT 6.2.0 (Supported on Cray XC, XE and XK systems)
   Perftools 6.2.0
   Papi 5.3.1
   Apprentice2 for Windows7 6.2.0
   Apprentice2 for Mac 6.2.0

Cray Scientific and Math Libraries
CSML 7.3.0   (Supported on Cray XC, XE and XK systems)
   acml 5.3.1 (XE/XK only)
   csmlversion 1.0
   fftw 2.1.5.7
   fftw 3.3.4.0
   petsc 3.4.4.0
   trilinos 11.8.1.0
   cray-libsci 13.0.0
   tpsl 1.4.1
   libsci_acc 3.0.2 (Cray XK and XC only)

Allinea's Distributed Debugging Tool
DDT Debugger 4.2.0.3 (Supported on Cray XC, XE and XK systems)
   ddt- 4.2.0.3_36484

TotalView Debugger
TotalView 8.13.0
   cray-totalview-8.13.0-totalview-support-1.2.0.1
PGI Compiler 14.4.0
For Cray XE and XK systems:
PGI 14.4.0

Third party products for the Programming environment 5.42
Third Party Products 5.42 (Supported on Cray XC, XE and XK systems)
cray-gdb 7.5.1
Flexnet license manager software 11.10.0
cray-hdf5 1.8.13
cray-netcdf 4.3.2
parallel-netcdf 1.4.1
iobuf 2.0.5
java jdk1.7.0_45
libonesided-ntk 1.5.0
cray-gcc-gmp 4.3.2
cray-gcc-mpc 0.8.1
cray-gcc-mpfr 2.4.2
cray-gcc 4.9.0
xt-pathscaleup 4.0.13 (Cray XE/XK with CLE 4.2 and earlier OS only)

Cray Developer Toolkit
(Supported on Cray XC systems)
CDT 1.16

Cray Application Developer’s Environment
(Supported on Cray XE and XK systems)
CADE 6.32

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