



Cray Compiling Environment 8.3 Release Overview and Installation Guide

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Part I: Release Overview

Introduction [1]

This document is an overview of the Cray Compiling Environment 8.3 release for the Cray XE, Cray XK, and Cray XC series systems.

This document does **not** describe hardware, software, installation of related products, or products that Cray does not provide.

1.1 Emphasis for the Cray Compiling Environment 8.3 Release

The Cray Compiling Environment (CCE) release provides the following enhancements:

- Continuing support for the *OpenACC Application Programming Interface, Version 2.0* specification, with performance enhancements, and support for command line control over assembly and link options.
- New Cray specific UPC functionality.
- Performance improvements for Cray XE, Cray XK, and Cray XC series systems.

1.2 Cray Compiling Environment 8.3 Release Package Description

The Cray Compiling Environment 8.3 consists of:

- Cray Fortran Compiler, version 8.3
- Cray C and C++ Compiler, version 8.3
- CrayLibs (libraries and utilities), version 8.3
- Cray documentation, described in [Chapter 4, Documentation on page 15](#)

All software is installed by means of scripts and RPM Package Manager (RPM) files. For more detail about Cray Compiling Environment 8.3 release package, refer to [Chapter 5, Release Package on page 19](#).

Software Enhancements [2]

This chapter describes software enhancements provided with the Cray Compiling Environment 8.3 release.

2.1 Performance Enhancements

- Certain performance-critical math intrinsics were enhanced for Cray XC Series systems at default optimization. In some cases, additional speedups are available with the `-hfp3` and `-hfp4` options.
- Floating-point performance on accelerators may be improved when compiling with `-hfp4`, which implies the CUDA `-use_fast_math` option for all accelerator math routines. The improved performance may come at the cost of reduced accuracy.
- Nested conditional code now vectorizes to arbitrary depth, limited only by architectural considerations.
- Loop nests with many read-only expressions may notice improved performance.
- Compile time has been reduced for some large OpenMP programs.

2.2 Accelerator Support

This release offers the following features:

- The `craype-accel-host` module supports compiling and running an OpenACC application on the host X86 processor. This provides source code portability between systems with and without an accelerator. The accelerator directives are automatically converted at compile time to OpenMP equivalent directives.
- The `-Wx, arg` option can be used to pass command line arguments to the PTX assembler for OpenACC applications.
- The `-Wc, arg` option can be used to pass command line arguments to the CUDA linker for OpenACC applications.
- The `-h acc_model=fast_addr` performance option is now safe for all OpenACC applications and is enabled by default.
- OpenACC constructs allow limited use of Fortran character strings.

This release continues to support the *OpenACC Application Programming Interface, Version 2.0* specification. Refer to the OpenACC home page at <http://www.openacc-standard.org/>. Under the Download area, select the *OpenACC 2.0 Specification*.

The Cray specific interfaces that have been adopted by OpenACC 2.0 are deprecated and will be removed in a future release.

See the `intro_openacc(7)` man page for the most current information regarding this implementation of OpenACC.

2.3 PGAS Support

The new `cray_upc_sheap_info()` call provides symmetric heap usage information to UPC applications. See the `cray_upc_sheap_info(3c)` manpage.

The new `cray_upc_shared_cast()` call creates a pointer-to-shared from a pointer-to-local, providing the inverse functionality to `upc_cast`. See the `cray_upc_shared_cast(3c)` man page.

This release supports the UPC 1.3 specification. The UPC 1.3 standard is available on the UPC specification website, <http://code.google.com/p/upc-specification>. See the `intro_pgas(7)` man page for more information regarding support for PGAS programming models.

2.4 Compiler Command Line Changes

The following command line changes apply to CCE 8.3.

- The `-h develop` option selects compiler optimization levels to balance compile time against application execution time. Use this option during application development, when quick turnaround is desired. It minimizes compile time at the cost of execution time performance.
- The `-h flex_mp=strict` option provides a level of repeatability between the conservative and intolerant levels.
- The `-h concurrent` option is equivalent to adding a `CONCURRENT` directive (pragma) before every loop in the file, including loops created from array syntax. This option provides significant performance improvements for some codes. Use with care as improper usage may result in application errors.
- The `-Wx, arg` option can be used to pass command line arguments to the PTX assembler for OpenACC applications.
- The `-Wc, arg` option can be used to pass command line arguments to the CUDA linker for OpenACC applications.

2.5 Changed Defaults

- The `-h acc_model=fast_addr` option is now default which improves performance for OpenACC applications.
- The Fortran command line now sets `-em` by default. Therefore, the Fortran compiler creates `.mod` files to hold module files for future compiles.

2.6 Instruction Set Support

The compiler now supports intrinsics for the FMA and AVX2 instructions on targets that support those instruction sets. See the `intro_asm_intrin(7)` man page.

Compatibilities and Differences [3]

This chapter describes compatibility issues and functionality changes to be aware of when upgrading from earlier releases of this software.

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.

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.

This chapter describes the documentation that supports the Cray Compiling Environment 8.3 release.

4.1 Accessing Product Documentation

With each software release, Cray provides books and man pages, and in some cases, third-party documentation. These documents are provided in the following ways:

- | | |
|---------------------------|--|
| CrayPort | CrayPort is the external Cray website for registered users that offers documentation for each product. CrayPort has portal pages for each product that contains links to all of the documents that are associated to that product. CrayPort enables you to quickly access and search Cray books, man pages, and in some cases, third-party documentation. You access CrayPort by using the following URL:

http://crayport.cray.com |
| CrayDoc | CrayDoc is the Cray documentation delivery system. CrayDoc enables you to quickly access and search Cray books, man pages, and in some cases, third-party documentation. Access the HTML and PDF documentation via CrayDoc at the following locations. <ul style="list-style-type: none">• The local network location defined by your system administrator• The CrayDoc public website: http://docs.cray.com |
| Man pages | Man pages are textual help files available from the command line on Cray machines. To access man pages, enter the man command followed by the name of the man page. For more information about man pages, see the man(1) man page by entering:

<code>% man man</code> |
| Third-party documentation | Third-party documentation that is not provided through CrayPort or CrayDoc is included with the third-party product. |

4.2 Cray Developed Publications Provided with This Release

The publications provided with this release are listed in [Table 1](#), which also indicates whether each publications was updated. Publications are provided in HTML and PDF formats.

Table 1. Books Provided with This Release

Book Title	Number	Updated
<i>Cray Compiling Environment Release Overview and Installation Guide</i> (this document)	S-5212-83	Yes
<i>Cray C and C++ Reference Manual</i>	S-2179-83	Yes
<i>Cray Fortran Reference Manual</i>	S-3901-83	Yes

4.3 Additional Documentation Resources

[Table 2](#) lists additional resources for obtaining documentation not included with this release package.

Table 2. Additional Documentation Resources

Product	Documentation Source
Example:	
GNU compilers	Documentation for the GNU C and Fortran compilers is available at http://gcc.gnu.org/onlinedocs/
glibc	glibc documentation is available at http://gcc.gnu.org/onlinedocs
GLIB	GLIB documentation is available at http://developer.gnome.org/glib/stable
RPM	RPM documentation is available at http://www.rpm.org

4.4 Changes to Man Pages

4.4.1 New Cray Man Pages

Cray man pages new with this release:

- `cray_upc_shared_cast(3c)`
- `cray_upc_sheap_info(3c)`
- `cray_upc_team_split(3c)`
- `cray_upc_team_t(3c)`
- `upc_thread_info(3c)`

4.4.2 Removed Cray Man Page

Cray man page removed with this release:

- `upc_thread_castable(3c)`

4.4.3 Changed Cray Man Pages

Cray man pages changed with this release:

- `craycc(1)`
- `crayCC(1)`
- `crayftn(1)`
- `intro_directives(7)`
- `openacc.examples(7)`
- `intro_pgas(7)`
- `intro_asm_intrin(7)`
- `optimize(7)`

4.5 Other Related Documents Available

The following publications contain additional information to help set up the Cray Compiling Environment 8.3; they are not provided with this release but are supplied with other products purchased from Cray:

- *Cray Programming Environments Installation Guide* (S-2372)
- *Cray Programming Environment User's Guide* (S-2529)
- *Managing System Software for the Cray Linux Environment* (S-2393)

Release Package [5]

5.1 Hardware and Software Requirements

The CCE 8.3 release is supported on the following software releases:

Table 3. Required CLE Versions

System	CLE
Cray XE	4.2.UP00, 5.2.UP00 and later
Cray XK	4.2.UP00, 5.2UP00 and later
Cray XC	5.1.UP00 and later

The Cray Compiling Environment 8.3 release requires the following supporting asynchronous software products. Required versions are listed below.

Table 4. Required Asynchronous Products

Product	Cray XE	Cray XK	Cray XC
craype	2.1.2 (CLE 5.2)	2.1.2 (CLE 5.2)	2.1.2 (CLE 5.1 or 5.2)
xt-asyncpe	5.27 (CLE 4.2)	5.27 (CLE 4.2)	N/A
PMI	5.0.1	5.0.1	5.0.1
LibSci	13.0.0	13.0.0	13.0.0
FlexNet	11.10.0	11.10.0	11.10.0
gcc	4.8.1	4.8.1	4.8.1

The Cray Compiling Environment 8.3 release requires the following minimum versions of these **optional** products:

Table 5. Optional Asynchronous Products

Product	Cray XE, Cray XK, and Cray XC30 Series Systems
HDF5	1.8.13
NETcdf	4.3.2
parallel-NETcdf	1.4.1
MPT	7.0.0
GA	5.1.0.5
LibSci_acc	3.0.2
TPSL	1.4.1
PETSc	3.4.4.0
Trilinos	11.8.1.0
fftw3	3.3.4.0
fftw2	2.1.5.7
Perftools	6.2.0
Reveal	1.4

5.2 Contents of the Release Package

The release package includes:

- Cray Fortran Compiler, version 8.3
- Cray C and C++ Compiler, version 8.3
- CrayLibs (libraries and utilities), version 8.3
- CrayDoc documentation, described in [Chapter 4, Documentation on page 15](#)

5.3 Licensing

The Cray Compiling Environment 8.3 is licensed under a software license agreement which is specific to the Cray Compiling Environment software. Upgrades to this product are provided only when a software support agreement for this Cray software is in place.

The software license agreement is enforced by FlexNet license manager software. [Table 6](#) shows the licensing scope for Cray Compiling Environment 8.3. A new license key is required for initially installing Cray Compiling Environment software and when upgrading from a previous release to a new major release. For information on installing the FlexNet Server Software, see [Appendix A, Installing and Managing FlexNet on page 29](#).

To request new FlexNet license manager keys for Cray Compiling Environment, contact license_keys@cray.com.

Table 6. Licensing Scope for Programming Environment Products

License for Product	Host Platform	Concurrent Users
Cray Compiling Environment 8.3	Cray XE, Cray XK, Cray XC series systems	Unlimited or 5

For more information about contractual licensing and pricing, contact your Cray sales representative, or send e-mail to crayinfo@cray.com.

Part II: Installation

Installing Cray Compiling Environment 8.3 [6]

Cray Compiling Environment 8.3 is installed on the shared root. You must have root permissions in order to install this software. Cray Compiling Environment 8.3 requires that asynchronous products are installed on the system. See [Table 4](#).

The CCE software release consists of the downloadable rpm file:

- `cce-8.3.0-N.x86_64.rpm` or later

Please refer to the most recent version of the *Cray Programming Environments Installation Guide* (S-2372) available at <http://docs.cray.com/>. For installations on Cray Development and Login (CDL) nodes (formerly esLogin node) also refer to *Installing CLE Support Package on a Cray Development and Login (CDL) Node* (S-2528).

This release includes *Coarray C++*, a template library that implements the coarray concept in C++. The template library specifications are contained on a set of *.html pages that the CCE installation copies to `/opt/cray/cce/version/doc/html/` on the Cray platform; they may be copied to any location which provides HTML web content for your site, or any location that can be accessed by site local web browsers.

6.1 Installing the License Key

To activate the software license, insert the FlexNet software license key information provided by Cray into a FlexNet license file on the system. The FlexNet license file contains data that is used to determine whether a licensed software product is allowed to run.

The license file contains the following information:

- FlexNet software license key for the Cray product
- Initial installation instructions
- Update instructions
- License manager utilities
- Technical Support information

Cray recommends the license file be named `/opt/cray/cce/cce.lic`. These instructions assume that the FlexNet license manager is running, that the license file is located in the directory `/opt/cray/cce`, and that the file is named `cce.lic`.

If you do not have FlexNet license manager already installed on your network, go to [Appendix A, Installing and Managing FlexNet on page 29](#).

Procedure 1. Adding a new key to a license file

1. Log in to the license server as admin or root.
2. Locate the existing license file, if any.

```
# ls /opt/cray/cce
```

If the directory does not exist,

```
# mkdir -p /opt/cray/cce
```

3. In `/opt/cray/cce`, create the plain text file named `cce.lic`. Copy the FlexNet license key received from Cray (typically in an e-mail message) to `cce.lic`.

4. Set the file access permissions to 644.

```
# chmod 644 /opt/cray/cce/cce.lic
```

5. Update the FlexNet license server to use the new key. Verify that the license server is running.

```
# lmstat
```

If the server is not running, go to [Appendix A, Installing and Managing FlexNet on page 29](#).

Assuming the server is running, reread the license file.

```
# lmrreread
```

The license is now ready to use.

6.2 Using Cray Compiling Environment 8.3

After the Cray Compiling Environment 8.3 rpm files are installed and the license is activated, load the `PrgEnv-cray` module to use CCE.

Load the `craype-accel-nvidiaversion` module to set the necessary compiler options and targets to use the accelerator.

Use either the `ftn` or `cc` command to compile. The module environment forces dynamic linking.

Because of the multiple compiling environments potentially available on Cray systems, the `ftn(1)`, `cc(1)`, and `CC(1)` man pages provide basic introductions to the compiler environment. For information about the Cray compiler command-line options, see the `crayftn(1)`, `craycc(1)`, and `crayCC(1)` man pages.

For more detailed information about the Cray compiler options, directives, pragmas, and optimizations, see *Cray Fortran Reference Manual* and *Cray C and C++ Reference Manual*.

The Cray Compiling Environment 8.3 compilation targets are `istanbul`, `mc8`, `mc12`, `interlagos`, `interlagos-cu`, `abudhabi`, `abudhabi-cu`, `ivybridge` and `sandybridge`.

The targeting modules (`craype-ivybridge`, or `craype-interlagos`, for example) set `target_system`. If the `target_system` is set during compilation of any source file, the same `target_system` must also be specified during linking and loading. For example, if users are compiling code for use on `ivybridge` nodes, they must load the `craype-ivybridge` module and use the same module at link and load time.

Installing and Managing FlexNet [A]

The Cray Compiling Environment requires FlexNet license manager.

If FlexNet license manager is not installed on your system, download the following packages provided in the Cray Compiling Environment 8.3 package:

- `cray-flexnet-installation-instructions.txt`
- `cray-flexnet-daemon-11.10.0-1.0000.3631.4.1.gem.x86_64.rpm`
- `cray-flexnet-manager-11.10.0-1.0000.3631.4.1.gem.x86_64.rpm`
- `cray-flexnet-publisher-switch-11.10.0-1.0000.3631.4.1.gem.x86_64.rpm`
- `cray-flexnet-utils-11.10.0-1.0000.3631.4.1.gem.x86_64.rpm`

Note: New licenses for CCE or PerfTools are not required when upgrading the FlexNet Server Software only.

See the FlexNet Publisher License Administration Guide at http://www.globes.com/support/utilities/fnp_LicAdmin_11_12_1.pdf.

Follow the instructions in the `cray-flexnet-installation-instructions.txt` file.

A.1 License Management Utilities and Files

Use the following commands to administer the license manager software:

<code>lmdown</code>	Shut down the licensing daemons
<code>lmgrd</code>	Invoke the licensing daemon
<code>lmhostid</code>	Display the host ID of a system
<code>lmremove</code>	Return a license to the license pool
<code>lmreread</code>	Update license daemons with new license data
<code>lmstat</code>	Report current status of the license daemon
<code>lmver</code>	Display the FlexNet version being used

Note: These commands are arguments passed to `lmutil`. If any of these commands do not exist on your license server, you can create them by making a symbolic link to `lmutil`. For example:

```
% ln -s lmutil command name
```

A.2 Combining License Files

If using three-server redundancy, use separate license files with different TCP/IP ports for the licensed software products from each vendor. (Licensed software products from the same vendor can share license files.)

If using a single server, license files may be combined. To do so, edit all license files that have matching `SERVER` lines into one file, and delete the extra `SERVER` lines (the port number does not have to match). Place all `DAEMON` lines after the `SERVER` line.

A.3 Resolving Problems

Verify the installation first. Then examine the log file:

- Verify that the license file is `/opt/cray/cce/cce.lic`. If this is not the location or name of the license file, each user must have `CRAYLMD_LICENSE_FILE` set to the correct path and name.
- Verify that the license file has a `FEATURE` line for the product that must be licensed.
- Use the `ps` command and the `lmstat` utility to verify that the servers specified in the license file are running.

Examine the log file. Look for the following messages:

- `Inconsistent encryption code for <name>` — The information encoded in the encryption code for the specified feature, server, or daemon is inconsistent with the information provided in the license file. Recheck the associated `FEATURE`, `SERVER`, or `DAEMON` line in your license file.
- `license daemon: execl failed` — The `lmgrd` path specified on the `DAEMON` line in the license file is not valid. Verify that the license file contains the correct path.
- `Retrying socket bind` — Either the TCP port number is already in use by another process, two `lmgrd` daemons were started with license files that specify the same TCP port, or the port is waiting to timeout after a recently executed `lmgrd` command. This message typically appears when you stop and then immediately try to restart `lmgrd`. In this case, wait a few minutes, to allow TCP time to relinquish the port.

If this fails to correct the problem, check the `SERVER` line in the license file. If another process needs the specified port, edit the license file to specify a different port. If no port is specified, the default port is 27000.