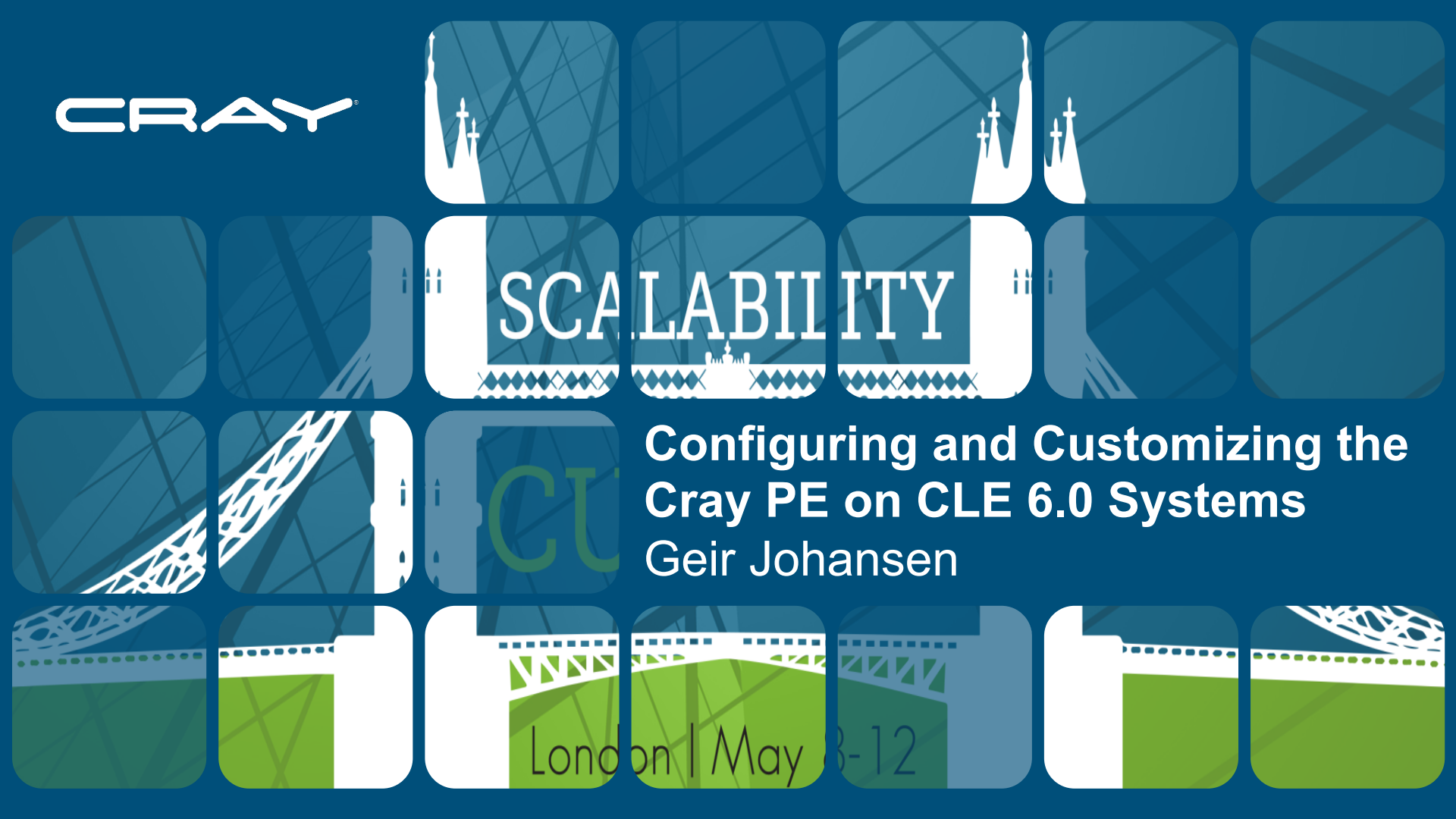
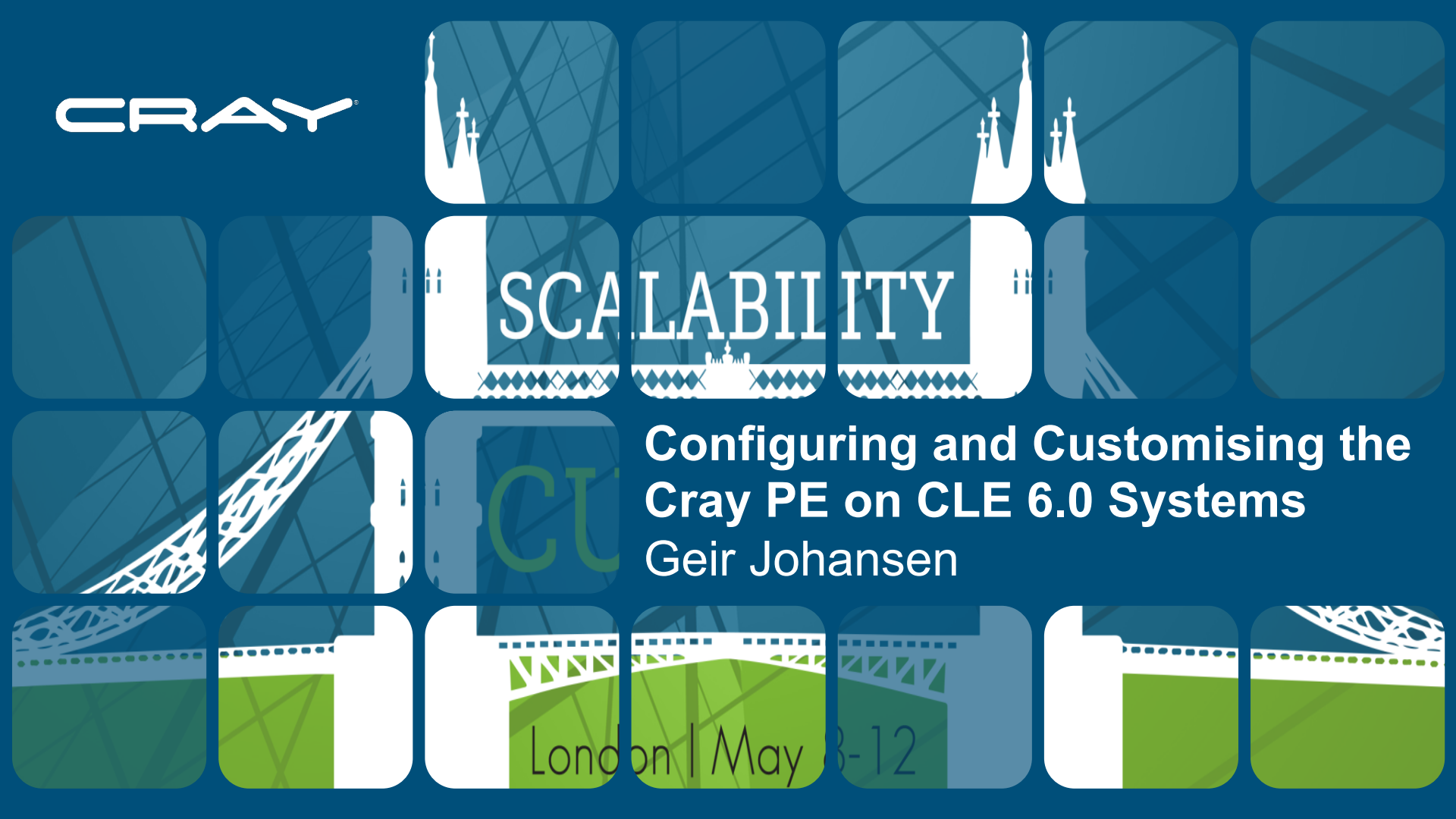


Configuring and Customizing the Cray PE on CLE 6.0 Systems

Geir Johansen



Configuring and Customising the Cray PE on CLE 6.0 Systems

Geir Johansen

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**

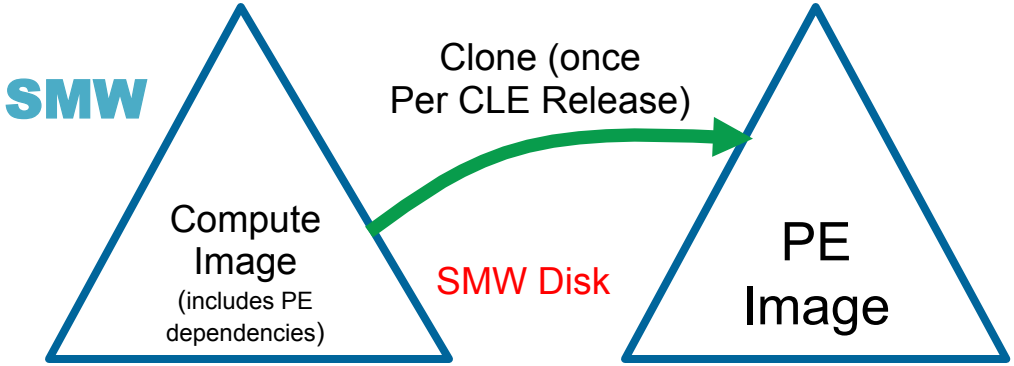
CLE 6.0 Installation & Configuration Info @ CUG

- *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

CLE6.0/SMW 8.0 Cray Management System

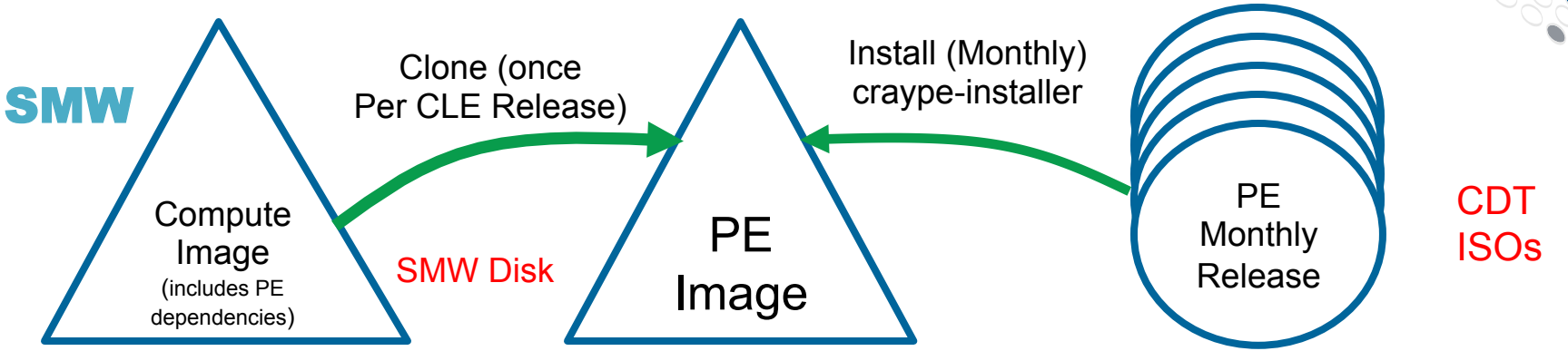
- CLE 6.0 system installation and configuration methodology is significantly different than previous versions of CLE.
- Move away from proprietary tools to Linux tools (rpm, zypper, yum, …)
- Processes can be shared across platforms (XC, SMW, eLogin, …)

CLE 6.0 PE Management



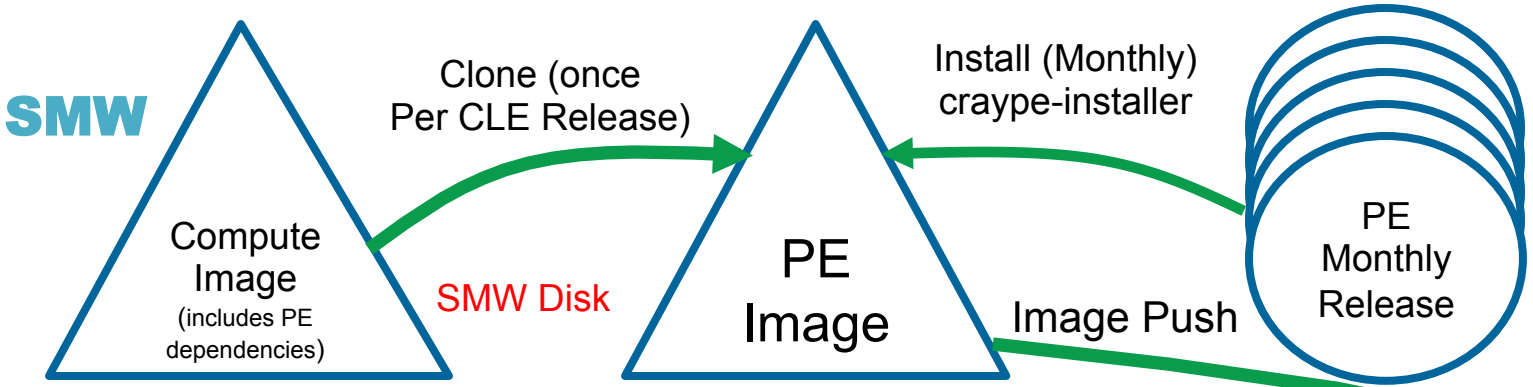
- PE installation takes place on SMW,
- No longer installed on a shared root on boot node
- PE software installed into a *PE root image*
- System agnostic process – same PE image root can be used on different systems
- Cloning feature – easier to test new PE releases, revert back to previous PE releases

CLE 6.0 PE Management



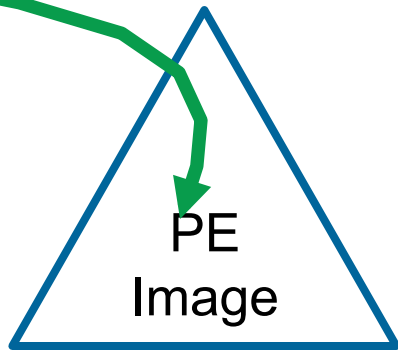
- Same Cray Developer Toolkit (CDT) ISOs are used for CLE 5.2 and CLE 6.0
- `craype-installer` will continued to be used to install the Cray PE
- PE software installed into a *PE root image*
- For CLE 6.0: the `install-cdt.yaml` configuration file has a new variable IMAGE_DIRECTORIES that designates the PE root image
- Cray PE software now installed into `/opt/cray/pe` directory

CLE 6.0 PE Management



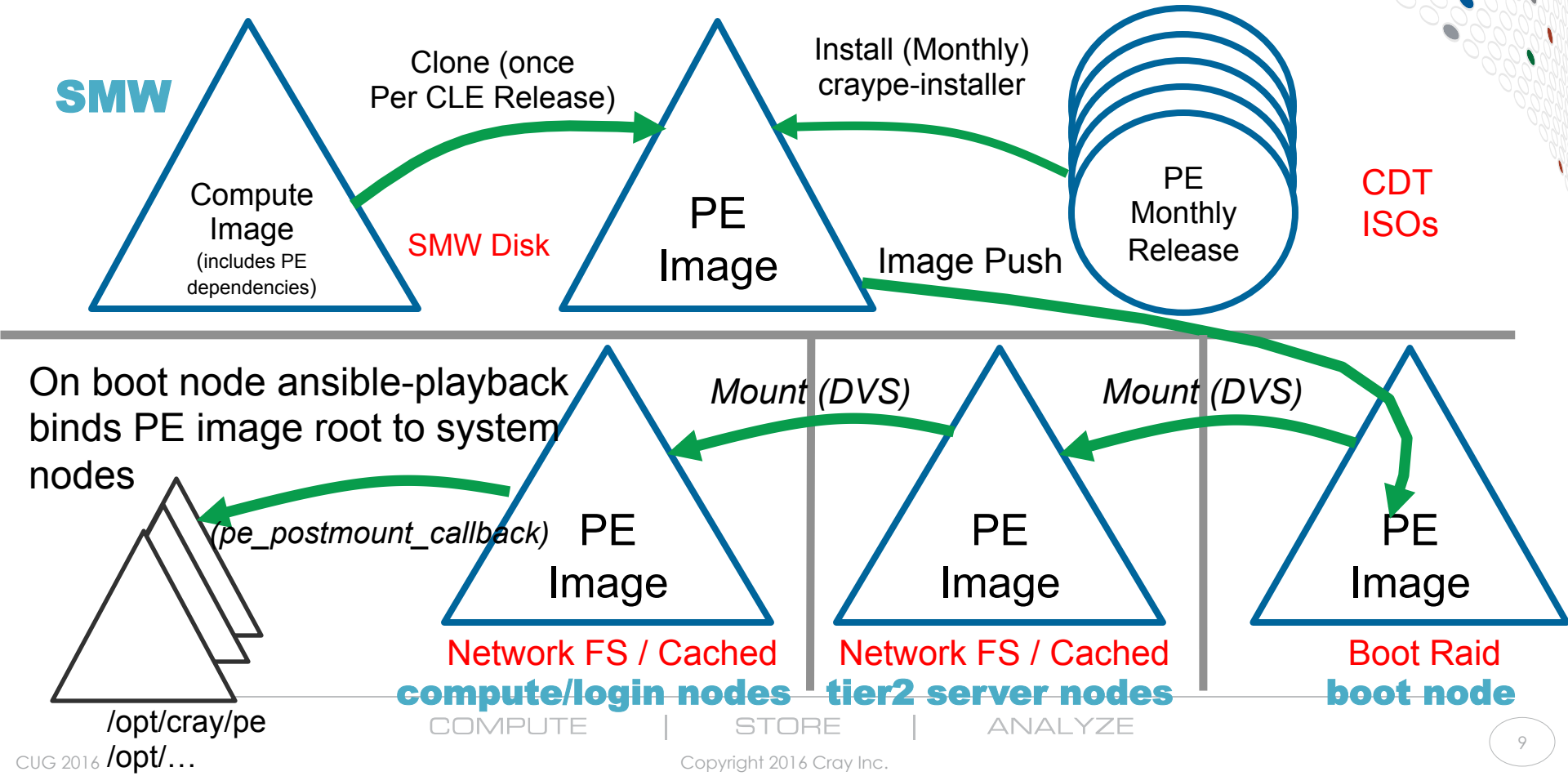
- Once installation has completed (including PE third party software), PE image root pushed to the boot node:

```
smw# image push –dest boot <PE image root>
```



Boot Raid
boot node

CLE 6.0 PE Management



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 moduefiles.
- 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`

site-config example

```
$ 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
$
```

CLE 6.0 PrgEnv modulefile features

- **PrgEnv modulefiles (i.e PrgEnv-cray, PrgEnv-intel, …) now released in CDT and not CLE 6.0**
  - CLE 5.2 wil continue used 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

```
$ 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)
$
```

GNU Autoconf -- configure

- 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 situtation.

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.

```
$ 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 -h
ipa0" 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

```
$ 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
-I$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
$
```

boost modulefile and craype integration

- **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:**

```
$ 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:

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

mpi4py example


```
$ 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 Programing 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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