

Cray Compiling Environment 8.1 Release Overview and Installation Guide

© 2012 Cray Inc. All Rights Reserved. This document or parts thereof may not be reproduced in any form unless permitted by contract or by written permission of Cray Inc.

U.S. GOVERNMENT RESTRICTED RIGHTS NOTICE

The Computer Software is delivered as "Commercial Computer Software" as defined in DFARS 48 CFR 252.227-7014.

All Computer Software and Computer Software Documentation acquired by or for the U.S. Government is provided with Restricted Rights. Use, duplication or disclosure by the U.S. Government is subject to the restrictions described in FAR 48 CFR 52.227-14 or DFARS 48 CFR 252.227-7014, as applicable.

Technical Data acquired by or for the U.S. Government, if any, is provided with Limited Rights. Use, duplication or disclosure by the U.S. Government is subject to the restrictions described in FAR 48 CFR 52.227-14 or DFARS 48 CFR 252.227-7013, as applicable.

Cray and Sonexion are federally registered trademarks and Active Manager, Cray Apprentice2, Cray Apprentice2 Desktop, Cray C++ Compiling System, Cray CX, Cray CX1, Cray CX1-iWS, Cray CX1-LC, Cray CX1000, Cray CX1000-C, Cray CX1000-G, Cray CX1000-S, Cray CX1000-SC, Cray CX1000-SM, Cray CX1000-HN, Cray Fortran Compiler, Cray Linux Environment, Cray SHMEM, Cray X1, Cray X1E, Cray X2, Cray XD1, Cray XE, Cray XEm, Cray XE5, Cray XE5m, Cray XE6, Cray XE6m, Cray XK6, Cray XK6m, Cray XMT, Cray XT, Cray XT, Cray XTm, Cray XT3, Cray XT4, Cray XT5, Cray XT5h, Cray XT5m, Cray XT6, Cray XT6m, CrayDoc, CrayPort, CRInform, ECOphlex, LibSci, NodeKARE, RapidArray, The Way to Better Science, Threadstorm, uRiKA, UNICOS/lc, and YarcData are trademarks of Cray Inc.

AMD Opteron is a trademark of Advanced Micro Devices, Inc. FlexNet is a trademark of Flexera Software. GNU is a trademark of The Free Software Foundation. Gemini, Intel and Kepler are a trademarks of Intel Corporation in the United States and/or ot her countries. Google is a trademark of Google. ISO is a trademark of International Organization for Standardization (Organisation Internationale de Normalisation). Linux is a trademark of Linus Torvalds. OpenACC and NVIDIA are trademarks of NVIDIA Corporation. PETSc is a trademark of Copyright (C) 1995-2004 University of Chicago. PGI is a trademark of The Portland Group Compiler Technology, STMicroelectronics, Inc. Platform is a trademark of Platform Computing Corporation. UNIX, the "X device," X Window System, and X/Open are trademarks of The Open Group in the United States and other countries. All other trademarks are the property of their respective owners.

Contents

	Page
Part I: Release Overview	
Introduction [1]	7
1.1 Emphasis for the Cray Compiling Environment 8.1 Release	7
1.2 Cray Compiling Environment 8.1 Release Package Description	7
Software Enhancements [2]	9
2.1 Performance Enhancements	9
2.2 Fortran Standard Compliance	10
2.2.1 Extensions to the Fortran Standard	10
2.3 OpenMP API Specification	10
2.4 ISO C++ Standard (2003)	11
2.5 Accelerator Support	11
2.5.1 OpenACC Directives	11
2.5.2 Fortran Intrinsics	11
2.5.3 Module Support	11
2.5.4 OpenMP Accelerator Directives Deprecated	12
2.6 Compiler Command Line Changes	12
2.7 New Environment Variables	13
2.8 New Compiler Directives	13
Compatibilities and Differences [3]	15
Documentation [4]	17
4.1 Accessing Product Documentation	17
4.2 Cray-developed Books Provided with This Release	18
4.3 Additional Documentation Resources	18
4.4 Changes to Man Pages	18
4.4.1 New Cray Man Pages	18
4.4.2 Changed Cray Man Pages	19
4.5 Other Related Documents Available	19

	Page
Release Package [5]	21
5.1 Hardware and Software Requirements	 21
5.2 Contents of the Release Package	 22
5.3 Licensing	 22
5.4 Third-party License Notices	 22
5.4.1 LLVM	 23
5.4.2 tcmalloc (google-perftools)	 24
5.4.3 AMD LibM 3.0.1	 25
5.4.4 AMD ACML-MV 4.4.1	 25
Part II: Installation	
Installing Cray Compiling Environment 8.1 [6]	29
6.1 Installing the RPM Files	 29
6.2 Installing the License Key	 31
6.3 Changing the Default Programming Environment	 32
6.3.1 Configuring the /etc/*rc.local Files on a Cray Linux Environment (CLE) System	 33
6.3.2 Configuring the /etc/*rc.local Files on a Standalone Linux System with cade-prgenv-4.0.*	 34
6.4 Using Cray Compiling Environment 8.1	34
6.4.1 Compiling and Linking an Application which Contains Accelerator Directives	 35
Appendix A Installing and Managing FlexNet	37
A.1 License Management Utilities and Files	 37
A.2 Combining License Files	 38
A.3 Resolving Problems	 38
Procedures	
Procedure 1. Installing the RPM files	 29
Procedure 2. Adding a new key to a license file	 32
Tables	
Table 1. Books Provided with This Release	 18
Table 2. Additional Documentation Resources	 18
Table 3. Licensing Scope for Programming Environment Products	 22

Part I: Release Overview

This document provides an overview of the Cray Compiling Environment 8.1 release for the Cray XE and Cray XK 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 8.1 Release

The *Cray Compiling Environment* release provides the following key enhancements:

- New features as specified by the 2008 Fortran standard. This compiler conforms to the Fortran 2008 standard (ISO/IEC 1539-1:2010).
- Enhanced support for accelerators on Cray Systems, including complete support for the *OpenACC Application Programming Interface, Version 1.0.*
- Performance improvements for Cray XE and Cray XK systems
- Support for the AMD Abu Dhabi CPU
- Support for the Intel Sandy Bridge CPU
- Support for the NVIDIA Kepler GPU

1.2 Cray Compiling Environment 8.1 Release Package Description

The Cray Compiling Environment 8.1 consists of:

- Cray Fortran Compiler, version 8.1
- Cray C and C++ Compiler, version 8.1
- CrayLibs (libraries and utilities), version 8.1
- CrayDoc software suite and the documentation, described in Chapter 4,
 Documentation on page 17

All software is installed by means of scripts and RPM Package Manager (RPM) files. For more detail about Cray Compiling Environment 8.1 release package, refer to Chapter 5, Release Package on page 21.

Software Enhancements [2]

This chapter describes the software enhancements provided with the Cray Compiling Environment 8.1 release.

2.1 Performance Enhancements

- Optimization has been improved for targets supporting AVX, especially for kernels using mixed width data types.
- Address computations have been improved to make better use of native hardware capabilities.
- The detection, enforcement, and use of aligned memory operations has been significantly optimized for better application performance.
- Performance of EXP libraries for 64-bit data types on Interlagos CPUs has been improved.
- Additional intrinsics where arguments can be determined are now evaluated at compile time.
- Performance of some reduction operations has been greatly improved by exploiting more instruction level parallelism.
- Autothreading (-hautothread) at thread level 3 (-O thread3 or -h thread3) is enhanced to parallelize some small loops with potential cross iteration dependence.
- Performance of adjacent reads has been improved by reducing the number of calls to the Fortran IO library.
- Portions of the optimizer have been redesigned for improved support of
 applications requiring bit reproducibility when changing the number of MPI ranks
 and OpenMP threads. -hflex_mp=conservative is now much more likely
 to result in application bit reproducibility, with a minimal impact on performance
 and -hflex_mp=intolerant has considerably improved performance for
 some applications, without a loss of bit reproducibility.
- The OpenACC cache directive and the cache_nt clause of the loop_info directive are now supported for NVIDIA accelerator targets, allowing the user to tune cache usage on the accelerator.

- Additional UPC and Fortran coarray shared data structures are now automatically grouped into block transfers, yielding improved data transfer speeds.
- Improvement to conflict detection for writes to UPC shared data, or to Fortran coarrays, allows applications to achieve faster message rates for the common case of no write conflicts.

2.2 Fortran Standard Compliance

The Cray Fortran compiler supports ISO/IEC 1539-1:2010, the Fortran 2008 standard.

2.2.1 Extensions to the Fortran Standard

• The maximum rank is equal to 31 - arrays can have up to 31 dimensions. The standard requires a maximum rank of 15.

2.3 OpenMP API Specification

Cray Compiling Environment 8.1 supports *OpenMP Application Program Interface*, *Version 3.1*. All OpenMP library procedures and directives, except for limitations in a few directive clauses, are supported.

This release adds support for the following feature, not described by the API specification:

omp_set_wait_policy()

A new Cray-specific OpenMP interface, <code>cray_omp_set_wait_policy</code>, introduces the ability to change the OpenMP wait policy dynamically during a program's execution. This routine allows dynamic modification of the <code>wait-policy-var</code> internal control variable (ICV) value, which corresponds to the <code>OMP_WAIT_POLICY</code> environment variable.

2.4 ISO C++ Standard (2003)

The Cray C++ compiler accepts the C++ language as defined by the ISO/IEC 14882:2003 standard, except for exported templates. C++ supports the ISO 2003 Standard Template Library (STL) headers but abrogates support for pre-standard template headers that have the .h extension.

Note: C++ codes that use the pre-standard template headers must be updated to the ISO C++ standard.

The -h gnu option enables the compiler to recognize a subset of the GCC version 4.4.4 extensions to C listed in the GCC C language extensions table. The default is -h nognu. For descriptions of the GCC C language extensions, see http://gcc.gnu.org/onlinedocs.

2.5 Accelerator Support

2.5.1 OpenACC Directives

This release supports the *OpenACC Application Programming Interface, Version 1.0* specification developed by PGI, Cray Inc., and NVIDIA, with support from CAPS entreprise. Refer to the OpenACC home page at http://www.openacc-standard.org/. Under the Downloads link, select the *OpenACC 1.0 Specification*.

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

2.5.2 Fortran Intrinsics

Certain Fortran intrinsic routines will run on the accelerator if they are encountered within an accelerated region. Support for the intrinsics MAXLOC, MINLOC, MAXVAL, and MINVAL was added in this release. The main limitation is that argument DIM must not be specified.

2.5.3 Module Support

To compile an application that includes accelerator directives, ensure that PrgEnv-cray module is loaded and that it includes CCE 8.1. Then, either load the craype-accel-nvidia20 module for Fermi support or the craype-accel-nvidia35 module for Kepler support.

Use either the ftn or cc command to compile.

2.5.4 OpenMP Accelerator Directives Deprecated

The OpenMP accelerator directives are currently being discussed in the OpenMP Language Committee and the specification is currently in a state of flux. The OpenMP accelerator directives, as currently implemented, are deprecated and will be removed in a future CCE release. Please use the OpenACC accelerator directives instead.

2.6 Compiler Command Line Changes

The following command line changes apply to CCE 8.1

- The compiler supports a more aggressive floating point and complex arithmetic optimization level, adding the -h fp4 option.
- h [no]keep_frame_pointer command line option prevents call stack frame from being optimized out of a function so CrayPat sampling is able to trace call stack back to entry point.
- The -h mpin option enables or disables an optimization that converts blocking MPI send and receive operations to their non-blocking counterparts paired with a wait operation, and schedules these operations to overlap communication and computation. The default is -hmpi0.
- Interprocedural analysis (IPA) level 5 enables cloning directives. Previously they
 were enabled at IPA level 4.
- The -h acc_model=option[:option] ... explicitly controls execution and memory model utilized by the accelerator support system. The option arguments identify the type of behavior desired. There are three option sets, only one member of a set may be used at a time; however, all three sets may be used together.

Fortran Only

- The -hcaf option to recognize coarray syntax is on by default. A new predefined macro _CRAY_COARRAY defined when -hcaf is in effect.
- The command line option -r i intersperses loop optimization messages within the loopmark listing.
- The -eD option enables all debugging options.
- New command line option -eb causes the compiler to issue a warning message rather than an error message for procedure call with TARGET, VOLATILE, ASYNCHRONOUS dummy arguments without an explicit interface definition.
- S no longer requires or accepts the specification of an output file. The options

 eS and -S now have the same effect. No changes were made to -eS. This change makes the Cray Fortran -S option consistent with other compilers.

C Only

• The -h bounds option provides checking of UPC shared array accesses to ensure that they are within acceptable boundaries. The -h nobounds option disables these checks.

2.7 New Environment Variables

NO_STOP_MESSAGE

If set, and if the STOP [$stop_code$] statement in the Fortran code does **not** specify the optional $stop_code$, then STOP messages are not produced when this statement is executed.

2.8 New Compiler Directives

• The general prefetch directive instructs the compiler to generate explicit prefetch instructions which load data from memory into cache prior to read or write access. See the prefetch(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.

- The -hcaf option to recognize coarray syntax is on by default. In previous releases, the default was -hnocaf.
- OpenMP accelerator directives, as currently implemented, are deprecated and will be removed in a future CCE release.
- Some system headers were removed from upc.h, including stdlib.h which includes sys/types.h. Do not rely on upc.h to include other system headers. If your code requires sys/types.h, Include stdint.h if you were not previously doing so.

Documentation [4]

This chapter describes the documentation that supports the Cray Compiling Environment 8.1 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.

- 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:

% man man

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 Books Provided with This Release

The books provided with this release are listed in Table 1, which also indicates whether each book was updated. Books are provided in HTML and PDF formats.

Table 1. Books Provided with This Release

Book Title	Number	Updated
Cray Compiling Environment Release Overview and Installation Guide (this document)	S-5212-81	Yes
Cray C and C++ Reference Manual	S-2179-81	Yes
Cray Fortran Reference Manual	S-3901-81	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

These man pages are new with this release:

- prefetch(7): A general directive which instructs the compiler to generate explicit prefetch instructions.
- OpenACC.EXAMPLES(7): Example OpenACC codes.
- execute_command_line(3i): Runs a shell command.

4.4.2 Changed Cray Man Pages

The following Cray man pages were changed with this release:

- craycc(1)
- crayCC(1)
- crayftn(1)
- amo(3i)
- intro_intrin(3i)
- intro_quad_precision(3i)
- num_images(3i)
- this_image(3i)
- intro_directives(7)
- intro_openacc(7)
- intro_openmp_acc(7)
- intro_pgas(7)

4.5 Other Related Documents Available

The following publications contain additional information that may be helpful in setting up your Cray Compiling Environment 8.1 environment; they are not provided with this release but are supplied with other products purchased from Cray:

- Cray Application Developer's Environment Installation Guide
- Cray Application Developer's Environment User's Guide
- Managing System Software for Cray XE and Cray XK Systems

5.1 Hardware and Software Requirements

The CCE 8.1.0 release is supported on Cray XE systems that run the Cray Linux Environment (CLE) operating system, version 3.1 and later, and on Cray XK systems that run the CLE operating system, version 4.0.UP01 and later. The Cray Compiling Environment 8.1 release requires the following supporting asynchronous software products:

- Cray Compiler Drivers (xt-asyncpe) 5.12 or later
- GNU Compiler Collection (GCC) 4.4.4 must be installed, but must NOT be the default GCC
- PMI 3.0.0 or later
- Cray Scientific Libraries (LibSci) 11.0.00 or later
- FlexNet License Manager 11.10.0 or later is recommended (available in Third Party Products 5.24 package)

The Cray Compiling Environment 8.1 release requires minimum versions of the following products, if these products are used:

- Cray Portable Extensible Toolkit for Scientific Computation (PETSc) 3.1.05 or later
- hdf5-netcdf 1.8 (HDF5 1.85 and netcdf 4.1.1)
- MPT 5.2.3 or later
- ACML 4.4.0 or later. To use ACML 5.0, GCC 4.6.1 must be installed.
- Cray Performance Measurement and Analysis Tools 5.3.0
- Cray Performance Measurement and Analysis Tools 6.0.0 is required for Reveal

5.2 Contents of the Release Package

The release package includes:

- Cray Fortran Compiler, version 8.1
- Cray C and C++ Compiler, version 8.1
- CrayLibs (libraries and utilities), version 8.1
- CrayDoc software suite and the documentation, described in Chapter 4, Documentation on page 17

5.3 Licensing

The Cray Compiling Environment 8.1 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 3 shows the licensing scope for Cray Compiling Environment 8.1. 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 (8.1). For information on installing the FlexNet Server Software, see Appendix A, Installing and Managing FlexNet on page 37.

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

Table 3. Licensing Scope for Programming Environment Products

License for Product	Host Platform	Concurrent Users
Cray Compiling Environment 8.1	Cray XE and Cray XK 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.

5.4 Third-party License Notices

The Cray Compiling Environment 8.1 release includes the following third-party software pursuant to the following third-party license notices.

5.4.1 LLVM

LLVM Release License

University of Illinois/NCSA Open Source License

Copyright (c) 2003-2008 University of Illinois at Urbana-Champaign. All rights reserved.

Developed by:

LLVM Team

University of Illinois at Urbana-Champaign

http://llvm.org

Permission is hereby granted, free of charge, to any person obtaining a copy of this software and associated documentation files (the "Software"), to deal with the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so, subject to the following conditions:

- * Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimers.
- * Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimers in the documentation and/or other materials provided with the distribution.
- * Neither the names of the LLVM Team, University of Illinois at Urbana-Champaign, nor the names of its contributors may be used to endorse or promote products derived from this Software without specific prior written permission.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE CONTRIBUTORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS WITH THE SOFTWARE.

5.4.2 tcmalloc (google-perftools)

Copyright (c) 2005, Google Inc. All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- * Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- * Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
- * Neither the name of Google Inc. nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

5.4.3 AMD LibM 3.0.1

Modified BSD License (2011):

Copyright (c) 2008-2011, Advanced Micro Devices, Inc. All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.

Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.

Neither the name of the copyright holder nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT HOLDER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

5.4.4 AMD ACML-MV 4.4.1

Copyright (c) 2006 Advanced Micro Devices, Inc.

All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- * Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- * Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
- * Neither the name of Advanced Micro Devices, Inc. nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

Part II: Installation

Installing Cray Compiling Environment 8.1 [6]

Cray Compiling Environment 8.1 is distributed on DVD. It is also available as one or more downloadable files. The instructions in this chapter assume you are working with a DVD. If you are working with either a single iso file or a tar file composed of individual rpm files, adjust the instructions accordingly.

Cray Compiling Environment 8.1 is installed on the shared root. You must have root permissions in order to install this software.

Use these rpm files:

• cce-8.1.0-N.x86_64.rpm or later

Additionally, Cray Compiling Environment 8.1 requires that the following asynchronous products be installed on your system:

- Cray Scientific Libraries (LibSci) 11.0.00 or later
- Cray Compiler Drivers (xt-asyncpe) 5.12 or later
- GNU Compiler Collection (GCC) 4.4.4

6.1 Installing the RPM Files

Procedure 1. Installing the RPM files

1. Log on to the SMW as root.

```
% ssh root@smw
```

2. Load and mount the distribution media, if necessary.

```
smw:~# mount /dev/cdrom /media/cdrom
```

3. Create a temporary directory on the boot node for the installation files, if one does not already exist.

```
smw:~# ssh boot mkdir /tmp/install.cce
```

4. Copy the installation files from the distribution media to the boot node.

```
smw:~# scp -pr /media/cdrom/cce-version.x86_64.rpm \
boot:/tmp/install.cce
```

5. (Optional) If you need to install asynchronous products, copy these files as needed.

```
smw:~# scp -pr /media/cdrom/xt-gcc-version.x86_64.rpm \
/media/cdrom/xt-asyncpe-version.i386.rpm \
/media/cdrom/xt-libsci-version.x86_64.rpm \
/media/cdrom/cray-mpt-version.x86_64.rpm \
boot:/tmp/install.cce
```

6. Unmount and remove the distribution media.

```
smw:~# umount /media/cdrom
```

7. Log into the boot node as root.

```
smw:~# ssh root@boot
```

8. Change to your temporary directory.

```
boot001:~# cd /tmp/install.cce
```

9. Create a target directory on the shared root and copy the installation files from your temporary directory to the shared root.

```
boot001/:/tmp/install.cce # mkdir -p /rr/current/software/install.cce
boot001/:/tmp/install.cce # cp -p cce-version.x86_64.rpm \
/rr/current/software/install.cce
```

10. (Optional) If you are installing asynchronous products, copy these files as needed.

```
boot001/:/tmp/install.cce # cp -p xt-gcc-version.x86_64.rpm \
xt-asyncpe-version.x86_64.rpm \
xt-libsci-version.x86_64.rpm \
cray-mpt-version.x86_64.rpm \
/rr/current/software/install.cce
```

11. Open an xtopview session.

```
boot001/:/tmp/install.cce # xtopview
```

12. Change to the temporary directory you created on the shared root.

```
default/:/# cd /software/install.cce
```

13. Use the rpm command to install the files.

Note: When running rpm from within xtopview, the rpm utility issues a warning that it cannot find /rr/current. This warning may safely be ignored.

Install CCE:

```
default/:/software/install.cce # rpm -ivh cce-8.1.0-version.x86_64.rpm

Set newly installed CCE to be default:

YarcData-logo_a-cray-compan.gifdefault/:/software/install.cce #
/opt/cray/admin-pe/set_default_files/set_default_cce_8.1.0
```

(Optional) If installing asynchronous products, use these commands as needed:

```
default/:/software/install.cce # rpm -ivh xt-gcc-version.x86_64.rpm
default/:/software/install.cce # rpm -ivh xt-asyncpe-version.i386.rpm
default/:/software/install.cce # rpm -iv xt-libsci-version.x86_64.rpm
```

Set newly installed *product* to be default:

```
default/:/software/install.cce #
/opt/cray/admin-pe/set_default_files/set_default_product_version
```

14. Exit from the xtopview session:

```
default/:/software/install.cce # exit
```

15. Log out of the boot node:

```
boot001/:/tmp/install.cce # exit
logout
Connection to boot closed.
smw:~#
```

16. Log out of the SMW.

```
smw:~# exit
logout
...
```

6.2 Installing the License Key

To activate your software license, you must insert the FlexNet software license key information provided by Cray into a FlexNet license file on your 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:

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

Cray recommends that you name your license file /opt/cray/cce/cce.lic. These instructions assume that the FlexNet license manager is already running, that your 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 37.

Procedure 2. Adding a new key to a license file

- 1. Log in to your license server as admin or root.
- 2. Locate your existing license file, if any.
 - # ls /opt/cray/cce

If the directory does not exist, make it.

- # mkdir -p /opt/cray/cce
- 3. In /opt/cray/cce, create the plain text file cce.lic. Copy your FlexNet license key you received from Cray (typically in an email message) to cce.lic.
- 4. Set the file access permissions to 644.
 - # chmod 644 /opt/cray/cce/cce.lic
- 5. Update your 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 37.

Assuming the server is running, reread the license file.

lmreread

Your license is now ready to use.

6.3 Changing the Default Programming Environment

The installation of the cade-prgenv RPM creates a section in the /etc/bash.bashrc.local and /etc/csh.cshrc.local scripts called the **PE-set-up** block. The user should not modify this block.

To change the default PE, and add more PE user defaults, the site administrator may add appropriate instructions by editing the /etc/*rc.local files within the SITE-set-up block only. Also refer to *Managing System Software for Cray XE and Cray XK Systems*, Section 5.7.

Cray Linux Environment (CLE) 4.0 release modifies the default programming environment in CLE 4.0 as follows:

- The programming environment requires that a default CPU target be specified in the SITE-set-up block of the /etc/*rc.local files.
- The CLE 4.0 and 4.1 environments support only network target gemini.
- The module, xt-mpich2, is no longer loaded as part of the default PrgEnv-*
 product list. This is to accommodate site preferences for xt-shmem or
 xt-mpich2 as the site default.

6.3.1 Configuring the /etc/*rc.local Files on a Cray Linux Environment (CLE) System

The network type is set correctly by the operating system installation and does not need to be reset.

The default link type is static.

Note: On CLE 4.0.UP01, the default programming environment (PE) is PrgEnv-pgi, unless set differently in the SITE-set-up block of the /etc/*rc.local files.

On CLE 4.0.UP02 and later, the default programming environment (PE) is PrgEnv-cray, unless set differently in the SITE-set-up block of the /etc/*rc.local files.

On the Cray XE system, the following configuration loads the xt-mpich2 module and ensures that code is generated for a mc12 target.

```
##BEGIN SITE-set-up ADD SITE DEFAULTS HERE
# Site specific set up in this section.
module load xt-mpich2
module load craype-mc12
##END SITE-set-up
```

If you want to change the default PE settings to PrgEnv-cray, SHMEM, CPU target xyz, and dynamic linking, add the following to the SITE-set-up block in bash.bashrc.local and csh.cshrc.local:

```
##BEGIN SITE-set-up ADD SITE DEFAULTS HERE
# Site specific set up in this section.
if (! ${?PELOCAL_PRGENV} ) then
  module unload PrgEnv-pgi
  module load PrgEnv-cray
  setenv PELOCAL_PRGENV true
  set -r PELOCAL_PRGENV=$PELOCAL_PRGENV
endif
module load xt-shmem
module load craype-xyz
setenv XTPE_LINK_TYPE dynamic
# OR: export XTPE_LINK_TYPE=dynamic
##END SITE-set-up
```

The instructions in the SITE-set-up block are not altered by operating system installations. The SITE-set-up block is evaluated after the PE-set-up block, so make sure new instructions do not conflict with the ones in the PE-set-up block.

6.3.2 Configuring the /etc/*rc.local Files on a Standalone Linux System with cade-prgenv-4.0.*

The installation of the cade-prgenv RPM adds the following line to the *rc.local files.

```
module use /opt/cray/xt-asyncpe/default/modulefiles;export \texttt{XTOS\_VERSION=4.0.} version
```

The XTOS_VERSION is updated with each cade-prgenv-4.0.* update.

Administrators may add additional settings after this line.

The default link type is static.

A CPU target must be defined. The choice of processor module depends on which system the user intends to use as a runtime system for the application they build. The default network type is gemini in a 4.0.* programming environment.

Systems that are used for cross compiling for several different processor targets might set the default processor type to interlagos. Users on these systems will choose to target a processor and will explicitly load a processor module choice which will override the default.

To set the default programming environment to PrgEnv-cray, link=dynamic, SHMEM, and cpu=mc12, add the following lines to /etc/bash.bashrc.local and /etc/csh.cshrc.local:

```
module use /opt/cray/xt-asyncpe/default/modulefiles
module load PrgEnv-cray
module load craype-mc12
module load xt-shmem
setenv XTPE_LINK_TYPE dynamic
# OR: export XTPE_LINK_TYPE=dynamic
```

6.4 Using Cray Compiling Environment 8.1

After the Cray Compiling Environment 8.1 rpm files are installed and the license is activated, users can load the PrgEnv-cray module.

The Cray compilers are invoked by using the ftn or cc commands.

Because of the multiple compiling environments potentially available on Cray XE 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 8.1 compilers produce code that can be executed on 64-bit AMD Opteron processors. The valid compilation targets are barcelona, shanghai, istanbul, mc8, mc12, interlagos, interlagos-cu, abudhabi, abudhabi-cu, and sandybridge.

The targeting modules (craype-mc8, 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 eight-core (mc8) or twelve-core (mc12) systems, they must load the craype-mc8, or craype-mc12 module and use the same module at link and load time.

6.4.1 Compiling and Linking an Application which Contains Accelerator Directives

To compile an application which uses the accelerator directives, ensure that PrgEnv-cray module is loaded. Load the appropriate *target_system* module corresponding to the host processor (craype-interlagos, for example). The *target_system* modules ensure that corresponding targeted libraries will be linked.

Then, either load the craype-accel-nvidia20 module for Fermi support or the craype-accel-nvidia35 module for Kepler support.

Use either the ftn or cc command to compile.

Installing and Managing FlexNet [A]

The Cray Compiling Environment requires FlexNet license manager.

If you do not already have this software installed on your system, download these packages provided in the Cray Compiling Environment 8.1 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: You do not need new licenses for CCE or PerfTools when upgrading the FlexNet Server Software only.

Refer to section 5.3 to determine when new licenses are needed. 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:

1mdown Shut down the licensing daemons

lmgrd Invoke the licensing daemon

lmhostid Display the host ID of a system

1mremove Return a license to the license pool

1mreread Update license daemons with new license data

lmstat Report current status of the license daemon

lmver Display the FlexNet version being used

Note: These commands are actually arguments passed to lmutil. If any 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 you are using three-server redundancy, you must 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 you are using a single server, you can combine license files. To do so, edit all license files that have matching SERVER lines (the port number does not have to match) into one file, and delete the extra SERVER lines. Place all DAEMON lines after the SERVER line.

A.3 Resolving Problems

If you are having problems with your license key, check your 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 your license file, each user must have
 CRAYLMD_LICENSE_FILE set to the path and name that you are using.
- Verify that the license file has a FEATURE line for the product you are trying to use.
- Use the ps command and the lmstat utility to verify that the servers specified in your license file are running.

When you 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.