Design, Implementation, and Experiences of Third-Party Software Administration at the ORNL NCCS

Nick Jones
Mark Fahey

National Center for Computational Sciences
Oak Ridge National Laboratory

May 7, 2008

The Problem

- **No standardized workflow for software installations**

- **Software updates are labor intensive**

- **Hard to maintain up to date documentation**

- **Manual software inventories**

- **Very little reporting data is available in real time**

CUG 2008 Crossing the Boundaries

Design Goals

- **Automated building, testing, and linking**

- **Inventory of currently installed software**

- **Ability to do batch operations**
  - **i.e. Rebuild current version of all applications compiled with PGI**

- **Easily maintainable**

- **Automate generation of many user documents such as the NCCS.gov software status page**

CUG 2008 Crossing the Boundaries

How we did it

- **Directory Hierarchy**

- **Scripts to rebuild, relink, and retest each application**

- **Installer documents and automates their work**

- **Scripts to automate builds, tests, reports**

- **Enforce the rules**

CUG 2008 Crossing the Boundaries

Directory Structure

- **<root>/<machine>/<app>/<ver>/<build>**

  - **root := /sw**

- **The machine folder may or may not be machine specific**

  - **Our XT4 systems all use the `xt` tree**

- **The structure is not used by end users**

  - **For that we use GNU Modules**

CUG 2008 Crossing the Boundaries
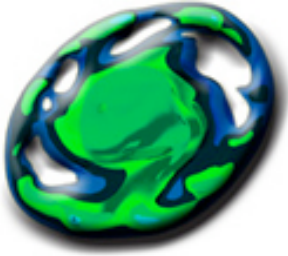
swtools

- **Scripts**
  - `swaddpackage, swaddbuild`
  - `swbuild, swlink, swtest`
  - `swdriver, swreport, swlog`

- **Based around textfiles that are written by the application installer**
  - **Application level:** `description, versions`
  - **Build level:** `rebuild, relink, retest, dependencies,` **and** `status`

CUG 2008 Crossing the Boundaries

Batch Operations

- **These scripts allow us to do advanced batch operations**

```
nai@jaguar1:~> swbuild -a szip -v 2.1 -b sles*

-------------------------------------build-------------------------------------

/sw/xt/szip/2.1/sles9.2_pgi7.0.7/rebuild        : passed (0)

/sw/xt/szip/2.1/sles9.2_pgi6.2.5/rebuild        : passed (0)

/sw/xt/szip/2.1/sles9.2_pathscale3.0/rebuild    : passed (0)

/sw/xt/szip/2.1/sles9.2_gnu4.2.1/rebuild        : passed (0)

nai@jaguar1:~> swtest -a szip -v 2.1 -b sles*

-------------------------------------test-------------------------------------

/sw/xt/szip/2.1/sles9.2_pgi7.0.7/retest         : passed (0)

/sw/xt/szip/2.1/sles9.2_pgi6.2.5/retest         : passed (0)

/sw/xt/szip/2.1/sles9.2_pathscale3.0/retest     : passed (0)

/sw/xt/szip/2.1/sles9.2_gnu4.2.1/retest         : passed (0)
```

CUG 2008 Crossing the Boundaries

What if…?

nai@jaguar1:~> **swdriver build test report-conform -a all –v current -b sles***

```
---------------------------------------build-------------------------------------------
/sw/ewok/szip/2.0/rhel4.5+pgi7.0.3/rebuild          : passed (0)
/sw/ewok/szip/2.0/rhel4.5+pgi6.2.5/rebuild          : passed (0)
/sw/ewok/szip/2.0/rhel4.5+pathscale3.0/rebuild      : passed (0)
…….
---------------------------------------test--------------------------------------------
/sw/ewok/szip/2.0/rhel4.5+pgi7.0.3/retest           : passed (0)
/sw/ewok/szip/2.0/rhel4.5+pgi6.2.5/retest           : passed (0)
/sw/ewok/szip/2.0/rhel4.5+pathscale3.0/retest       : passed (0)
…….
---------------------------------report-conform--------------------------------
/ewok
  /szip
    /2.0
       /rhel4.5+pgi7.0.3
       /rhel4.5+pgi6.2.5
       /rhel4.5+pathscale3.0
```

CUG 2008 Crossing the
Boundaries

Reporting Data

- **Automated generation of inventory pages for www.NCCS.gov**

- **Alphabetical view**

- **Category view**

- **Lists status of installed builds**

- **Lists the level of support we provide**

CUG 2008 Crossing the Boundaries

Applications

Click here for the Category View

	XT	BGP	ANALYSIS-X86
ARPACK	X		
ATLAS	X		
AZTEC	X		
BLACS	X		
BLAS	X		
CMAKE	X		
CRAYPAT	X		
DOXYGEN	X		
FERRET	X		
FFTPACK	X		
FFTW	X	X	
FPMPI	X		
GAMESS	X		
GCC	X	X	X
GLOBALARRAYS	X		
GNUPLOT	X	X	X
GRACE	X		
HDF5	X	X	X
HYPRE	X		
IDL	X		X
IMAGEMAGICK	X		X
JAVA-JDK	X		

Alphabetical View

CUG 2008 Crossing the Boundaries

OAK RIDGE
National Laboratory

Category View

Program Dev

	XT	BGP	ANALYSIS-X86
COMPILERS			
GCC	X	X	X
PATHSCALE	X		X
PGI	X		X
XLC		X	
XLF		X	
LANGUAGES			
JAVA-JDK	X		
JAVA-JRE	X	X	X
NUMERICPYTHON	X		
PYTHON	X	X	X
TOOLS			
CMAKE	X		
DOXYGEN	X		
QT	X		
SUBVERSION	X	X	X
VIM	X	X	

Program Development

	XT	BGP	ANALYSIS-X86
MVAPICH2			X
OMPI	X		X

Science Apps

CUG 2008 Crossing the Boundaries

OAK RIDGE National Laboratory

Application Pages

HDF5

Category: Libraries-IO

Description

The Hierarchical Data Format (HDF) project involves the development and support of software and file formats for scientific data management. The HDF software includes I/O libraries and tools for analyzing, visualizing, and converting scientific data.

There are two HDF formats, HDF (4.x and previous releases) and HDF5. These formats are completely different and NOT compatible, but conversion software is available for converting HDF4 data to HDF5, and vice versa.

For more information see the HDF home page.

Use

HDF5 is available on jaguar as a module. See the modules page for more information on modules. There are parallel and serial versions of HDF5. The parallel module is suffixed with "_par". Any binaries provided in the parallel module must be run with aprun, however any binaries in provided in the serial module are run without aprun.

Once a HDF module has been loaded the following examples can be used to compile and link your program (hdf5example.f90) to the HDF libraries.

For parallel HDF5:

```
FORTRAN
  ftn hyperslab.f90 ${HDF5_FLIB}
      OR
  h5pfc hyperslab.f90
```

The environment variables given above are set in the module file - they are locally defined.

```
C
  cc -o hdf5example.x hdf5example.c ${HDF5_CLIB}
      OR
```

Application Pages

CUG 2008 Crossing the Boundaries

```
h5pcc -o hdf5example.x hdf5example.c

Note the difference between HDF5_FLIB and HDF5_CLIB for Fortran and C, respectively.
```

Support

This package has the following support level : Supported

Available Versions

VERSION	AVAILABLE BUILDS			
	PGI	PATHSCALE	GNU	OTHER
1.6.5	pgi6.2.5 v pgi6.2.5_par u pgi7.0.7 v pgi7.0.7_par v	pathscale3.0 v pathscale3.0_par v	gnu4.2.1_par v gnu4.2.1 v	
1.6.6	pgi7.0.7_par v pgi7.0.7 v	pathscale3.0 u pathscale3.0_par u	gnu4.2.1_par v gnu4.2.1 v	
1.6.7	pgi7.0.7 v pgi7.0.7_par v	pathscale3.0 u pathscale3.0_par u	gnu4.2.1_par v gnu4.2.1 v	
1.8.0	pgi7.0.7_i8 v			

Experiences to Date

- **Began development in January**

- **Written completely in Python, with a few shell scripts**

- **Unveiled to other NCCS staff in March**

- **17 Staff reinstalled 60 applications in three weeks**

- **Staff have been using it for 2 months**

CUG 2008 Crossing the Boundaries

Challenges

- **Permissions**

- **Sensitive applications**

- **Binary applications**

- **Compiler naming schemes**

- **Vendor provided applications**

- **Web Integration (Wordpress/Drupal)**

CUG 2008 Crossing the
Boundaries

Problems with the `man`

- **SLES `man` does not support having "+" symbols in the `$MANPATH`**

- **Decided to migrate all installed builds to use "_" as the delimiter**

  - `cnl2.0+pgi7.1.5` **became** `cnl2.0_pgi7.1.5`

  - **Began work on a Friday afternoon**

  - **Recompiled and retested approximately 120 builds by Saturday night, including parallel builds**

CUG 2008 Crossing the Boundaries

OAK RIDGE
National Laboratory

Moving Forward

- **Others systems to migrate onto: Smoky, Lens, Everest, BGP**

- **Resolve Application Dependencies**

- **Preparation for Baker/petaflop system**

- **Integrate into new Web Content management system**

- **Used to test existing XT4 builds on upgraded quad core XT4**

  - **Batch operation and we know what to expect now**

  - **But really need to recompile apps with barcelona-64 option and mpt3**

CUG 2008 Crossing the Boundaries

Conclusions

- **Overall a great success**

- **Positively impacting day-to-day business**

- **Lots of complexity**

- **Exceptions to every rule**

CUG 2008 Crossing the Boundaries

Questions?

faheymr@ornl.gov

CUG 2008 Crossing the Boundaries