Using Spack to Manage Software on Cray Supercomputers

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May 9th, 2017
State of Software in HPC

- Scientific software large and complex (multiple dependencies)
- HPC teams support different versions of software
- Same packages installed but built with different compilers/libraries/etc
Tools for HPC Software

- **Package managers for HPC**
  - Smithy (ORNL)
  - SWTools (ORNL)
  - EasyBuild (UGhent)
  - Maali (Pawsey)
  - Spack (LLNL)
The Supercomputing PACKage Manager
• Spack included many features of interest to us at NERSC
  – Easy to install and use
  – Packages are flexible
    • Build a range of versions for each package.
    • LLNL our close neighbors!
    • Todd Gamblin and Greg Becker (lead developers)
• Lacked compatibility with our Cray systems
  – Work needed to adapt Spack to Cray systems
  – Originally used on LLNL Linux clusters
Package template files

- Allow different options to be chosen
- Can pick and choose dependencies, variants, compilers.
- Automatic patching
- Control over combinatorial space of a package.
- Wrapper for common file and build functions
  - configure(), make()
- Can modify build environment for package and it’s dependents.
from spack import *

class Libelf(AutotoolsPackage):
    """libelf lets you read, modify or create ELF object files in an architecture-independent way. The library takes care of size and endian issues, e.g. you can process a file for SPARC processors on an Intel-based system.""

    homepage = "http://www.mr511.de/software/english.html"
    url = "http://www.mr511.de/software"

    version('0.8.13', '4136d7b4c04df68b686570afa26988ac')
    version('0.8.12', 'e21f8273d9f5f6d43a59878dc274fec7')

    provides('elf')

    def configure_args(self):
        args = ['--enable-shared',
                '--disable-dependency-tracking',
                '--disable-debug']
        return args

    def install(self, spec, prefix):
        make('install', parallel=False)
## Spack Spec Syntax

<table>
<thead>
<tr>
<th>Spec Type</th>
<th>Spec Symbol</th>
<th>CLI Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>package</td>
<td>package-name</td>
<td>python</td>
</tr>
<tr>
<td>version</td>
<td>@</td>
<td>python@2.7.13</td>
</tr>
<tr>
<td>compiler</td>
<td>%</td>
<td>python@2.7.13%gcc</td>
</tr>
<tr>
<td>architecture</td>
<td>arch=</td>
<td>python@2.7.13%gcc arch=cray-CNL-haswell</td>
</tr>
<tr>
<td>variant</td>
<td>+/-</td>
<td>python@2.7.13%gcc arch=cray-CNL-haswell</td>
</tr>
<tr>
<td>compiler flags</td>
<td>ldflags=, cflags=, cxxflags=, cppflags=</td>
<td>python@2.7.13%gcc arch=cray-CNL-haswell cflags=-02</td>
</tr>
</tbody>
</table>

Each parameter constrains the spec
Full control over the combinatorial space of a package.
$ spack spec blast-plus

• Spec represents a directed acyclic graph
• Concretization algorithm
  • Fixed-point

Blast-plus@2.6.0%gcc@4.9.3+bzip2+freetype+gnutls+jpeg+lzo+openssl+pcre/perl+png+python-static+zlib arch=cray-CNL-ivybridge
  ^bzip2@1.0.6%gcc@4.9.3+shared arch=cray-CNL-ivybridge
  ^freetype@2.7.1%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^libpng@1.6.29%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^zlib@1.2.11%gcc@4.9.3+pic+shared arch=cray-CNL-ivybridge
^pkg-config@0.29.2%gcc@4.9.3+internal_glib arch=cray-CNL-ivybridge
  ^gnutls@3.5.10%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^nettle@3.2%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^gmp@6.1.2%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^m4@1.4.18%gcc@4.9.3+sigsegv arch=cray-CNL-ivybridge
  ^libsigsegv@2.11%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^jpeg@9b%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^lzo@2.09%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^openssl@1.0.2k%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^pcre@8.40%gcc@4.9.3+utf arch=cray-CNL-ivybridge
  ^perl@5.24.1%gcc@4.9.3+cp pam arch=cray-CNL-ivybridge
  ^gdbm@1.13%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^python@2.7.13%gcc@4.9.3-tk-ucs4 arch=cray-CNL-ivybridge
  ^ncurses@6.0%gcc@4.9.3-sym links arch=cray-CNL-ivybridge
  ^readline@7.0%gcc@4.9.3 arch=cray-CNL-ivybridge
  ^sqlite@3.18.0%gcc@4.9.3 arch=cray-CNL-ivybridge
Installing Packages w/ Spack

- Easy as `spack install mpileaks`
- Spack compiler wrappers handle lib, include and RPATHs, and compiler flags.
- Each package has unique DAG-hash for provenance
  - Directory tree generated for you
- Generates modulefiles in a post-hook after install method completed.
  - Supports Lmod, Dotkit, TCL
Spack Configuration

- Spack allows flexibility and customization
- Configuration files
  - packages.yaml
  - modules.yaml
  - compilers.yaml
  - config.yaml
Spack Community

• When presented at SC ’15 Spack supported only 300 packages. Now over 1,400 packages are supported.
• Spack is in US Exascale Computing Project.
• Over 75% of packages are contributed externally.
Cray Programming Environment
Cray Programming Environment

• NERSC houses two Cray-XCs (Edison and Cori)
• Cori named top 5 most powerful supercomputer
  – as of November 2016

• Cori Architecture
  – Intel Xeon (Haswell) and Intel Xeon Phi (Knight’s Landing)
  – Burst Buffer
  – 250 Unique packages maintained on these systems
TCL Modules Environment

- Dynamically modify the user’s environment
- Vital for compiling codes
  - Swap in and out of Programming Environments
  - Load necessary Cray optimized libraries.
  - Load target processors for cross-compiling.
NERSC default modules

Default Modules Found on Cori
1) modules/3.2.10.5
2) nsg/1.2.0
3) intel/17.0.2.174
4) craype-network-aries
5) craype/2.5.7
6) cray-libsci/16.09.1
7) udreg/2.3.2-7.54
8) ugni/6.0.15-2.2
9) pmi/5.0.10-1.0000
10) dmapp/7.1.1-39.37
11) gni-headers/5.0.11-2.2
12) xpmem/2.1.1_gf9c9084-2.38
13) job/2.1.1_gclad964-2.175
14) dvs2.7_2.1.6
15) alps/6.3.4-2.21
16) rca/2.1.6_g2c60fbf-2.265
17) atp/2.0.3
18) PrgEnv-intel/6.0.3
19) craype-haswell
20) cray-shmem/7.4.4
21) cray-mpich/7.4.4
• Three types of PrgEnv modules
  – PrgEnv-intel
  – PrgEnv-gnu
  – PrgEnv-cray

• Load corresponding compiler: Intel, GCC, CCE

• Compiler module controls compiler version.
Target Modules

• Cray machines are heterogeneous structures
  – Front-end (login node) and back-end (compute nodes) vary in processor and operating system.

• Front-end (login nodes)
  – Basic tasks (I/O, filesystem tasks, loading data, compiling)

• Back-end (compute nodes)
  – High performance tasks
  – What your software should be optimized against
  – Special target flags in cray compilers placed based on loaded target.

• Target modules exist so you can cross-compile without submitting a job.
Cray and Third-Party Software

• Cray provides optimized software libraries
  – MPI (cray-mpich)
  – I/O Libraries (cray-netcdf, cray-hdf5)
  – Math libraries (cray-petsc, cray-trilinos)
  – Numerical routines (BLAS/LAPACK/SCALAPACK)
    • Cray-libsci, Intel-MKL

• Monthly upgrades

• Libraries necessary for compiled software.
Cray Compiler Wrappers

• Long complex line of –L and –l flags.
• Contain optimization flags for architecture and target processor.
• Recommended to compile code for compute nodes.
• Requires compiling with Cray provided executables
  – cc, CC, ftn
Spack on Cray

NERSC
Spack on Cray

- NERSC and LLNL collaboration to port Spack onto Cray.
  - Module support
  - Architecture Spec
  - Compiler Detection/Wrapper Handling
  - Use of Cray packages
  - MPI support
  - Static and Dynamic Linking
• Prior to v0.10 Spack could load own modules but not system modules.

• Python wrapper for modulecmd
  – Takes as argument as shell name i.e Python, Ruby, Bash
  – Output can be parsed by that shell

• Can load and unload modules
  – PrgEnv-gnu/intel/cce
  – Target modules.
- Previous versions of arch spec were just strings
- Spack uniquely provides support for compiling against different architectures.
- Auto-detected
- Cori defaults:
  - arch=cray-CNL-haswell
- Genepool defaults:
  - arch=linux-debian6-x86_64
Improved Compiler Detection and Wrapper Handling

- Detection previously made through $PATH.
- modulecmd python avail (gcc/intel/cce)
- Point wrappers to cc, CC, ftn rather than direct compiler path.
- Add operating system/target to compiler metadata.
Spacc Compiler Wrappers

Package Process

do_install()

install dep1  install dep2  install root package

Fork

cc  CC  ftn

Build

Setup environment

CC=spack/env/cray/cc  SPACK_CC=cc
CXX=spack/env/cray/CC  SPACK_CXX=cc
F77=spack/env/cray/ftn  SPACK_F77=ftn
FC=spack/env/cray/ftn  SPACK_FC=ftn
PKG_CONFIG_PATH= ...  PATH=spack/env:$PATH

install()

Spacc Compiler Wrappers

(spack/env/cray/cc, spack/env/cray/CC, spack/env/ftn)

-1/dep1-prefix/include
-L/dep1-prefix/lib
-Wl, rpath=/dep1-prefix/lib
-craype-verbose (cray compiler wrappers)

./configure  make  make install
Support for Cray Packages

- Existing logic already present in packages.yaml
- Declare packages as modules
  - Spack can load the required module
  - Deduce path from modules
packages.yaml

```yaml
packages:
  mpich:
    buildable: false
    modules:
      - mpich@7.3.2%intel@17.0.0.098: cray-mpich/7.3.2
      - mpich@7.4.1%cce@8.4.4: cray-mpich/7.4.1
      - mpich@7.4.1%gcc@6.1.0: cray-mpich/7.4.1
  python:
    buildable: false
    paths:
      - python@2.7.12%gcc@6.1.0: /global/common/software/python
      - python@2.7.12%intel@17.0.0.098: /global/common/software/python
      - python@2.7.12%cce@8.4.4: /global/common/software/python
```

Message Passing Interface

• **Cray provides Module Passing Toolkit (MPT)**
  – cray-mpich, cray-shmem

• **MPI Compiler: cc, CC, ftn.**

• **User chooses how to compile**
  – Register MPI cray-mpich in packages.yaml.
  – Use Spack built MPI

• **Package writing for MPI is made simple**
  – env[‘CC’] = spec[‘mpi’].mpicc
  – env[‘CXX’] = spec[‘mpi’].mpicxx
Static and Dynamic Linking

• Default static linking
  – Causes problems with most build system assumptions.

• $\text{CRAYPE\_LINK\_TYPE}=\text{dynamic}$
  – Cray builds work like Linux builds
  – Spack doesn’t preclude static linking
    • Static flags added by build system.
Spack at NERSC and ORNL
NERSC Usage

• Pseudo-user SWOWNER
  – Login as pseudo-user and install packages
  – Special read and write

• NERSC own github repo
  – Forked from LLNL branch
  – Change our fork and merge changes into main repo

• Can use SWOWNER Spack or your own

• Future plans to offer Spack as module to users
• Mainly used at OLCF and NCRC
• Number of packages installed with Spack
  – 7/193 Titan (Cray XK7)
  – 5/73 Eos
• On non-Cray 48/59 packages installed w/ Spack.
• Single Spack instance used per host.
• Future use to allow users to use Spack with limited permissions.
Results at NERSC

• Setting up Spack can be burdensome  
  – Hard to make configurations for all platforms

• Platform specific compilers needed  
  – Most sites support multiple platforms

• Modulefiles needs better customization  
  – No logic to switch between programming environments

• Installation directory tree needs customization  
  – Most sites have canonical path for installs

• Minimal stack on Edison/Cori  
  – Not ready for production. Yet!

• ORNL wants to move to production as well!
Results at ORNL

• Spack mostly used on non-Cray systems
• Move towards Spack on Cray is slow.
• Lower number of packages present on Titan and Eos.
Related Package Managers

• **EasyBuild** – Ghent University (Used at most CUG sites)
  – Easyconfigs, easyblocks

• **Maali** – Pawsey Supercomputing
  – Collection of bash scripts

• **Smithy** – ORNL
  – Port based package manager specifically for Crays
## Comparison

<table>
<thead>
<tr>
<th></th>
<th>EasyBuild</th>
<th>Spack</th>
<th>Maali</th>
<th>Smithy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Installs dependencies</td>
<td>Y</td>
<td>Y</td>
<td>N</td>
<td>N</td>
</tr>
<tr>
<td>Combinatorial Stack</td>
<td>Y</td>
<td>Y</td>
<td>N</td>
<td>N</td>
</tr>
<tr>
<td>Programming Language</td>
<td>Python</td>
<td>Python</td>
<td>Bash</td>
<td>Ruby</td>
</tr>
<tr>
<td>Generates modulefiles</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Manipulates Cray modules</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Dependency Resolution</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>N</td>
</tr>
<tr>
<td>Version</td>
<td>v3.2.0 (stable)</td>
<td>V0.10 (alpha)</td>
<td>release_1.x</td>
<td>v1.6.5</td>
</tr>
</tbody>
</table>
Conclusions
Conclusions

• Spack is alpha software
• Future work still needed on Spack to accommodate our needs
  – Default system package configuration
  – Modulefile logic for swapping PrgEnvs
  – Custom install naming scheme (PR submitted!)
  – Getting static builds is hard!
• Package builds are unstable
  – NERSC plans on nightly tests on Cray
• Spack support for containers in Shifter.
  – Use Spack as a package manager in images
• Adopting a new tool is a slow process!