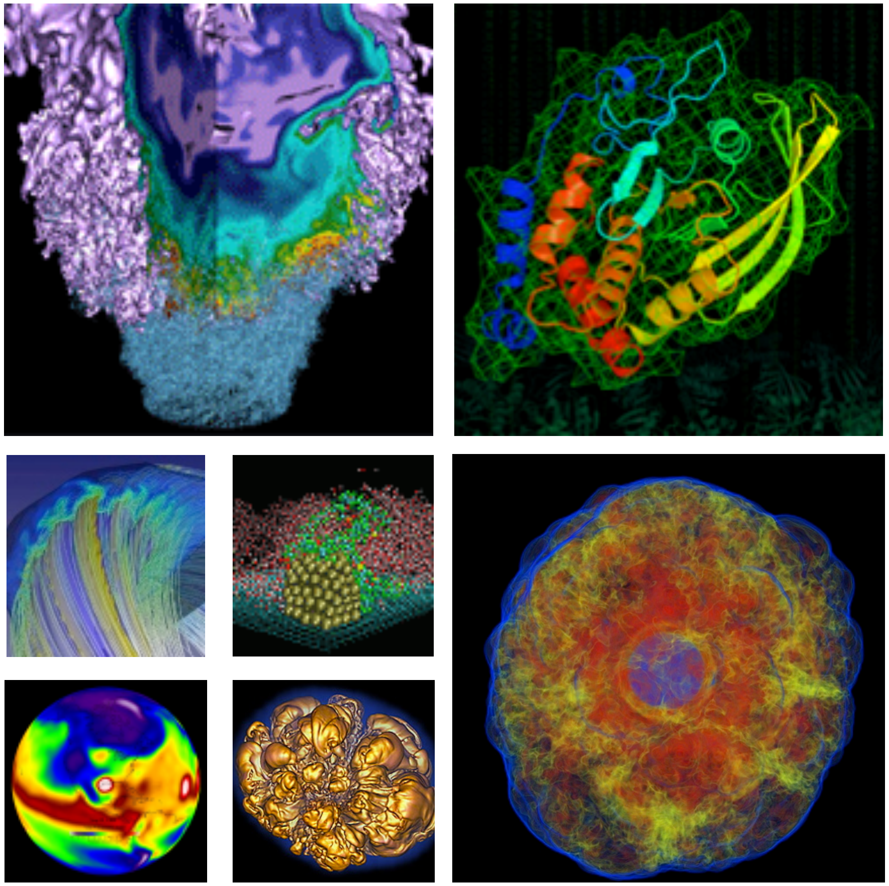
Using Spack to Manage Software on Cray Supercomputers



May 9th, 2017

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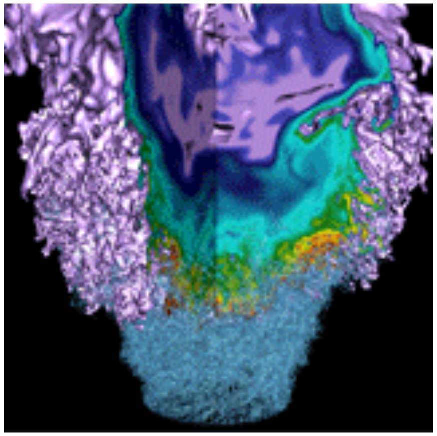
State of Software in HPC

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

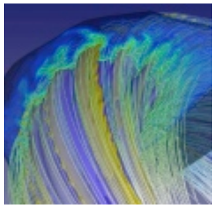
Tools for HPC Software

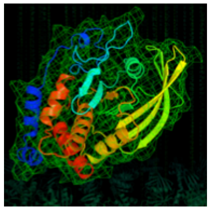
- **Package managers for HPC**
  - Smithy (ORNL)
  - SWTools (ORNL)
  - EasyBuild (UGhent)
  - Maali (Pawsey)
  - Spack (LLNL)

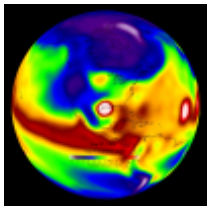
The Supercomputing PACKage Manager

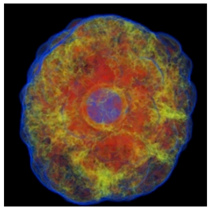


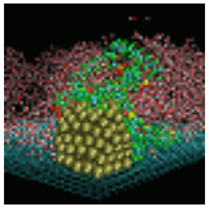
NERSC











SuperComputing PACKage Manager

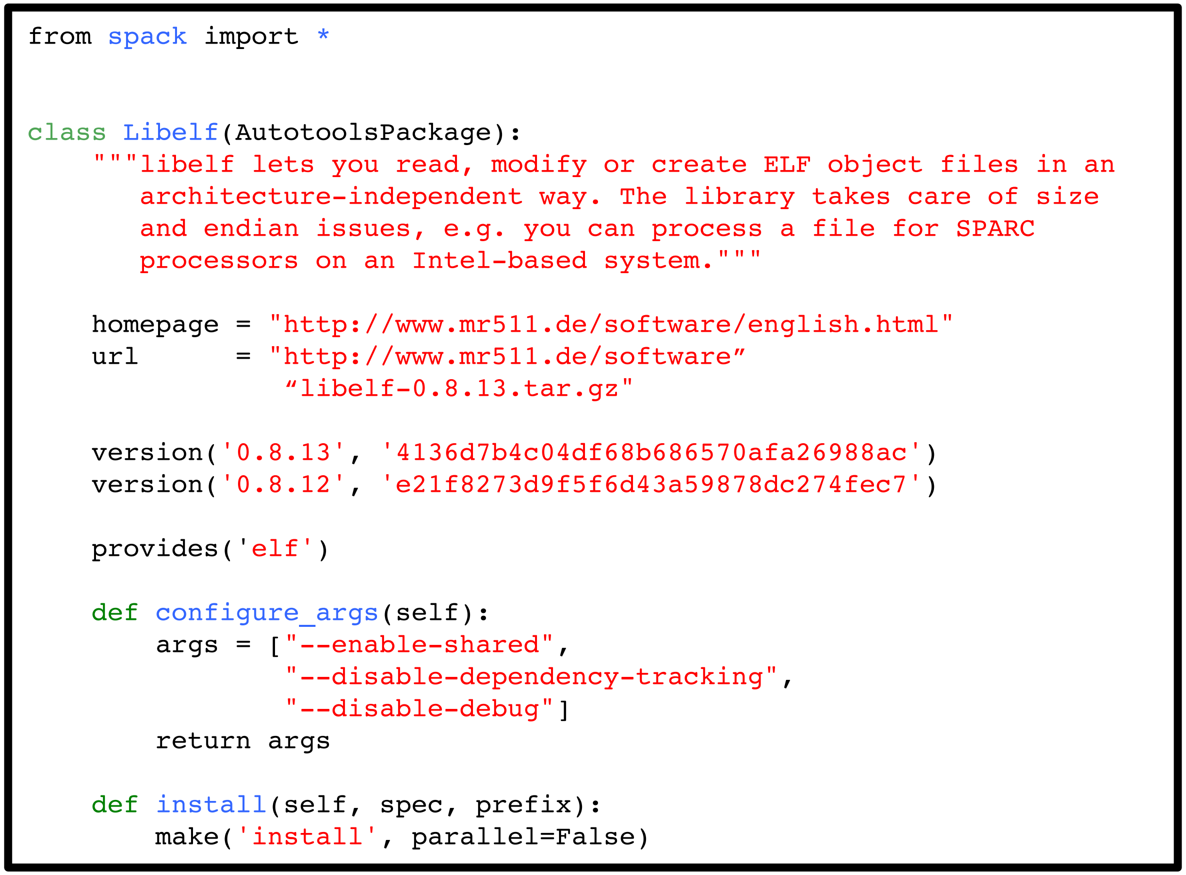
- **Spack included many features of interest to us at NERSC**
  - Easy to install and use
  - Packages are flexible
    - Build a range of versions for each package.
    - LLNL our close neighbors!
    - Todd Gamblin and Greg Becker (lead developers)
- **Lacked compatibility with our Cray systems**
  - 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.**

Package template file

Example of a package template file



```
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”
                “libelf-0.8.13.tar.gz"

    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

Spec Type	Spec Symbol	CLI Usage
package	package-name	python
version	@	python@2.7.13
compiler	%	python@2.7.13%gcc
architecture	arch=	python@2.7.13%gcc arch=cray-CNL-haswell
variant	+/-	python@2.7.13%gcc +tk arch=cray-CNL-haswell
compiler flags	ldflags=, cflags=, cxxflags=, cppflags=	python@2.7.13%gcc +tk arch=cray-CNL-haswell cflags=-02

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+openss
l+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+cpanm 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~symlinks 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

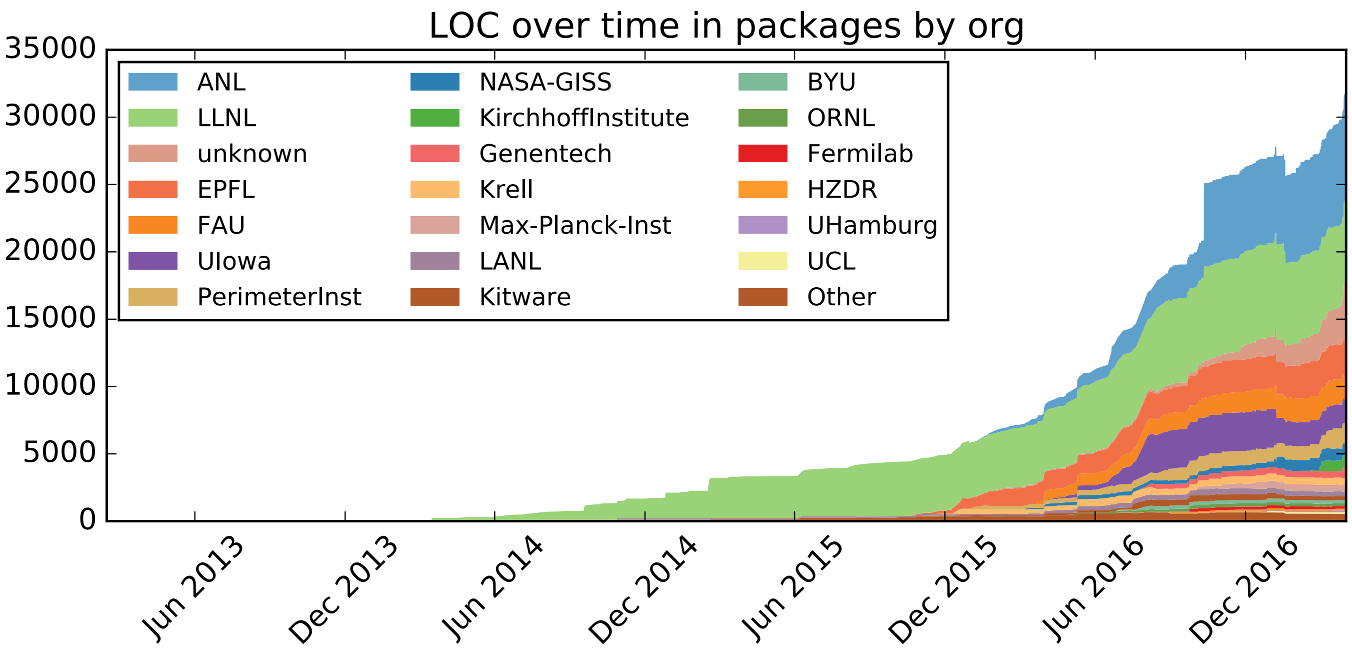
- **Easy as `spack install mpileaks`**
- **Spack compiler wrappers handle lib, include and RPATHs, and compiler flags.**
- **Each package has unique DAG-hash for provenance**
  - Directory tree generated for you
- **Generates modulefiles in a post-hook after install method completed.**
  - Supports Lmod,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

Spack Configuration

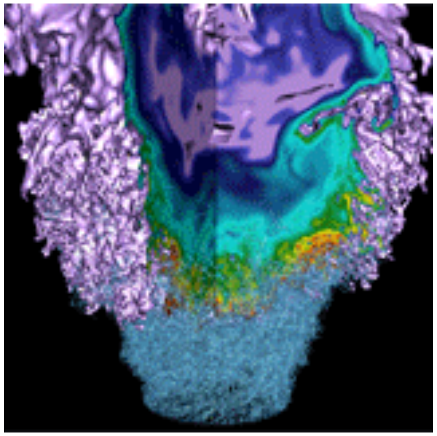
- **Spack allows flexibility and customization**
- **Configuration files**
  - packages.yaml
  - modules.yaml
  - compilers.yaml
  - config.yaml

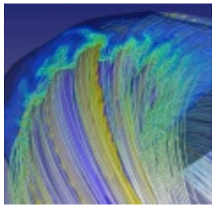
Spack Community

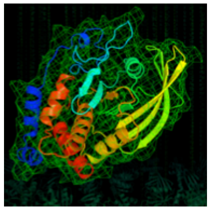
- When presented at SC ’15 Spack supported only 300 packages. Now over 1,400 packages are supported.
- Spack is in US Exascale Computing Project.
- Over 75% of packages are contributed externally.

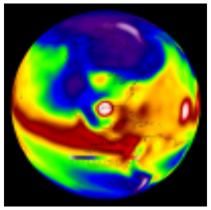


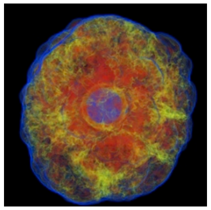
Cray Programming Environment

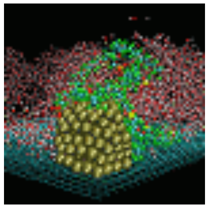












Cray Programming Environment

- **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             12) xpmem/2.1.1_gf9c9084-2.38
2) nsg/1.2.0                    13) job/2.1.1_gc1ad964-2.175
3) intel/17.0.2.174             14) dvs2.7_2.1.6
4) craype-network-aries         15) alps/6.3.4-2.21
5) craype/2.5.7                 16) rca/2.1.6_g2c60fbf-2.265
6) cray-libsci/16.09.1          17) atp/2.0.3
7) udreg/2.3.2-7.54             18) PrgEnv-intel/6.0.3
8) ugni/6.0.15-2.2              19) craype-haswell
9) pmi/5.0.10-1.0000           20) cray-shmem/7.4.4
10) dmapp/7.1.1-39.37           21) cray-mpich/7.4.4
11) gni-headers/5.0.11-2.2
```

Programming Environment Modules

- **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.**

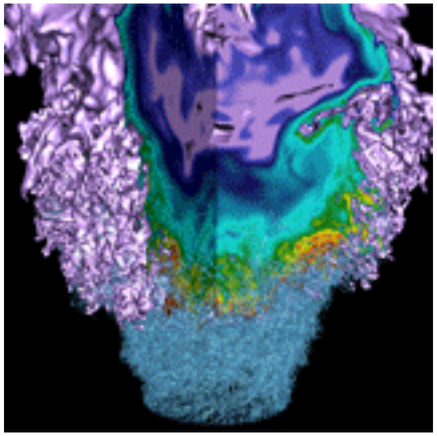
Cray and Third-Party Software

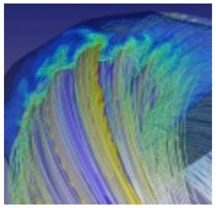
- **Cray provides optimized software libraries**
  - MPI (cray-mpich)
  - I/O Libraries (cray-netcdf, cray-hdf5)
  - Math libraries (cray-petsc, cray-trilinos)
  - Numerical routines (BLAS/LAPACK/SCALAPACK)
    - Cray-libsci, Intel-MKL
- **Monthly upgrades**
- **Libraries necessary for compiled software.**

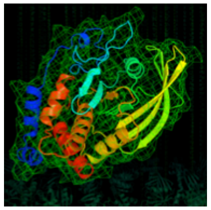
Cray Compiler Wrappers

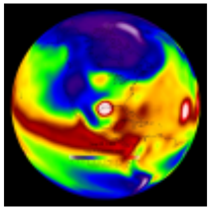
- **Long complex line of –L and –I flags.**
- **Contain optimization flags for architecture and target processor.**
- **Recommended to compile code for compute nodes.**
- **Requires compiling with Cray provided executables**
  - cc, CC, ftn

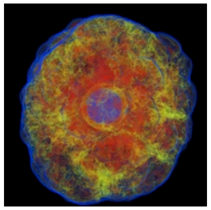
Spack on Cray

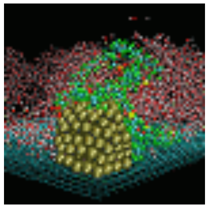












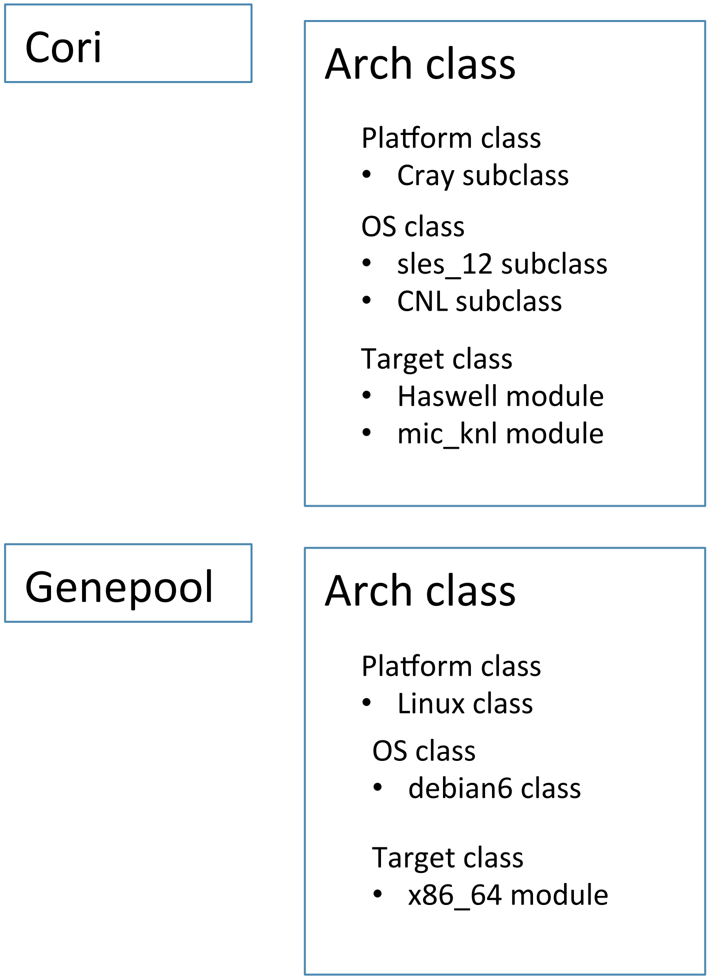
Spack on Cray

- **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

Modules Support

- **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.

Architecture Spec



Cori

Arch class

Platform class
- Cray subclass

OS class
- sles_12 subclass
- CNL subclass

Target class
- Haswell module
- mic_knl module

Genepool

Arch class

Platform class
- Linux class

OS class
- debian6 class

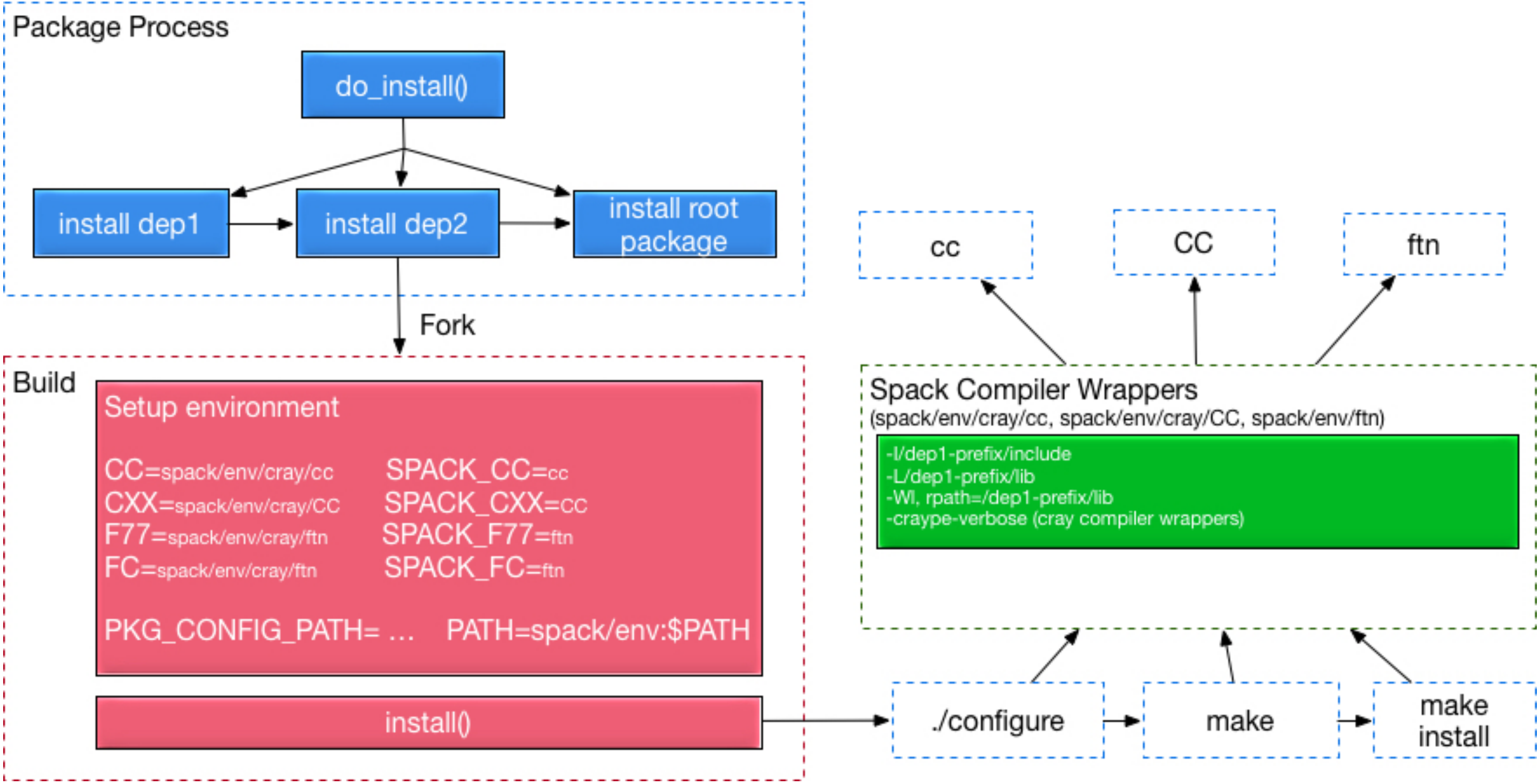
Target class
- x86_64 module

- **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 meta-data.

Spack Compiler Wrappers



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

```
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
```

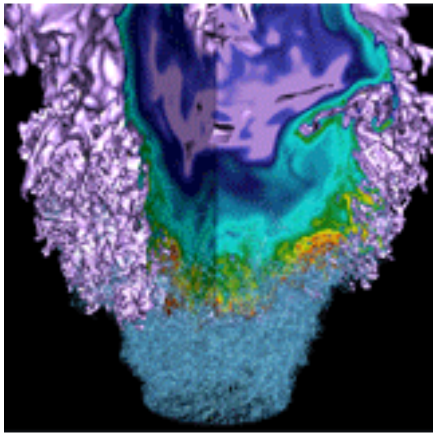
Message Passing Interface

- **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.
- **$CRAYPE_LINK_TYPE=dynamic**
  - Cray builds work like Linux builds
  - Spack doesn’t preclude static linking
    - Static flags added by build system.

Spack at NERSC and ORNL



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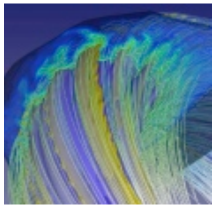
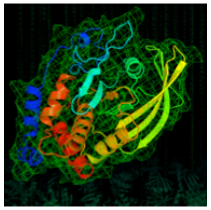
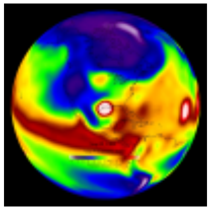
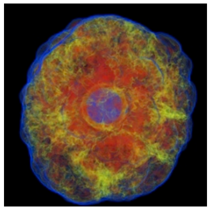
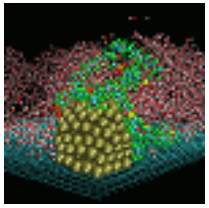










NERSC Usage

- **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**

ORNL Usage

- **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.

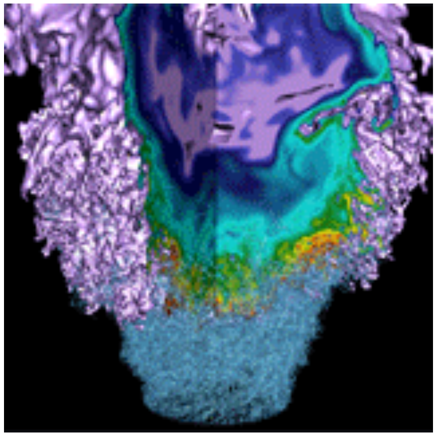
Related Package Managers

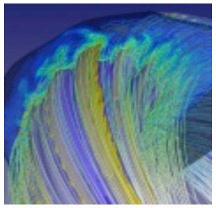
- **EasyBuild – Ghent University (Used at most CUG sites)**
  - Easyconfigs, easyblocks
- **Maali – Pawsey Supercomputing**
  - Collection of bash scripts
- **Smithy – ORNL**
  - Port based package manager specifically for Crays

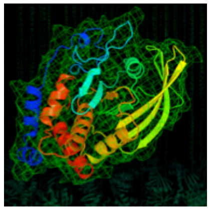
Comparison

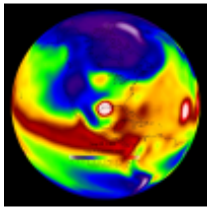
	EasyBuild	Spack	Maali	Smithy
Installs dependencies	Y	Y	N	N
Combinatorial Stack	Y	Y	N	N
Programming Language	Python	Python	Bash	Ruby
Generates modulefiles	Y	Y	Y	Y
Manipulates Cray modules	Y	Y	Y	Y
Dependency Resolution	N	Y	N	N
Version	v3.2.0 (stable)	V0.10 (alpha)	release_1.x	v1.6.5

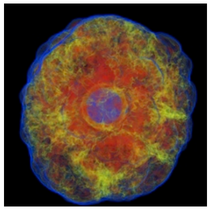
Conclusions

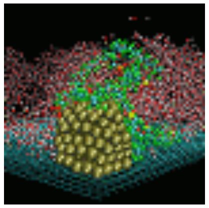












Conclusions

- **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!**

NERSC

National Energy Research Scientific Computing Center