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Cray Compiling Environment Release Overview and Installation Guide (8.5)

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1 Cray Compiling Environment 8.5 Release Overview Introduction

This publication is an overview of the Cray Compiling Environment 8.5 release for the Cray XE, Cray XK, Cray XC, Cray CS series systems, and Cray Envoy systems.

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

Emphasis for the Cray Compiling Environment 8.5 Release

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

- Support for the C11 language standard.
- Support for the device (accelerator) features in the OpenMP 4.5 specification.
- Support for the Intel[®] Xeon Phi[™] processor (formerly codenamed Knights Landing or KNL).
- Support for Cray Envoy systems.
- Functional support for PGAS languages (UPC, Fortran 2008 and C++ coarrays) on Cray CS series systems.
- Performance improvements for all supported systems.

Cray Compiling Environment 8.5 Release Package Description

The Cray Compiling Environment 8.5 consists of:

- Cray Fortran Compiler, version 8.5
- Cray C and C++ Compiler, version 8.5
- CrayLibs (libraries and utilities), version 8.5
- Cray Compiling Environment 8.5 Documentation Overview

All software is installed by means of scripts and RPM Package Manager (RPM) files. For more detail about Cray Compiling Environment 8.5 release package, refer to the *Cray Compiling Environment 8.5 Release Package Overview* on page 10.

2 Cray Compiling Environment 8.5 Software Enhancements

This topic describes software enhancements provided with the Cray Compiling Environment 8.5 release.

Performance Enhancements

- Loops that have been hand unrolled will now vectorize under certain conditions.
- Automatic cloning is now enabled by default. If the compiler is unable to inline a call, and the compiler determines there is an execution performance advantage to cloning the call site, it will do so automatically. Messages will appear in the .lst file explaining why the compiler decided to clone a given call site.
- Enhanced inlining (available at -hipa4) for C++ codes can yield improved performance. This often comes at a compile time increase.
- Partial OpenMP 4.5 support allows for improved performance on accelerators, through the use of asynchronous target constructs and more efficient handling of implicit scalar-variable data transfers.

C and C++ Support

This release adds support for the C11 language standard. To enable C11 features, use the -h std=c11 command line option. If not specified, the default is -h std=c99.

Support for the gcc extension attribute ((aligned(<const>))) has been added.

The optimize pragma directive is now supported for C and C++ applications. In previous releases, this directive was supported in Fortran only. This allows for control of optimizations in a program unit. See the *C* and C++ *Reference Manual S-2179* and the optimize (7) man page for more information.

OpenMP Support

This release adds support for the device (accelerator) features in the OpenMP 4.5 specification. Features of note include:

- The target enter data and target exit data constructs
- The nowait and depend clauses on the target construct
- The private and firstprivate clause on the target construct
- The is device ptr clause on the target construct
- The defaultmap clause on the target construct
- The nowait and depend clauses on the target construct
- The use device ptr clause on the target construct
- The lastprivate clause on the distribute construct

- The to and link clauses on the declare target directive
- The always map type modifier on the map clause
- The release and delete map types on the map clause for the target exit data construct
- The directive name modifier on if clauses
- The device memory routines, including omp_target_alloc, omp_target_free, omp_target_is_present, omp_target_memcpy, omp_target_memcpy_rect, omp_target_associate_ptr, and omp_target_disassociate_ptr.

The OpenMP 4.5 standard is available on the OpenMP website, http://openmp.org/wp/openmp-specifications/.

Intel[®] Xeon Phi[™] Support

This release adds support for the Intel[®] Xeon Phi[™] processor (formerly codenamed Knights Landing or KNL).

- The AVX512F instruction set is supported through automatic vectorization. Load the craype-mic-knl module to target KNL processors including AVX512F support.
- The new memory directive provides a mechanism for users to place variables and memory allocations in KNL "high-bandwidth" MCDRAM memory. See the memory (7) man page for more information.

PGAS Support

Functional support for PGAS languages (UPC, Fortran 2008, and C++ coarrays) on Cray CS series systems has been added in this release. Performance has not been optimized. This provides functional portability for PGAS applications. See the intro_pgas(7) man page for more information regarding support for PGAS programming models.

Compiler Command Line Changes

The following command line changes apply to CCE 8.5:

The -Wx option can be used to limit the number of registers used by kernels. In some cases this can improve both occupancy and performance. For example, -Wx, "--maxregcount=64" would limit all the kernels generated within the source file to use at most 64 registers.

The -Wc option can be used to add ptx/cubin files to the link step. This can be used to allow OpenACC kernels to make use of CUDA code compiled with nvcc.

3 Cray Compiling Environment 8.5 Compatibilities and Differences

There are no changes in CCE 8.5 that impact compatibility with CCE 8.4.

CCE supports OpenMP 3.1 constructs through the GNU interface. This allows users to link gcc-compiled libraries that contain OpenMP 3.1 constructs, with CCE compiled applications. In previous CCE releases, CCE provided OpenMP 3.1 compatibility with gcc 4.8. CCE 8.5 now provides OpenMP 3.1 compatibility with gcc 4.9 and gcc 5.x.

4 Cray Compiling Environment 8.5 Documentation Overview

This topic describes the documentation that supports the Cray Compiling Environment 8.5 release.

Access Product Documentation

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

Cray Documentation Portal	The Cray Documentation Portal is the Cray documentation delivery system. Access the HTML and PDF documentation via the Cray Documentation Portal at <i>https://pubs.cray.com/</i> .
	Legacy documentation (as well as man pages, and in some cases, third-party documentation) can be found on the CrayDoc website: <i>http://docs.cray.com</i> or through the local network location defined by the system administrator.
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 the quick access and search of Cray books, man pages, and in some cases, third-party documentation. Access CrayPort by using the following URL: <i>http://crayport.cray.com</i> .
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:
	% man man
Third-party documentation	Third-party documentation that is not provided through CrayPort or CrayDoc is included with the third-party product.

Cray Developed Publications Provided with this Release

The publications provided with this release are listed in the table below, which also indicates whether each publication was updated. Publications are provided in HTML and PDF formats.

Table 1. Publications Provided with this Release

Book Title	Number	Updated
Cray Compiling Environment Release Overview and Installation Guide (this document)	8.5	Yes

Book Title	Number	Updated
Cray C and C++ Reference Manual	8.5	Yes
Cray Fortran Reference Manual	8.5	Yes

Additional Documentation Resources

The below table lists additional resources for obtaining documentation not included with this release package.

Table 2. Additional Documentation Resources

Product	Documentation Source
GNU compilers	Documentation for the GNU C and Fortran compilers is available at <i>http://gcc.gnu.org/onlinedocs/</i>
glibc	glibe 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

New Cray Man Pages

Cray man pages new with this release:

• memory(7)

Changed Cray Man Pages

Cray man pages changed with this release:

- craycc(1)
- crayCC(1)
- crayftn(1)
- intro openacc(7)
- intro directives(7)
- optimize(7)

Other Related Documents Available

The following publications contain additional information to help set up the Cray Compiling Environment 8.5; they are not provided with this release but are supplied with other products purchased from Cray:

- Cray Programming Environments Installation Guide (16.06)
- Cray Programming Environment User's Guide (S-2529)
- Managing System Software for the Cray Linux Environment (S-2393)
- Installing the Cray Programming Environment for Cray CS Systems (S-2800)

• PE Installation on Envoy Guide

5 Cray Compiling Environment 8.5 Release Package Overview

Hardware and Software Requirements

The Cray Compiling Environment 8.5 release is supported on the following software releases:

Table 3. Required OS Versions

System	os
Cray XE	CLE 5.2
Сгау ХК	CLE 5.2
Cray XC	CLE 5.2 or CLE 6.0
Cray CS	CentOS 6.7/7.1 and RedHat 6.7/7.1
Cray Envoy	SLES12 SP1

The Cray Compiling Environment 8.5 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	Cray CS	Cray Envoy
craype	2.5.4	2.5.4	2.5.4	2.5.4	2.5.4
РМІ	5.0.10	5.0.10	5.0.10	N/A	N/A
LibSci	16.06	16.06	16.06	16.06	16.06
FlexNet	11.13.1.1	11.13.1.1	11.13.1.1	11.13.1.1	11.13.1.1
gcc	4.8.1	4.8.1	4.8.1	4.8.1	4.8.1

The Cray Compiling Environment 8.5 release requires the following minimum versions of these **optional** products:

Table 5. Optional Asynchronous Products

Product	
HDF5	1.8.16
NETcdf	4.4.0

Product	
parallel-NETcdf	1.6.1
МРТ	7.3.3
GA	5.3.0.5
LibSci_acc	16.03.1
TPSL	16.03.1
PETSc	3.6.3.0
Trilinos	12.2.1.0
fftw3	3.3.4.7
fftw2	2.1.5.9
Perftools	6.4.0

Contents of the Release Package

The release package includes:

- Cray Fortran Compiler, version 8.5
- Cray C and C++ Compiler, version 8.5
- CrayLibs (libraries and utilities), version 8.5
- CrayDoc documentation, described in the Cray Compiling Environment 8.5 Documentation Overview topic.

Licensing

The Cray Compiling Environment 8.5 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. The table below shows the licensing scope for Cray Compiling Environment 8.5. 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 *Install and Manage FlexNet*.

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 8.5	Cray XE, Cray XK, Cray XC, Cray CS, Cray Envoy systems	5 or unlimited

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

6 Install Cray Compiling Environment 8.5

Cray Compiling Environment 8.5 is installed on the shared root. root permissions are necessary in order to install this software. Cray Compiling Environment 8.5 requires that asynchronous products are installed on the system.

To install the CCE programming environment:

• CLE 5.2, Cray CS series systems:

rpm -ivh --prefix=/opt/cray cce-8.5.0-N.x86_64.rpm

To make CCE 8.5.0 the default version of CCE, execute:

/opt/cray/admin-pe/set default files/set default cce 8.5.0

CLE 6.0 and Cray Envoy systems:

rpm -ivh cce-8.5.0-N.x86_64.rpm

• To make CCE 8.5.0 the default version of CCE, execute:

/opt/cray/pe/admin-pe/set default files/set default cce 8.5.0

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). For Cray CS systems, please refer to the most recent version of *Installing the Cray Programming Environment for Cray CS Systems (S-2800)*.

For Cray Envoy systems, please refer to the most recent version of PE Installation on Envoy Guide.

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 the site, or any location that can be accessed by site local web browsers.

6.1 Install the License Key

Prerequisites

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 the FlexNet license manager isn't installed on the network, see Install and Manage FlexNet.

Procedure

- 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. Create the plain text file named cce.lic in /opt/cray/cce.
 - a. 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, see Install and Manage FlexNet.

Assuming the server is running, reread the license file.

lmreread

The license is now ready to use.

6.2 Use of the Cray Compiling Environment 8.5

After the Cray Compiling Environment 8.5 rpm files are installed and the license is activated, load the PrgEnvcray module to use CCE.

Load the craype-accel-nvidiaversion module to set the necessary compiler options and targets. When using an accelerator, the module environment forces dynamic linking.

Use either ftn or cc command to compile.

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 more 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 8.5 compilation targets are istanbul, mc8, mc12, interlagos, interlagos-cu, abudhabi, abudhabi-cu, ivybridge, sandybridge, haswell, broadwell, and arm-thunderx.

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.

7 Install and Manage FlexNet

The Cray Compiling Environment requires FlexNet license manager.

If FlexNet license manager is not installed on the system, download the following packages provided in the Cray Compiling Environment 8.5 package:

- cray-flexnet-installation-instructions.txt
- cray-flexnet-daemon-11.12.1-1.0000.9037.2.1.ari.x86 64.rpm
- cray-flexnet-manager-11.12.1-1.0000.9037.2.1.ari.x86 64.rpm
- cray-flexnet-publisher-switch-11.12.1-1.0000.9037.2.1.ari.x86 64.rpm
- cray-flexnet-utils-11.12.1-1.0000.9037.2.1.ari.x86 64.rpm

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

See the FlexNet Publisher License Administration Guide at *https://www.synopsys.com/support/Ll/Licensing/ Documents/Dockeys/enduser.pdf*.

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

License Management Utilities and Files

Use the following commands to administer the license manager software:

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

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

% ln -s lmutil *command name*

Combine 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.

Resolve 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 the 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 after stopping and then immediately trying 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.