Configuring and Customizing the Cray PE on CLE 6.0 Systems
Geir Johansen
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Agenda

● Purpose
  ● Outline changes to the Cray Programming Environment in CLE 6.0
  ● Provide current information on customization of the programming environment

● Benefit/Value
  ● Talk is targeted for site administrators, and system consultants responsible for assisting their user community in building and analyzing programs.

● CLE 6.0 PE installation and configuration
● New CLE 6.0 PrgEnv modulefile features
● Topics in porting and integrating third party software with Cray PE
● Summary
● Q&A
CLE 6.0 Installation & Configuration Info @ CUG

- Cray Management System for XC Systems with SMW 8.0/CLE 6.0 -- Cray Tutorial
- eLogin Made Easy - An Introduction and Tutorial on the new Cray External Login Node – Cray tutorial
- Crossing the Rhine - Moving to CLE 6.0 System Management -- NERSC presentation
- How to Automate and not Manage under Rhine/Redwood -- LANL presentation
CLE 6.0 system installation and configuration methodology is significantly different than previous versions of CLE.

- Move away from proprietary tools to Linux tools (rpm, zypper, yum, ...)
- Processes can be shared across platforms (XC, SMW, eLogin, ...)
**CLE 6.0 PE Management**

- PE installation takes place on SMW,
- No longer installed on a shared root on boot node
- PE software installed into a **PE root image**
- System agnostic process – same PE image root can be used on different systems
- Cloning feature – easier to test new PE releases, revert back to previous PE releases
Same Cray Developer Toolkit (CDT) ISOs are used for CLE 5.2 and CLE 6.0
• craype-installer will continued to be used to install the Cray PE
• PE software installed into a *PE root image*
• For CLE 6.0: the *install-cdt.yaml* configuration file has a new variable *IMAGE_DIRECTORIES* that designates the PE root image
• Cray PE software now installed into */opt/cray/pe* directory
Once installation has completed (including PE third party software), PE image root pushed to the boot node:

\[ \text{smw# image push --dest boot <PE image root>} \]
CLE 6.0 PE Management

SMW

Compute Image (includes PE dependencies)

Clone (once Per CLE Release)

PE Image

Install (Monthly) craype-installer

PE Monthly Release

SMW Disk

Image Push

CDT ISOs

On boot node ansible-playback binds PE image root to system nodes

Mount (DVS)

Network FS / Cached

PE Image

Mount (DVS)

Network FS / Cached

PE Image

Mount (DVS)

PE Image

/computenode

/installnode

Mount (DVS)

Network FS / Cached

/computenode

/installnode

/onboodnode

Mount (DVS)

Network FS / Cached

/computenode

/installnode

/onboodnode

(pe_postmount_callback)

/opt/cray/pe

/opt/…
Installation of Third Party PE Software

- Performed on SMW by using `chroot` to access the PE root image
- PGI Compiler example:
  ```
  smw# cp pgi-16.4.0-*.rpm <PE root image>/var/tmp
  smw# chroot <PE root image> rpm -ivh /var/tmp/pgi-16.4.0-*.rpm
  ```

- Intel compiler -- not system agnostic, needs access to install system’s /dev file. Workaround:
  ```
  smw # mount --bind /dev <PE root image>/dev
  ```
CLE 6.0 Shell Initialization (rc) Files to Load Programming Environment Modulefiles

- Typically site administrators will initialize `/etc/bash.bashrc.local` and `/etc/csh.cshrc.local` to automatically load programming environment modulefiles.
- In CLE 6.0, the file `/etc/opt/cray/pe/admin-pe/site-config` is used to specify the modulefiles to be loaded when a user logs in.
- Supports bash (sh), csh, tcsh, zsh, ksh (lksh, mksh, pdksh)
- Task performed by `/opt/cray/pe/bin/setup_shell_rcs.sh`
$ cat /etc/opt/cray/pe/admin-pe/site-config
# Defines the Programming Environment modules
# that will automatically be loaded.
module add PrgEnv-cray
module add atp
module add cray-mpich
module add craype-haswell
module add perftools-base
module add forge
module add slurm
$

site-config example
CLE 6.0 PrgEnv modulefile features

- PrgEnv modulefiles (i.e. PrgEnv-crty, PrgEnv-intel, …) now released in CDT and not CLE 6.0
  - CLE 5.2 will continue to use PrgEnv modulefiles released with CLE 5.2

- SITE_MODULE_NAMES environment variable
  - User specified modulefiles to be swapped during a PrgEnv module swap

- cdt modulefiles
  - Specify modules from a specific CDT release

- Modules –S substring search
SITE_MODULE_NAMES

● Add modulefile name to the SITE_MODULE_NAMES environment variable results in the modulefile being unloaded and loaded during a module swap of PrgEnv

● Automatically done for Cray Programming Libraries that are loaded

● Insures that environment variables are set correctly for the compiler that is loaded

● craype compiler drivers also check which compiler, network target, and CPU target that is loaded for Cray Programming Environment libraries
SITE_MODULE_NAMES example

```bash
$ module load PrgEnv-cray
$ module load cray-netcdf cray-tpsl boost
$ export SITE_MODULE_NAMES=boost
$ module show PrgEnv-gnu 2>&1 | grep swap
module     swap craype/2.5.4
module     swap cray-mpich cray-mpich/7.3.3
module     swap cray-hdf5 cray-hdf5/1.8.16
module     swap cray-tpsl cray-tpsl/16.03.1
module     swap boost boost/1.59.0
$
cdt modulefiles

- Introduced in CLE 6.0
- modulefile for each Cray Developer toolkit (CDT) release
- Instructs module command to use software components from a specific CDT release
- Effectively changes the set of default modulefiles
cdt modulefile example

$ module load cdt/16.3
$ module load cray-mpich
$ module list 2>&1 | grep mpich
  22) cray-mpich/7.3.2
$ module load cdt/16.4
$ module swap cray-mpich cray-mpich
$ module list 2>&1 | grep mpich
  22) cray-mpich/7.3.3
$
Module command substring search

● Introduced in modules 3.2.10.4 (CDT 16.04)
● Available for CLE 5.2

$ module avail trilinos
$ module avail -S trilinos

---------- /opt/cray/modulefiles ----------
cray-trilinos/12.2.1.0(default)
$
Version 2.63 (available on CLE 5.2) has Cray specific fixes/ CLE 6.0 has version 2.69.

Autoconf generated configure scripts often run slowly on Cray systems
  - Many Cray systems default to static linking
  - Several large networking (i.e. ugni) and programming environment (i.e. cray-libsci) libraries are linked

The configure ‘–C’ option creates a config.cache file. Subsequent executions using the ‘–config-cache’ option will avoid many of the configure tests.

Some applications support the configure directive ‘cross_compiling=yes’, may resolve issue where build machine does not match target machine. Becoming more supported, build for ARM is a big reason for this situation.
CMake 3.5

- Developed by Kitware Inc.
- In March 2016 released CMake 3.5.0:
  "The 3.5 release introduced a new platform file to increase the compatibility of CMake with the Cray Linux Environment (CLE). This file allows CMake to cross-compile code in the CLE to target compute nodes."
- `-DCMAKE_SYSTEM_NAME=CrayLinuxEnvironment
is specified on the the CMake command line
- Enables Cmake to use appropriate build settings with the PrgEnv modulefiles loaded
Downloading and building CMake

- CMake 3.5.1 that was downloaded from cmake.org.
- CC and CXX environment variables were intentionally not set, so the build process defaults to directly calling the gcc and g++ compilers.

```bash
$ tar xzvf cmake-3.5.1.tar.gz
$ cd cmake-3.5.1
$ module load gcc  # load a current version of GCC
$ export PE_INSTALL=<Installation directory for PE tools>
$ mkdir -p $PE_INSTALL/cmake/3.5.1
$ ./configure --prefix=$PE_INSTALL/cmake/3.5.1
$ gmake install
```
Creating a CMake modulefile

$ module load craypkg-gen
$ craypkg-gen -m $PE_INSTALL/cmake/3.5.1
$ module use $PE_INSTALL/modulefiles
$ module load cmake
$ cmake --version

CMake version 3.5.1

CMake suite maintained and supported by Kitware (kitware.com/cmake).

$
Using craypkg-gen to integrate third party software with Cray Programming Environment

- **Custom Product Integration and the Cray Programming Environment** -- CUG 2015

- Creates modulefiles
  - Intel compiler
  - PGI compiler downloaded from PGI (not Cray)

- Generate pkg-config (*.pc) files
  - Allows integration with the CrayPE compiler drivers

- Create an RPM of the software
Boost C++ Library Example

- Open source C++ library
- Has a wide variety of libraries
- Available at boost.org
- Use craypkg-gen to:
  - Create pkgconfig files
  - Create modulefile
  - Create an RPM
Building Boost

$ tar xzvf boost_1_59_0.tar.gz
$ cd boost_1_59_0
$ export CC=cc
$ export CXX=CC
$ export PE_INSTALL=<PE_Installation Directory>
$ ./bootstrap.sh --prefix=$PE_INSTALL/boost/1.59.0/
CRAY --without-libraries=python cflags="-hgnu -hipa0" cxxflags="-hgnu -hipa0"
$ ./b2 toolset=cray link=static  #static
$ ./b2 toolset=cray.             #dynamic
$ ./b2 toolset=cray install
$
Creating pkgconfig_files for boost

- craypkg-gen ‘-p’ option
- Create pkgconfig/<library-name>.pc files in the software’s library directories
- Modulefile sets env. variable to point to these files
- CrayPE compiler drivers use them to set compiler options to find appropriate header files and libraries

```
$ module load craypkg-gen
$ craypkg-gen -p $PE_INSTALL/boost/1.59.0/CRAY
```
Creating boost modulefile

- craypkg-gen ‘-m’ option
- Initializes environment variables such as $PATH and $MANPATH
- Sets env. variables to point to the pkgconfig files
- Creates a set_default script
  - Used to make modulefile the default version

$ module load craypkg-gen
$ craypkg-gen -m $PE_INSTALL/boost/1.59.0
Building a boost RPM

- craypkg-gen ‘-r’ option
- RPM package can be installed on other systems
- Can be used to transfer software from a user’s local directory to a system directory
- ‘-prefix’ option used to specify destination directory

```
$ module load craypkg-gen
$ craypkg-gen -r $PE_INSTALL/boost/1.59.0
    --prefix=/opt/local
$ 
```
### boost modulefile and craype integration

```bash
$ module load PrgEnv-cray
$ module swap craype-network-aries craype-network-none
$ module unload cray-mpich cray-libsci
$ module use $PE_INSTALL/modulefiles
$ module load boost
$ cat main.c
int main() { }
$ cc -c -craype-verbose main.c
driver.cc -hcpu=ivybridge -hstatic -D__CRAY_IVYBRIDGE -D__CRAYXT_COMPUTE_LINUX_TARGET
-hnetwork=none -c main.c -Wl,--rpath=/opt/cray/cce/8.5.0/craylibs/x86-64
-hlast_user_arg -nostdinc -ibase=compiler /opt/cray/cce/8.5.0/CC/x86-64/
compiler_include_base -isystem /opt/cray/cce/8.5.0/craylibs/x86-64/include
-I/opt/gcc/4.8.1/snos/lib/gcc/x86_64-suse-linux/4.8.1/include
-I/opt/gcc/4.8.1/snos/lib/gcc/x86_64-suse-linux/4.8.1/include-fixed -isystem /usr/include
-ugcc_base=/opt/gcc/4.8.1/snos -uno_driver_libs
-$$PE_INSTALL/boost/1.59.0/CRAY/include -I/opt/cray/rca/1.0.0-2.0502.60530.1.62.ari/include
-I/opt/cray/cce/8.5.0/craylibs/x86-64/pkgconfig/../include -I/opt/cray/krca/1.0.0-2.0502.63139.4.31.ari/include
-I/opt/cray-hss-devel/7.2.0/include
$
```
Assuming that a GCC version of Boost 1.59.0 was also built and installed into $PE_INSTALL/boost/1.59.0/GNU, then a module swap to PrgEnv-gnu will result in the CC compiler driver automatically using the GCC version of the Boost library:

```bash
$ module swap PrgEnv-cray PrgEnv-gnu 2>/dev/error
$ module unload cray-libsci
$ cc -c -craype-verbose main.c
gcc -march=corei7-avx -static -D__CRAY_IVYBRIDGE -D__CRAYXT_COMPUTE_LINUX_TARGET -upthread_mutex_destroy -D__TARGET_LINUX__ -c main.c
-I$PE_INSTALL/boost/1.59.0/GNU/include
$  
```
 mpi4py example

● Allow python programs to use MPI library
● Can be downloaded from pypi.python.org
● Build instructions provided in the CUG paper
● To create mpi4py modulefile:

```
# craypkg-gen -m $PE_INSTALL/mpi4py/2.0.0
```

● Add following line to the mpi4py modulefile:

```python
prepend-path PYTHONPATH $PREFIX/lib64/python2.7/site-packages
```
mpi4py example

```python
$ cat test.py
from mpi4py import MPI
import os
import glob
COMM = MPI.COMM_WORLD
irank = COMM.Get_rank()
print 'Hello world from rank', irank
$ module use $PE_INSTALL/modulefiles
$ module load mpi4py
$ aprun -n 8 python test.py
Hello world from rank 2
Hello world from rank 4
Hello world from rank 5
Hello world from rank 6
Hello world from rank 7
Hello world from rank 3
Hello world from rank 0
Hello world from rank 1
Application 8209638 resources: utime ~0s, stime ~0s, Rss ~9892, inblocks ~4282, outblocks ~12
$
Future Opportunities

● **Craype-installer**
  ● Ability to remove older PE releases
  ● Finer granularity on selecting products to install or uninstall

● **PrgEnv modulefiles**
  ● Snapshot/Restore feature – ability to create user customized PrgEnv modulefiles

● **Address Autoconf Issues**
  ● Faster linker (gold, LLVM lld)
  ● Automatically detect configure scenario
Summary

- CLE 6.0 changes to Cray Programming Environment
  - Overview of installation
  - CLE 6.0 shell initialization files
- Enhancements to CLE 6.0 PrgEnv modulefiles
  - SITE_MODULE_NAMES
  - cdt modulefile
- Recent Topics in porting and integrating third party software with Cray PE
  - Issues with porting and GNU Autoconf
  - Cmake 3.5 compatibility with CLE
  - craypkg-gen examples
Q&A
Suggestions!
Feedback!

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