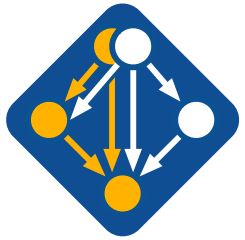

Managing HPC Software Complexity with Spack

Supercomputing 2016 Half-day Tutorial
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http://github.com/LLNL/spack

Lawrence Livermore National Laboratory

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Tutorial Materials

Materials: Download the latest version of slides and handouts at:

http://spack.readthedocs.io

Slides and hands-on scripts are in the "Tutorial" Section of the docs.

Other Resources:

- Spack GitHub repository: **http://github.com/LLNL/spack**
- Spack Documentation: **http://spack.readthedocs.io**

Tutorial Presenters & Contributors

Presenters

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Who is this Tutorial for?

People who want to use or distribute software for HPC!

1. **End Users of HPC Software**
   - Install and run HPC applications and tools
2. **HPC Application Teams**
   - Manage third-party dependency libraries
3. **Package Developers**
   - People who want to package their own software for distribution
4. **User support teams at HPC Centers**
   - People who deploy software for users at large HPC sites

HPC Software Complexity Prevents Reuse & Reduces Productivity

- Not much standardization in HPC: every machine/app has a different software stack
  - This is done to get the best **performance**
- HPC frequently trades reuse and usability for performance
  - Reusing a piece of software frequently requires you to port it to many new platforms
- Example environment for some LLNL codes:

48 third party packages x **3 MPI versions**: mvapich, mvapich2, OpenMPI x **3-ish Platforms**: Linux, BlueGene, Cray

x **Up to 7 compilers**: Intel, GCC, XLC, Clang, PGI, Cray, Pathscale x **Oh, and 2-3 versions of each package**

= **~7,500** combinations

Spack lowers barriers to software reuse by automating these builds!

What is the “production” environment for HPC?

- Someone’s home directory?
- LLNL? LANL? Sandia? ANL? LBL? TACC?
  - Environments at large-scale sites are very different.
- Which MPI implementation?
- Which compiler?
- Which dependencies?
- Which versions of dependencies?
  - Many applications require specific dependency versions.

Real answer: there isn’t a single production environment or a standard way to build.
Reusing someone else’s software is HARD.

Tutorial Overview

1.	Welcome & Overview	1:30 - 1:40
2.	For everyone: **Basics of Building and Linking**	1:40 - 1:55
3.	For everyone: **Spack Basics (hands on)**	1:55 - 2:40
4.	For everyone: **Core Spack Concepts**	2:40 - 3:00
5.	-- Break --	3:00 - 3:30
6.	For developers: **Making your own Spack Packages (hands on)**	3:30 - 4:15
7.	For HPC centers: **Deploying Spack at HPC Facilities (hands on)**	4:15 - 5:00

Why use a new tool?

1. Automate the process of building large software packages
2. Automate testing with different compilers and options
3. Leverage the work of others with shared build recipes
    1. Don’t repeat the same builds!
4. Distribute your software to a growing audience of HPC users

Spack is a flexible package manager for HPC

- How to install Spack:

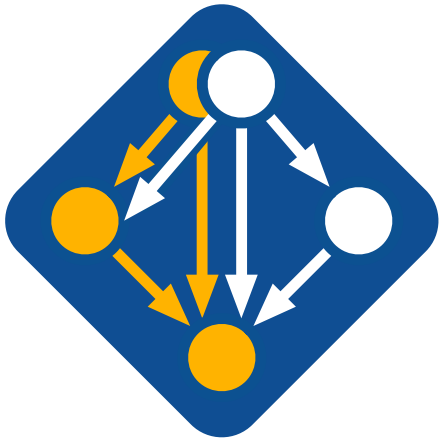
```
$ git clone https://github.com/LLNL/spack.git
$ . spack/share/spack/setup-env.sh
```

- How to install a package:

```
$ spack install hdf5
```

- HDF5 and its dependencies are installed within the Spack directory.

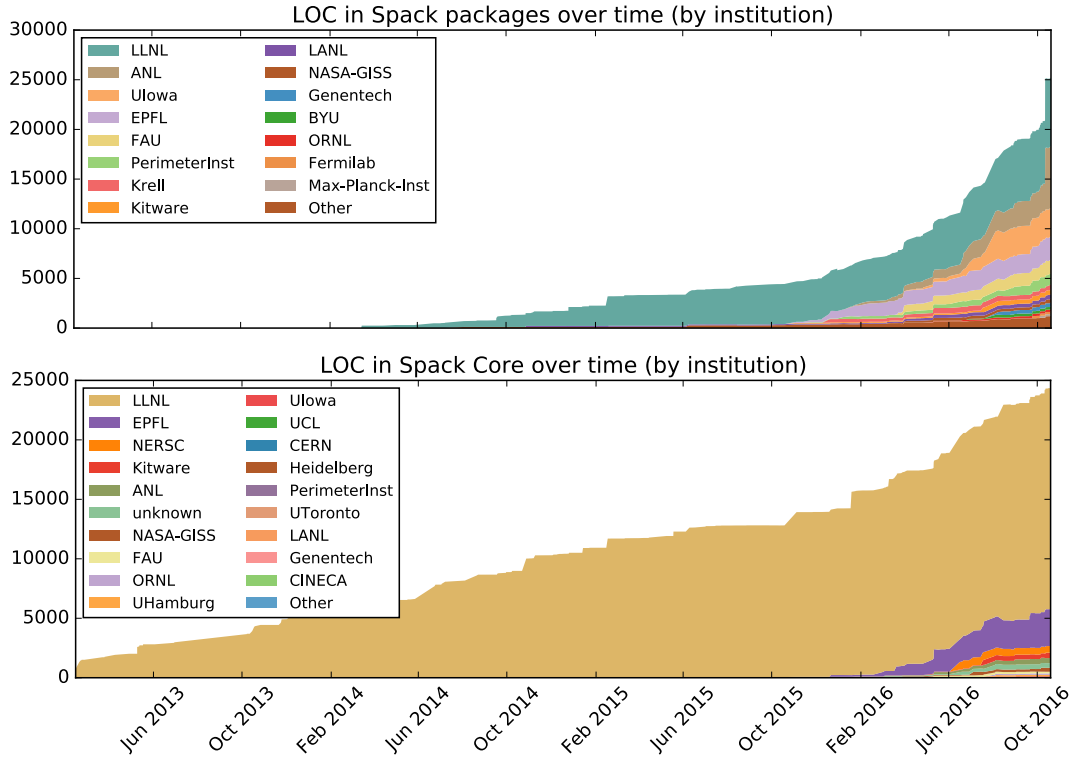
- Unlike typical package managers, Spack can also install many variants of the same build.
  - Different compilers
  - Different MPI implementations
  - Different build options



Get Spack!

http://github.com/LLNL/spack

Contributions to Spack have grown rapidly over the past year



- 1 year ago, LLNL provided most of the contributions to Spack
- Since last year, we've gone from 300 to 1,000 packages
- Over 75% of lines of code in packages are from external contributors.
  - Contributors add to the core as well.
- We are committed to sustaining Spack's open source ecosystem!

Join the Spack community!

- **20+ organizations**
  90+ contributors
  Sharing **1,016 packages** and growing

- **Spack can be a central repository for tools**
  - Make it easy for others to use them!
  - Build code the same way across HPC centers.

- **Spack is used in production at LLNL**
  - Livermore Computing
  - LLNL production multi-physics codes

- **Other organizations using Spack:**
  - **NERSC** using Spack on Cori: Cray support.
  - **EPFL** (Switzerland) contributing core features.
  - **Fermi, CERN, BNL**: high energy physics ecosystem.
  - **ANL** using Spack on production Linux clusters.
  - **NASA** packaging an Ice model code.
  - **ORNL** working with us on Spack for CORAL.
  - **Kitware**: core features, ParaView, UV-CDAT support

Related Work

Spack is not the first tool to automate builds
— Inspired by copious prior work

1. **"Functional" Package Managers**
   — Nix — https://nixos.org/
   — GNU Guix — https://www.gnu.org/s/guix/

2. **Build-from-source Package Managers**
   — Homebrew — http://brew.sh
   — MacPorts — https://www.macports.org

Other tools in the HPC Space:

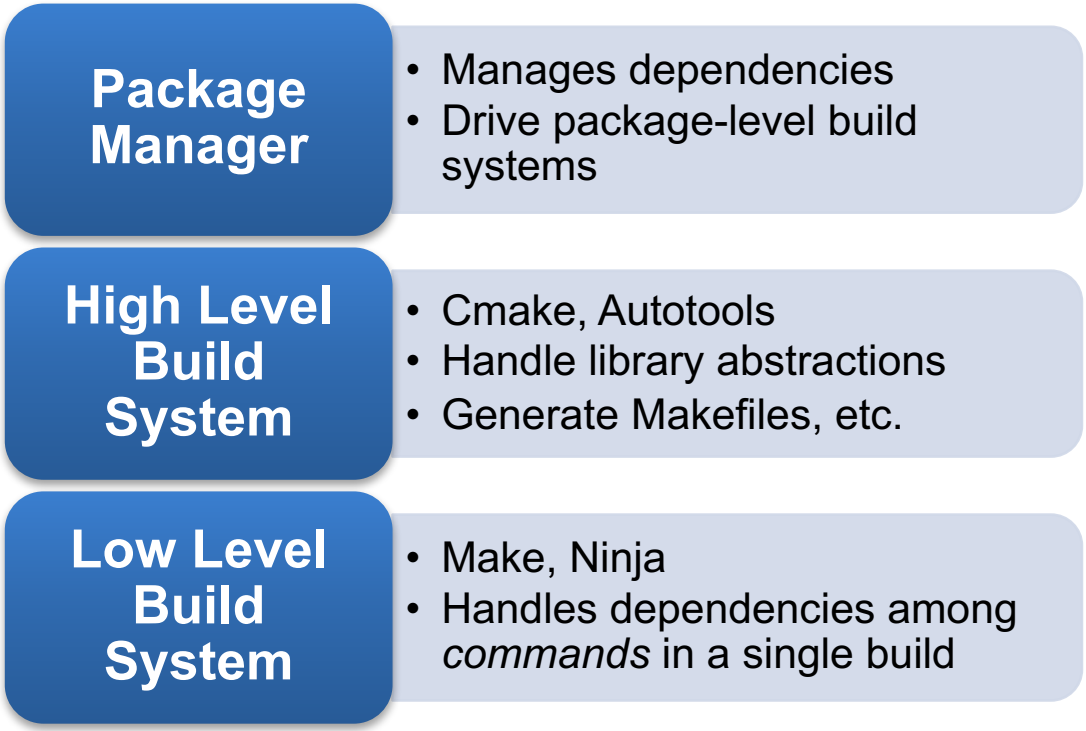
- **Easybuild** — http://hpcugent.github.io/easybuild/
  — An *installation* tool for HPC
  — Focused on HPC system administrators – different package model from Spack
  — Relies on a fixed software stack – harder to tweak recipes for experimentation

- **Hashdist** — https://hashdist.github.io

Building & Linking Basics

What's a package manager?

- Spack is a ***package manager***
  - **Does not** a replace Cmake/Autotools
  - Packages built by Spack can have any build system they want
- Spack manages *dependencies*
  - Drives package-level build systems
  - Ensures consistent builds
- Determining magic configure lines takes time
  - Spack is a cache of recipes



Static vs. shared libraries

- Static libraries: `libfoo.a`
  - .a files are archives of .o files (object files)
  - Linker includes needed parts of a static library in the output executable
  - No need to find dependencies at runtime – only at build time.
  - Can lead to large executables
  - Often hard to build a completely static executable on modern systems.

- Shared libraries: `libfoo.so` (Linux), `libfoo.dylib` (MacOS)
  - More complex build semantics, typically handled by the build system
  - Must be found by `ld.so` or `dyld` (dynamic linker) and loaded at runtime
    - Can cause lots of headaches with multiple versions
  - 2 main ways:
    - `LD_LIBRARY_PATH`: environment variable configured by user and/or module system
    - RPATH: paths embedded in executables and libraries, so that they know where to find their own dependencies.

API and ABI Compatibility

- **API: Application Programming Interface**
  - Source code functions and symbol names exposed by a library
  - If API of a dependency is backward compatible, source code need not be changed to use it
  - **May** need to recompile code to use a new version.

- **ABI: Application Binary Interface**
  - Calling conventions, register semantics, exception handling, etc.
  - Defined by how the compiler builds a library
    - Binaries generated by different compilers are typically ABI-incompatible.
  - May also include things like standard runtime libraries and compiler intrinsic functions
  - May also include values of hard-coded symbols/constants in headers.

- **HPC code, including MPI, is typically API-compatible but not ABI-compatible.**
  - Causes many build problems, especially for dynamically loaded libraries
  - Often need to rebuild to get around ABI problems
  - Leads to combinatorial builds of software at HPC sites.

3 major build systems to be aware of

1. Make (usually GNU Make)
   - https://www.gnu.org/software/make/
2. GNU Autotools
   - Automake: https://www.gnu.org/software/automake/
   - Autoconf: https://www.gnu.org/software/autoconf/
   - Libtool: https://www.gnu.org/software/libtool/
3. CMake:
   - https://cmake.org

Make and GNU Make

- Many projects opt to write their own Makefiles.
  - Can range from simple to very complicated
- Make declares some standard variables for various compilers
  - Many HPC projects don't respect them
  - No standard install prefix convention
  - Makefiles may not have install target
- Automating builds with Make usually requires editing files
  - Typical to use sed/awk/some other regular expression tool on Makefile
  - Can also use patches

Typical build incantation

```
<edit Makefile>
make PREFIX=/path/to/prefix
```

Configure options

```
None.  Typically must edit Makefiles.
```

Environment variables

CC	CFLAGS	LDFLAGS
CXX	CXXFLAGS	LIBS
FC	FFLAGS	CPP
F77	FFLAGS	

Autotools

- Three parts of autotools:
  - autoconf: generates a portable configure script to inspect build host
  - automake: high-level syntax for generating lower-level Makefiles.
  - libtool: abstraction for shared libraries
- Typical variables are similar to make
- Much more consistency among autotools projects
  - Wide use of standard variables and configure options
  - Standard install target, staging conventions.

Typical build incantation

```
./configure --prefix=/path/to/install_dir
make
make install
```

Configure options

```
./configure \
    --prefix=/path/to/install_dir \
    --with-package=/path/to/dependency \
    --enable-foo \
    --disable-bar
```

Environment variables

CC	CFLAGS	LDFLAGS
CXX	CXXFLAGS	LIBS
FC	FFLAGS	CPP
F77	FFLAGS	

CMake

- Gaining popularity
- Arguably easier to use (for developers) than autotools
- Similar standard options to autotools
  - different variable names
  - More configuration options
  - Abstracts platform-specific details of shared libraries
- Most CMake projects should be built “out of souce”
  - Separate build directory from source directory

Typical build incantation

```
mkdir BUILD && cd BUILD
cmake –DCMAKE_INSTALL_PREFIX=/path/to/install_dir ..
make
make install
```

Configure options

```
cmake \
    –D CMAKE_INSTALL_PREFIX=/path/to/install_dir \
    -D ENABLE_FOO=yes \
    -D ENABLE_BAR=no \
    ..
```

Common –D options

```
CMAKE_C_COMPILER            CMAKE_C_FLAGS
CMAKE_CXX_COMPILER          CMAKE_CXX_FLAGS
CMAKE_Fortran_COMPILER      CMAKE_Fortran_FLAGS
CMAKE_SHARED_LINKER_FLAGS   CMAKE_EXE_LINKER_FLAGS
CMAKE_STATIC_LINKER_FLAGS
```

Spack Basics

Spack provides a *spec* syntax to describe customized DAG configurations

```
$ spack install mpileaks                              unconstrained
$ spack install mpileaks@3.3                          @ custom version
$ spack install mpileaks@3.3 %gcc@4.7.3               % custom compiler
$ spack install mpileaks@3.3 %gcc@4.7.3 +threads      +/- build option
$ spack install mpileaks@3.3 cppflags=\"-O3\"         setting compiler flags
$ spack install mpileaks@3.3 os=CNL10 target=haswell  setting target for X-compile
$ spack install mpileaks@3.3 ^mpich@3.2 %gcc@4.9.3    ^ dependency information
```

- Each expression is a ***spec*** for a particular configuration
  - Each clause adds a constraint to the spec
  - Constraints are optional – specify only what you need.
  - Customize install on the command line!

- Spec syntax is recursive
  - Full control over the combinatorial build space

`spack list` shows what packages are available

```
$ spack list
==> 303 packages.
activeharmony   cgal             fish         gtkplus      libgd          mesa              openmpi          py-coverage       py-pycparser         qt          tcl
adept-utils     cgm              flex         harfbuzz     libgpg-error   metis             openspeedshop    py-cython         py-pyelftools        qthreads    texinfo
apex            cityhash         fltk         hdf          libjpeg-turbo  Mitos             openssl          py-dateutil       py-pygments          R           the_silver_searcher
arpack          cleverleaf       flux         hdf5         libjson-c      mpc               otf              py-epydoc         py-pylint            ravel       thrift
asciidoc        cloog            fontconfig   hwloc        libmng         mpe2              otf2             py-funcsigs       py-pypar             readline    tk
atk             cmake            freetype     hypre        libmonitor     mpfr              pango            py-genders        py-pyparsing         rose        tmux
atlas           cmocka           gasnet       icu          libNBC         mpibash           papi             py-gnuplot        py-pyqt              rsync       tmuxinator
atop            coreutils        gcc          icu4c        libpciaccess   mpich             paraver          py-h5py           py-pyside            ruby        trilinos
autoconf        cppcheck         gdb          ImageMagick  libpng         mpileaks          paraview         py-ipython        py-pytables          SAMRAI      uncrustify
automaded       cram             gdk-pixbuf   isl          libsodium      mrnet             parmetis         py-libxml2        py-python-daemon     samtools    util-linux
automake        cscope           geos         jdk          libtiff        mumps             parpack          py-lockfile       py-pytz              scalasca    valgrind
bear            cube             gflags       jemalloc     libtool        munge             patchelf         py-mako           py-rpy2              scorep      vim
bib2xhtml       curl             ghostscript  jpeg         libunwind      muster            pcre             py-matplotlib     py-scientificpython  scotch      vtk
binutils        czmq             git          judy         libuuid        mvapich2          pcre2            py-mock           py-scikit-learn      scr         wget
bison           damselfly        glib         julia        libxcb         nasm              pdt              py-mpi4py         py-scipy             silo        wx
boost           dbus             glm          launchmon    libxml2        ncdu              petsc            py-mx             py-setuptools        snappy      wxpropgrid
bowtie2         docbook-xml      global       lcms         libxshmfence   ncurses           pidx             py-mysqldb1       py-shiboken          sparsehash  xcb-proto
boxlib          doxygen          glog         leveldb      libxslt        netcdf            pixman           py-nose           py-sip               spindle     xerces-c
bzip2           dri2proto        glpk         libarchive   llvm           netgauge          pkg-config       py-numexpr        py-six               spot        xz
cairo           dtcmp            gmp          libcerf      llvm-lld       netlib-blas       pmgr_collective  py-numpy          py-sphinx            sqlite      yasm
callpath        dyninst          gmsh         libcircle    lmdb           netlib-lapack     postgresql       py-pandas         py-sympy             stat        zeromq
cblas           eigen            gnuplot      libdrm       lmod           netlib-scalapack  ppl              py-pbr            py-tappy             sundials    zlib
cbtf            elfutils         gnutls       libdwarf     lua            nettle            protobuf         py-periodictable  py-twisted           swig        zsh
cbtf-argonavis  elpa             gperf        libedit      lwgrp          ninja             py-astropy       py-pexpect        py-urwid             szip
cbtf-krell      expat            gperftools   libelf       lwm2           ompss             py-basemap       py-pil            py-virtualenv        tar
cbtf-lanl       extrae           graphlib     libevent     matio          ompt-openmp       py-biopython     py-pillow         py-yapf              task
cereal          exuberant-ctags  graphviz     libffi       mbedtls        opari2            py-blessings     py-pmw            python               taskd
cfitsio         fftw             gsl          libgcrypt    memaxes        openblas          py-cffi          py-pychecker      qhull                tau
```

- Spack has over 1000 packages now.

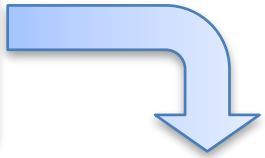
`spack find` shows what is installed

```
$ spack find
==> 103 installed packages.
-- linux-redhat6-x86_64 / gcc@4.4.7 ------------------------------
ImageMagick@6.8.9-10  glib@2.42.1        libtiff@4.0.3     pango@1.36.8          qt@4.8.6
SAMRAI@3.9.1          graphlib@2.0.0     libtool@2.4.2     parmetis@4.0.3        qt@5.4.0
adept-utils@1.0       gtkplus@2.24.25    libxcb@1.11       pixman@0.32.6         ravel@1.0.0
atk@2.14.0            harfbuzz@0.9.37    libxml2@2.9.2     py-dateutil@2.4.0     readline@6.3
boost@1.55.0          hdf5@1.8.13        llvm@3.0          py-ipython@2.3.1      scotch@6.0.3
cairo@1.14.0          icu@54.1           metis@5.1.0       py-nose@1.3.4         starpu@1.1.4
callpath@1.0.2        jpeg@9a            mpich@3.0.4       py-numpy@1.9.1        stat@2.1.0
dyninst@8.1.2         libdwarf@20130729  ncurses@5.9       py-pytz@2014.10       xz@5.2.0
dyninst@8.1.2         libelf@0.8.13      ocr@2015-02-16    py-setuptools@11.3.1  zlib@1.2.8
fontconfig@2.11.1     libffi@3.1         openssl@1.0.1h    py-six@1.9.0
freetype@2.5.3        libmng@2.0.2       otf@1.12.5salmon  python@2.7.8
gdk-pixbuf@2.31.2     libpng@1.6.16      otf2@1.4          qhull@1.0

-- linux-redhat6-x86_64 / gcc@4.8.2 ------------------------------
adept-utils@1.0.1  boost@1.55.0  cmake@5.6-special  libdwarf@20130729  mpich@3.0.4
adept-utils@1.0.1  cmake@5.6     dyninst@8.1.2      libelf@0.8.13      openmpi@1.8.2

-- linux-redhat6-x86_64 / intel@14.0.2 ---------------------------
hwloc@1.9  mpich@3.0.4  starpu@1.1.4

-- linux-redhat6-x86_64 / intel@15.0.0 ---------------------------
adept-utils@1.0.1  boost@1.55.0  libdwarf@20130729  libelf@0.8.13  mpich@3.0.4

-- linux-redhat6-x86_64 / intel@15.0.1 ---------------------------
adept-utils@1.0.1  callpath@1.0.2  libdwarf@20130729  mpich@3.0.4
boost@1.55.0       hwloc@1.9       libelf@0.8.13      starpu@1.1.4
```

- All the versions coexist!
  - Multiple versions of same package are ok.
- Packages are installed to automatically find correct dependencies.
- Binaries work *regardless of user's environment*.
- Spack also generates module files.
  - Don't *have* to use them.

Users can query the full dependency configuration of installed packages.

```
$ spack find callpath
==> 2 installed packages.
-- linux-x86_64 / clang@3.4 --------     -- linux-x86_64 / gcc@4.9.2 -------------
callpath@1.0.2                           callpath@1.0.2
```



Expand dependencies with `spack find -d`

```
$ spack find -dl callpath
==> 2 installed packages.
-- linux-x86_64 / clang@3.4 -----------     -- linux-x86_64 / gcc@4.9.2 -----------
xv2clz2    callpath@1.0.2                    udltshs    callpath@1.0.2
ckjazss        ^adept-utils@1.0.1            rfsu7fb        ^adept-utils@1.0.1
3ws43m4            ^boost@1.59.0             ybet64y            ^boost@1.55.0
ft7znm6            ^mpich@3.1.4              aa4ar6i            ^mpich@3.1.4
qqnuet3        ^dyninst@8.2.1                tmnnge5        ^dyninst@8.2.1
3ws43m4            ^boost@1.59.0             ybet64y            ^boost@1.55.0
g65rdud            ^libdwarf@20130729        g2mxrl2            ^libdwarf@20130729
cj5p5fk                ^libelf@0.8.13        ynpai3j                ^libelf@0.8.13
cj5p5fk            ^libelf@0.8.13            ynpai3j            ^libelf@0.8.13
g65rdud        ^libdwarf@20130729            g2mxrl2        ^libdwarf@20130729
cj5p5fk            ^libelf@0.8.13            ynpai3j            ^libelf@0.8.13
cj5p5fk        ^libelf@0.8.13                ynpai3j        ^libelf@0.8.13
ft7znm6        ^mpich@3.1.4                  aa4ar6i        ^mpich@3.1.4
```

- Architecture, compiler, versions, and variants may differ between builds.

Spack manages installed compilers

- Compilers are automatically detected
  - Automatic detection determined by OS
  - Linux: PATH
  - Cray: `module avail`
- Compilers can be manually added
  - Including Spack-built compilers

```
$ spack compilers
==> Available compilers
-- gcc ---------------------------------
gcc@4.2.1      gcc@4.9.3

-- clang -------------------------------
clang@6.0
```

compilers.yaml

```
compilers:
- compiler:
    modules: []
    operating_system: ubuntu14
    paths:
      cc: /usr/bin/gcc/4.9.3/gcc
      cxx: /usr/bin/gcc/4.9.3/g++
      f77: /usr/bin/gcc/4.9.3/gfortran
      fc: /usr/bin/gcc/4.9.3/gfortran
    spec: gcc@4.9.3
- compiler:
    modules: []
    operating_system: ubuntu14
    paths:
      cc: /usr/bin/clang/6.0/clang
      cxx: /usr/bin/clang/6.0/clang++
      f77: null
      fc: null
    spec: clang@6.0
- compiler:
    ...
```

Hands-on Time

Extensions and Python Support

- Spack installs packages in own prefix
- Some packages need to be installed within directory structure of other packages
  - i.e., Python modules installed in $prefix/lib/python-<version>/site-packages
  - Spack supports this via extensions

```
class PyNumpy(Package):
    """NumPy is the fundamental package for scientific computing with Python."""

    homepage = "https://numpy.org"
    url      = "https://pypi.python.org/packages/source/n/numpy/numpy-1.9.1.tar.gz"
    version('1.9.1', ' 78842b73560ec378142665e712ae4ad9')

    extends("python")

 def install(self, spec, prefix):
        setup_py("install", "--prefix={0}".format(prefix))
```

Spack extensions

- Examples of extension packages:
  - python libraries are a good example
  - R, Lua, perl
  - Need to maintain combinatorial versioning

```
spack/opt/
    linux-redhat6-x86_64/
        gcc-4.7.2/
            python-2.7.12-6y6vvaw/
                python/
            py-numpy-1.10.4-oaxix36/
                py-numpy/
...
```

```
$ spack activate py-numpy @1.10.4
```

- Symbolic link to Spack install location
- Automatically activate for correct version of dependency
  - Provenance information from DAG
  - Activate all dependencies that are extensions as well

```
spack/opt/
    linux-redhat6-x86_64/
        gcc-4.7.2/
            python-2.7.12-/
                python/
                py-numpy
            py-numpy-1.10.4-oaxix36/
                py-numpy/
...
```

Extensions must be activated into extendee

```
$ spack extensions python
==> python@2.7.12% gcc@4.9.3 ~tk~ucs4 arch=linux-redhat7-x86_64-i25k4oi
==> 118 extensions:
…
py-autopep8      py-docutils        py-mako            py-numpy        py-py2neo
…

==> 3 installed:
-- linux-redhat7-x86_64 / gcc@4.9.3 ----------------------------
py-nose@1.3.7  py-numpy@1.11.0  py-setuptools@20.7.0

==> None activated.

$ spack load python
$ python
Python 2.7.12 (default, Aug 26 2016, 15:12:42)
[GCC 4.9.3] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
Traceback (most recent call last): File "<stdin>", line 1, in <module>
ImportError: No module named numpy
>>>
```

- Python unaware of numpy installation

```
$ spack activate py-numpy
==> Activated extension py-numpy@1.11.0% gcc@4.9.3 +blas+lapack
arch=linux-redhat7-x86_64-77im5ny for python@2.7.12 ~tk~ucs4 % gcc@4.9.3
$ spack extensions python
==> python@2.7.12% gcc@4.9.3 ~tk~ucs4 arch=linux-redhat7-x86_64-i25k4oi
…
==> 1 currently activated:
-- linux-redhat7-x86_64 / gcc@4.9.3 ----------------------------

$ python
Python 2.7.12 (default, Aug 26 2016, 15:12:42)
[GCC 4.9.3] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> x = numpy.zeros(10)
>>>
```

- `activate` symlinks entire numpy prefix into Python installation
- Can alternatively load extension

```
$ spack load python
$ spack load py-numpy
```

Hands-on Time

Follow script at:

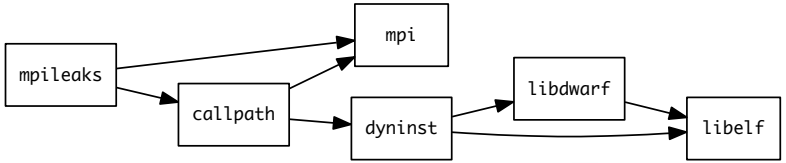
Core Spack Concepts

Most existing tools do not support combinatorial versioning

- Traditional binary package managers
  - RPM, yum, APT, yast, etc.
  - Designed to manage a single stack.
  - Install *one* version of each package in a single prefix (`/usr`).
  - Seamless upgrades to a *stable, well tested* stack
- Port systems
  - BSD Ports, portage, Macports, Homebrew, Gentoo, etc.
  - Minimal support for builds parameterized by compilers, dependency versions.
- Virtual Machines and Linux Containers (Docker)
  - Containers allow users to build environments for different applications.
  - Does not solve the build problem (someone has to build the image)
  - Performance, security, and upgrade issues prevent widespread HPC deployment.

Spack handles combinatorial software complexity.

Dependency DAG



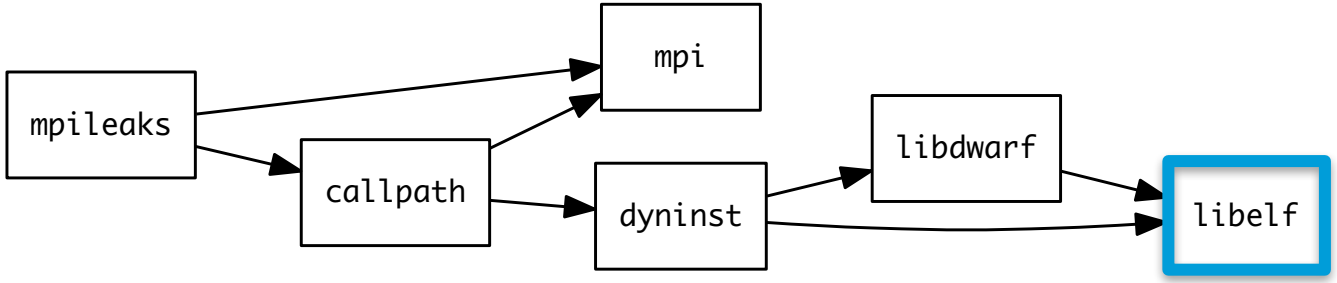
Installation Layout

Hash

```
spack/opt/
    linux-x86_64/
        gcc-4.7.2/
            mpileaks-1.1-
0f54bf34cadk/
        intel-14.1/
            hdf5-1.8.15-lkf14aq3nqiz/
    bgq/
        xl-12.1/
            hdf5-1-8.16-fqb3a15abrwx/
```

- Each unique dependency graph is a unique ***configuration***.
- Each configuration installed in a unique directory.
  - Configurations of the same package can coexist.
- **Hash** of entire directed acyclic graph (DAG) is appended to each prefix.
- Installed packages automatically find dependencies
  - Spack embeds RPATHs in binaries.
  - No need to use modules or set LD_LIBRARY_PATH
  - Things work *the way you built them*

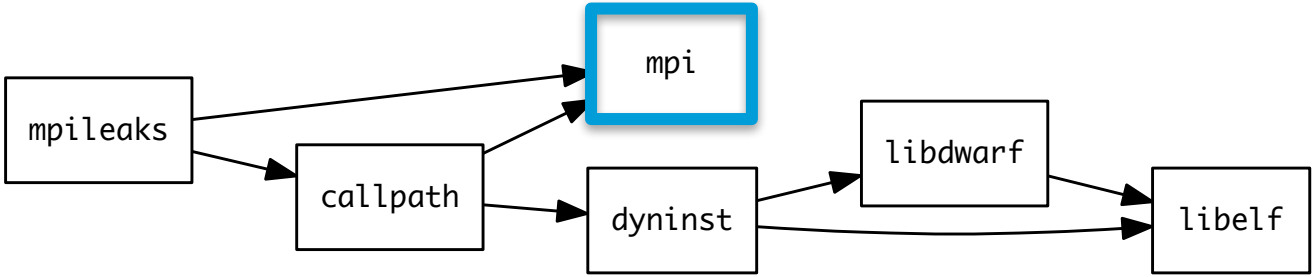
Spack Specs can constrain versions of dependencies




```
$ spack install mpileaks %intel@12.1 ^libelf@0.8.12
```

- Spack ensures *one* configuration of each library per DAG
  - Ensures ABI consistency.
  - User does not need to know DAG structure; only the dependency *names.*
- Spack can ensure that builds use the same compiler, or you can mix
  - Working on ensuring ABI compatibility when compilers are mixed.

Spack handles ABI-incompatible, versioned interfaces like MPI



- `mpi` is a *virtual dependency*
- Install the same package built with two different MPI implementations:

```
$ spack install mpileaks ^mvapich@1.9
```

```
$ spack install mpileaks ^openmpi@1.4:
```

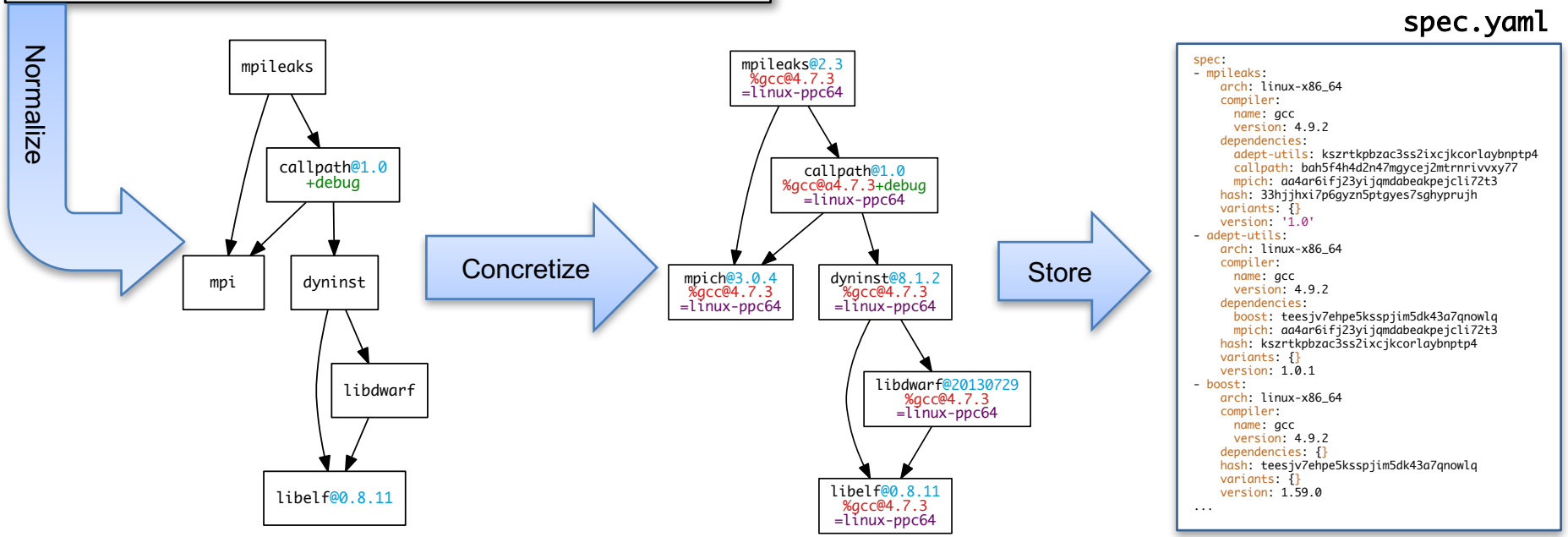
- Let Spack choose MPI implementation, as long as it provides MPI 2 interface:

```
$ spack install mpileaks ^mpi@2
```

Concretization fills in missing configuration details when the user is not explicit.

```
mpileaks ^callpath@1.0+debug ^libelf@0.8.11
```

User input: *abstract* spec with some constraints



Abstract, normalized spec with some dependencies.

Concrete spec is fully constrained and can be passed to install.

spec.yaml

```
spec:
- mpileaks:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      adept-utils: kszrtkpbzac3ss2ixcjkcorlaybnptp4
      callpath: bah5f4h4d2n47mgycej2mtrnrivvxy77
      mpich: aa4ar6ifj23yijqmdabeakpejcli72t3
    hash: 33hjjhxi7p6gyzn5ptgyes7sghyprujh
    variants: {}
    version: '1.0'
- adept-utils:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      boost: teesjv7ehpe5ksspjim5dk43a7qnowlq
      mpich: aa4ar6ifj23yijqmdabeakpejcli72t3
    hash: kszrtkpbzac3ss2ixcjkcorlaybnptp4
    variants: {}
    version: 1.0.1
- boost:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies: {}
    hash: teesjv7ehpe5ksspjim5dk43a7qnowlq
    variants: {}
    version: 1.59.0
...
```

Detailed provenance is stored with the installed package

Use spack spec to see the results of concretization

```
$ spack spec mpileaks
Input spec
--------------------------------
  mpileaks

Normalized
--------------------------------
  mpileaks
      ^adept-utils
          ^boost@1.42:
          ^mpi
      ^callpath
          ^dyninst
              ^libdwarf
                  ^libelf

Concretized
--------------------------------
  mpileaks@1.0%gcc@5.3.0 arch=darwin-elcapitan-x86_64
      ^adept-utils@1.0.1%gcc@5.3.0 arch=darwin-elcapitan-x86_64
          ^boost@1.61.0%gcc@5.3.0+atomic+chrono+date_time~debug+filesystem~graph
           ~icu_support+iostreams+locale+log+math~mpi+multithreaded+program_options
           ~python+random +regex+serialization+shared+signals+singlethreaded+system
           +test+thread+timer+wave arch=darwin-elcapitan-x86_64
              ^bzip2@1.0.6%gcc@5.3.0 arch=darwin-elcapitan-x86_64
              ^zlib@1.2.8%gcc@5.3.0 arch=darwin-elcapitan-x86_64
          ^openmpi@2.0.0%gcc@5.3.0~mxm~pmi~psm~psm2~slurm~sqlite3~thread_multiple~tm~verbs+vt arch=darwin-elcapitan-x86_64
              ^hwloc@1.11.3%gcc@5.3.0 arch=darwin-elcapitan-x86_64
                  ^libpciaccess@0.13.4%gcc@5.3.0 arch=darwin-elcapitan-x86_64
                      ^libtool@2.4.6%gcc@5.3.0 arch=darwin-elcapitan-x86_64
                          ^m4@1.4.17%gcc@5.3.0+sigsegv arch=darwin-elcapitan-x86_64
                              ^libsigsegv@2.10%gcc@5.3.0 arch=darwin-elcapitan-x86_64
      ^callpath@1.0.2%gcc@5.3.0 arch=darwin-elcapitan-x86_64
          ^dyninst@9.2.0%gcc@5.3.0~stat_dysect arch=darwin-elcapitan-x86_64
              ^libdwarf@20160507%gcc@5.3.0 arch=darwin-elcapitan-x86_64
                  ^libelf@0.8.13%gcc@5.3.0 arch=darwin-elcapitan-x86_64
```

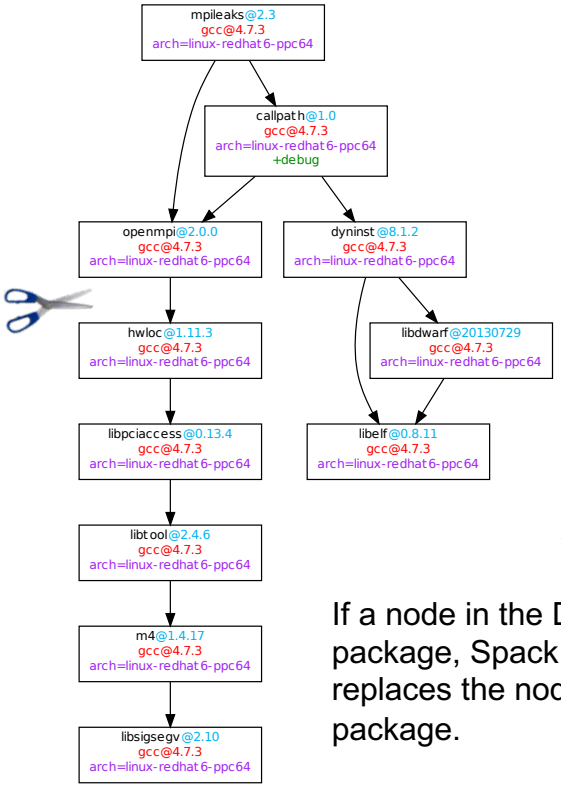
Building against externally installed software

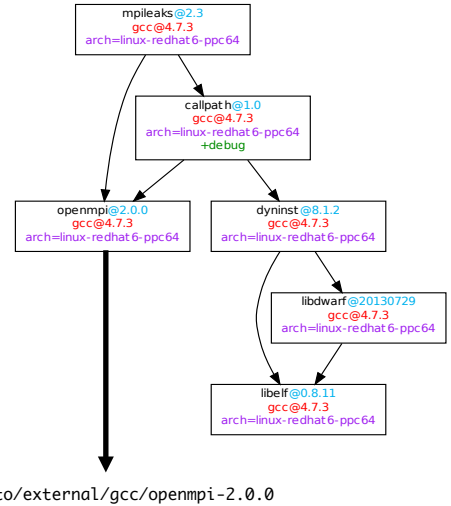
```
mpileaks ^callpath@1.0+debug
    ^openmpi ^libelf@0.8.11
```

packages.yaml

```
packages:
  mpi:
    buildable: False
  openmpi:
    buildable: False
    paths:
      openmpi@2.0.0 %gcc@4.7.3 arch=linux-redhat6-ppc64:
        /path/to/external/gcc/openmpi-2.0.0
      openmpi@1.10.3 %gcc@4.7.3 arch=linux-redhat6-ppc64:
        /path/to/external/gcc/openmpi-1.10.3
      openmpi@2.0.0 %intel@16.0.0 arch=linux-redhat6-ppc64:
        /path/to/external/intel/openmpi-2.0.0
      openmpi@1.10.3 %intel@16.0.0 arch=linux-redhat6-ppc64:
        /path/to/external/intel/openmpi-1.10.3
...
```

A user registers external packages with Spack.

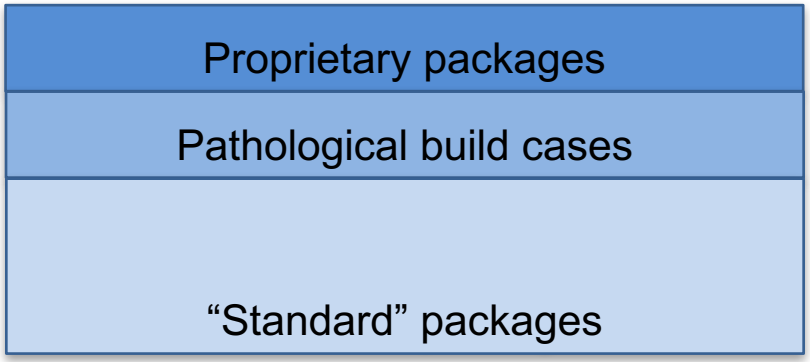




If a node in the DAG matches an registered external package, Spack prunes the DAG at that node and replaces the node with a reference to the external package.

Spack package repositories

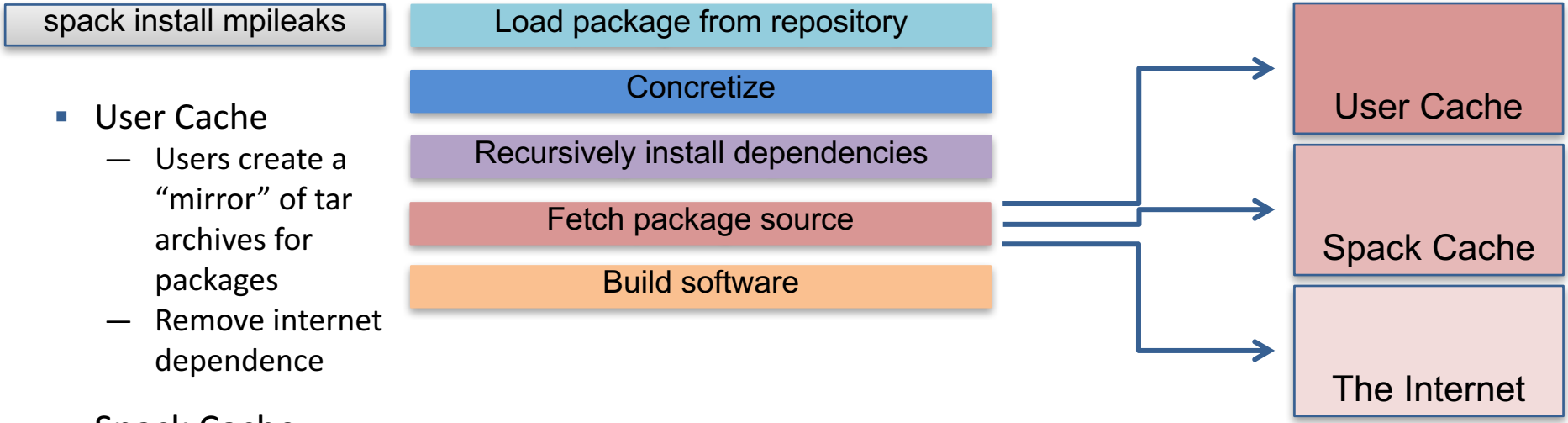
- Some packages can not be released publicly
- Some users have use cases that require ~~bizarre~~ custom builds
- Packaging issues should not prevent users from updating Spack
  - Solution: separate repositories
  - A repository is simply a directory of package files



`my_repo`

`spack/var/repos/builtin`

Fetching source code for spack



- User Cache
  - Users create a "mirror" of tar archives for packages
  - Remove internet dependence
- Spack Cache
  - Spack automatically caches tar archives for previously installed software
- The Internet
  - Spack packages can find source files online

Adding compiler flags (for compiler parameter studies)

```
$ spack install hdf5 cflags=\‘-O3 –g –fast –fpack-struct\’
```

- This would install HDF5 with the specified flags
  - Flags are injected via Spack’s compiler wrappers.
- Flags are propagated to dependencies automatically
  - Flags are included in the **DAG hash**
  - Each build is considered a **different version**
- This provides an easy harness for doing parameter studies for tuning codes
  - Previously working with large codes was very tedious.
- Supports cflags, cxxflags, fflags, cppflags, ldflags, and ldlibs
  - Added from CLI or config file

Spack provides hooks that enable tools to work with large codes.

Making your own Spack Packages

Creating your own Spack Packages

- Package is a recipe for building
- Each package is a Python class
  - Download information
  - Versions/Checksums
  - Build options
  - Dependencies
  - Build instructions
- Package collections are repos
  - Spack has a “builtin” repo in **$REPO/var/spack/repos/builtin**

$REPO/packages/zlib/package.py

```
from spack import *


class Zlib(Package):
    """A free, general-purpose, legally unencumbered lossless
       data-compression library."""

    homepage = "http://zlib.net"
    url      = "http://zlib.net/zlib-1.2.8.tar.gz"

    version('1.2.8', '44d667c142d7cda120332623eab69f40')

    depends_on(‘cmake’, type=‘build’)

    def install(self, spec, prefix):
        configure('--prefix={0}'.format(prefix))

        make()
        make('install')
```

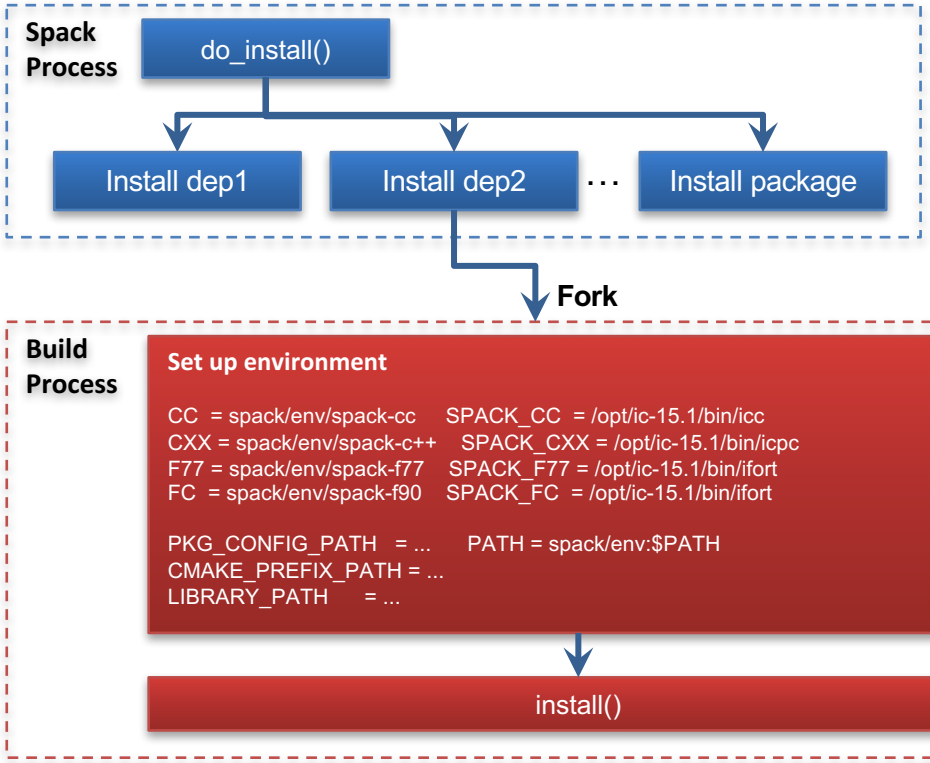
Packages are Parameterized

- Each package has one class
  - e.g., zlib for Intel compiler and zlib for GCC compiler are built with the same recipe.
- Can query what's being built.
- Compiler wrappers handle many details automatically.
  - Spack feeds compiler wrappers to (cc, c++, f90, …) to autoconf, cmake, gmake, …
  - Wrappers select compilers, dependencies, and options under the hood.

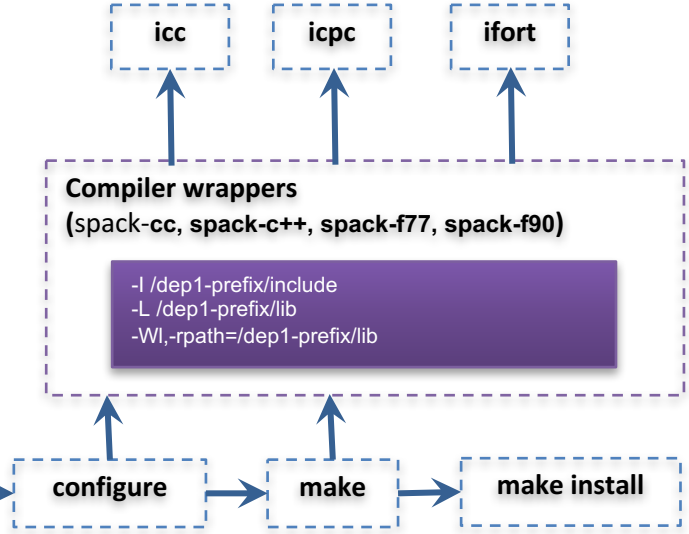
package.py

```
def install(self, spec, prefix):
    config_opts=['--prefix='+prefix]

    if '~shared' in self.spec:
        config_opts.append('--disable-shared')
    else:
        config_opts.append('--enable-shared')

    configure(config_opts)
    make()
    make('install')
```

Spack builds each package in its own compilation environment



- **Forked build process isolates environment for each build.**
- **Uses compiler wrappers to:**
  - Add include, lib, and RPATH flags
  - Ensure that dependencies are found automatically
  - Load Cray modules (use right compiler/system deps)



Writing Packages - Versions and URLs

$REPO/packages/mvapich/package.py

```
class Mvapich2(Package):
    homepage = "http://mvapich.cse.ohio-state.edu/"
    url = "http://mvapich.cse.ohio-state.edu/download/mvapich/mv2/mvapich2-2.2rc2.tar.gz"

    version('2.2rc2', 'f9082ffc3b853ad1b908cf7f169aa878')
    version('2.2b',   '5651e8b7a72d7c77ca68da48f3a5d108')
    version('2.2a',   'b8ceb4fc5f5a97add9b3ff1b9cbe39d2')
    version('2.1',    '0095ceecb19bbb7fb262131cb9c2cdd6')
    version('2.0',    '9fbb68a4111a8b6338e476dc657388b4')
```

- Package downloads are hashed with md5
  - or SHA-1, SHA-256, SHA-512
- Download URLs can be automatically extrapolated from URL.
  - Extra options can be provided if Spack can't extrapolate URLs
- Options can also be provided to fetch from VCS repositories

Writing Packages – Variants and Dependencies

$REPO/packages/petsc/package.py

```
class Petsc(Package):
    variant('mpi',     default=True,  description='Activates MPI support')
    variant('complex', default=False, description='Build with complex numbers')
    variant('hdf5',    default=True,  description='Activates support for HDF5 (only parallel)')

    depends_on('blas')
    depends_on('python@2.6:2.7')
    depends_on('mpi', when='+mpi')
```

- Variants are named, have default values and help text
- Other packages can be dependencies
  - **when** clause provides conditional dependencies
  - Can depend on specific versions or other variants

Writing Packages – Build Recipes

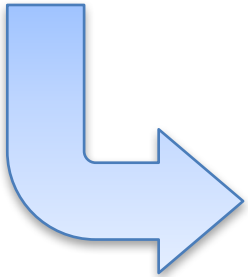
- Functions wrap common ops
  - cmake, configure, patch, make, …
  - **Executable** and **which** for new wrappers.
- Commands executed in clean environment
- Full Python functionality
  - Patch up source code
  - Make files and directories
  - Calculate flags
  - …

$REPO/packages/dyninst/package.py

```
def install(self, spec, prefix):
    with working_dir("build", create=True):
        cmake("..", *std_cmake_args)
        make()
        make("install")


@when('@:8.1')
def install(self, spec, prefix):
    configure("--prefix=" + prefix)
    make()
    make("install")
```

Create New Packages with spack create

```
$ spack create http://zlib.net/zlib-1.2.8.tar.gz
```



$REPO/packages/zlib/package.py

```
class Zlib(Package):
    # FIXME: Add a proper url for your package's homepage here.
    homepage = "http://www.example.com"
    url      = "http://zlib.net/zlib-1.2.8.tar.gz"
    version('1.2.8', '44d667c142d7cda120332623eab69f40')

    def install(self, spec, prefix):
        # FIXME: Modify the cmake line to suit your build system here.
```

- Spack create <url> will create a skeleton for a package
  - Spack reasons about URL, hash, version, build recipe.
- Spack edit <package> for subsequent changes

Hands-on Time

Deploying Spack at HPC Sites with Modules

What are module files?

- **Purpose of module files**
  - modify dynamically user's env
  - manage multiple versions of same library / application
  - minimal user interface
- **State of the art**
  - different file formats
  - different layouts
  - different tools
- **Spack support for module files**
  - TCL / Non-hierarchical layout
  - Lua / Hierarchical layout

	TCL Non-hierarchical	Lua Hierarchical
Generator name	`tcl`	`lmod`
Default folder	`share/spack/modules`	`share/spack/lmod`
Compatible tools	Env. modules LMod	LMod

How do module files look like?

```
$ module av

---  share/spack/modules/linux-Ubuntu14-x86_64 ---
autoconf-2.69-gcc-4.8-eud4m3w
ghostscript-9.18-gcc-4.8-5n627qp
lua-luaposix-33.4.0-gcc-4.8-s7lrtog
autoconf-2.69-gcc-6.1.0-wo3aeho
ghostscript-9.18-gcc-6.1.0-fsencrw
libpciaccess-0.13.4-clang-3.8.0-oqbf3i7
m4-1.4.17-clang-3.8.0-gstiykt
pkg-config-0.29.1-gcc-4.8-6zuabcp
automake-1.15-gcc-4.8-z42qh3r
gmp-6.1.1-gcc-4.8-xsezhyp
libpciaccess-0.13.4-gcc-4.8-62psbr2
m4-1.4.17-gcc-4.8-drmfctm
...
```

```
#%Module1.0
## Module file created by spack ...
##
## <full-spec>
##
module-whatis "autoconf @2.69"

proc ModulesHelp { } {
puts stderr " Autoconf -- system
configuration part of autotools"
}

prepend-path PATH "<full-prefix>/autoconf-
2.69-eud4m3weu6hfeu4o22xiwavnrarxjluo/bin"
prepend-path MANPATH ...
prepend-path CMAKE_PREFIX_PATH ...
```

Life cycle of module files within spack

```
def do_install(self, **kwargs):
    # Check if the package is already installed
    if self.installed:
        return
    # Recurse to install dependencies
    for x in self.dependencies():
        x.do_install(**kwargs)
    # Run pre-install hooks
    self.pre_install_hooks()
    # Real installation happens here
    self.install(self, self.spec, self.prefix)
    # Module files generation happens here
    self.post_install_hooks()
```

```
def do_uninstall(self, **kwargs):
    # Run pre-uninstall hooks
    self.pre_uninstall_hooks()

    # "Uninstall" package
    self.remove_prefix()

    # Deletion of module files
    # happens here
    self.post_install_hooks()
```

Package file API: package related content customization

```
def setup_dependent_environment(
    self, spack_env, run_env, extension_spec
):
    """Set up the compile and runtime environments
       for packages that depends on this one.
    """
    ...
       if extension_spec.package.extends(self.spec):
           run_env.prepend_path(
               'LUA_PATH',
               ';'.join(lua_patterns),
               separator=';'
           )
```

```
def setup_environment(
    self, spack_env, run_env
):
    """Set up the compile and runtime environments
       for a package.
    """
   ...
   ld_library_path = join_path(
       self.prefix, 'rlib', 'R', 'lib'
    )

    run_env.prepend_path(
        'LIBRARY_PATH', ld_library_path
    )
```

“modules.yaml”: site related customizations

```
modules:
  # Module generation needs to be activated
  # Every module type will have its own section
    enable :
      - tcl
      - lmod
    # Configurations common to all module types
    prefix_inspections:
      bin:
      - PATH
    tcl:
      # TCL specific section
    lmod:
      # LMOD specific section
```

Enable generation of tcl and lmod module files

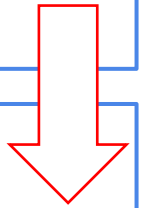
Options that are common to all types of module files

Options that are specific to tcl and lmod respectively

Inspection of package's installation prefix

```
modules:
      prefix_inspections:
        bin:
          - PATH
        man:
          - MANPATH
        share/man:
          - MANPATH
        lib:
          - LIBRARY_PATH
          - LD_LIBRARY_PATH
        ...
```

```
$ ls -l ${PREFIX_ROOT}/autoconf-2.69-eud4m3weu6h
    total 8
    drwxrwxr-x 2 mculpo mculpo 4096 ago 17 08:35 bin
    drwxrwxr-x 6 mculpo mculpo 4096 ago 17 08:35 share
```



```
prepend-path PATH "$PREFIX_ROOT/autoconf-2.69-
    eud4m3weu6h/bin"
prepend-path MANPATH "$PREFIX_ROOT/autoconf-2.69-
    eud4m3weu6h/share/man"
prepend-path CMAKE_PREFIX_PATH
    "$PREFIX_ROOT/autoconf-2.69-eud4m3weu6h"
```

Apply a rule to a set of packages: “anonymous specs”

```
modules:
     tcl:
       all:
         # Modifications that affect all packages
         # (always evaluated first)
       intel:
         # Modifications that affect all 'intel'
         # packages
       '^openmpi':
         # Modifications that affect all the packages
         # that depends on 'openmpi'
       '%gcc@4.4.7':
         # Modifications that affect all the packages
         # that are compiled with 'gcc@4.4.7'
```

anonymous specs

- specs possibly without root package
- used for constraint-matching purposes

Where are they used as a selection mechanism?

- module file suffixes
- prereq / autoload dependencies
- load external modules
- conflicts
- custom environment modifications

Refresh or remove module files: `spack module` command

```
$ spack module refresh -m tcl hdf5
    ==> You are about to regenerate tcl module files for:

    -- linux-Ubuntu14-x86_64 / gcc@4.8 --
    narq2au hdf5@1.10.0-patch1
    2qxlg4m hdf5@1.10.0-patch1

    -- linux-Ubuntu14-x86_64 / gcc@6.1.0 --
    o52kh5m hdf5@1.10.0-patch1

    ==> Do you want to proceed ? [y/n]
    y
    ==> Regenerating tcl module files
```

```
spack  module rm -m tcl hdf5
    ==> You are about to remove tcl module files the
    following specs:

    -- linux-Ubuntu14-x86_64 / gcc@4.8 --
    narq2au hdf5@1.10.0-patch1
    2qxlg4m hdf5@1.10.0-patch1

    -- linux-Ubuntu14-x86_64 / gcc@6.1.0 --
    o52kh5m hdf5@1.10.0-patch1

    ==> Do you want to proceed ? [y/n]
    y
```

Filter unwanted modifications to the environment

```
modules:
  enable:
    - tcl

  tcl:
    all:
      filter:
        # Exclude changes to any of these variables
        # in all packages, may be more selective
        environment_blacklist:
          - CPATH
          - LIBRARY_PATH
```

all:

- selects all packages

filter:

- reserved to gather filtering directives
- right now supports only what is shown

environment_blacklist:

- takes a list of env variables
- that won't be modified in module files

Prevent module files from being generated

```
modules:
    enable:
      - 'tcl'
    tcl:
      whitelist:
        - 'gcc'
        - 'llvm'
        - 'intel'
      blacklist:
        - '%gcc@4.4.7'
        - 'py-numpy'
        - 'py-scipy'
        - 'py-matplotlib'
        - 'py-pip'
```

Whitelisted entries take precedence over blacklisted ones

Blacklist modules using anonymous specs

```
==>     WHITELIST :
llvm@3.8.0%gcc@6.1.0+all_targets+clang+...
arch=linux-Ubuntu14-x86_64-gpwe4lu
[matches : llvm  ]

==>     WRITE :
llvm@3.8.0%gcc@6.1.0+all_targets+clang+...
   arch=linux-Ubuntu14-x86_64-gpwe4lu
[.../llvm-3.8.0-gcc-6.1.0-gpwe4lu]

==>     BLACKLIST :
lmod@6.4.5%gcc@4.8 arch=linux-Ubuntu14-x86_64-
   sth2wun
[matches : %gcc@4.8  ]
```

Change the naming of module files: control the hash length

```
modules:
     enable:
       - tcl
       - lmod
     tcl:
       hash_length : 7 # Default value
```

```
--- /modules/linux-Ubuntu14-x86_64 ---
autoconf-2.69-gcc-4.8-eud4m3w
ghostscript-9.18-gcc-4.8-5n627qp
libedit-3.1-gcc-6.1.0-hzefu25
lua-luaposix-33.4.0-gcc-4.8-s7lrtog
...
```

```
modules:
     enable:
       - tcl
       - lmod
     tcl:
       hash_length : 0
```

```
--- /modules/linux-Ubuntu14-x86_64 ---
autoconf-2.69-gcc-4.8
ghostscript-9.18-gcc-4.8
libedit-3.1-gcc-6.1.0
lua-luaposix-33.4.0-gcc-4.8
...
```

Change the naming of module files: add custom suffixes

```
modules:
   tcl:
     all:
       suffixes:
         # Add '-openmp' suffix if satisfies +openmp
         '+openmp': openmp
         # ... or if it satisfies ^fftw+openmp
         '^fftw+openmp': openmp
         # Add 'openblas' if depends on openblas
         '^openblas': openblas
     netlib-scalapack:
       suffixes:
         '^openmpi': openmpi
         '^mpich': mpich
```

suffixes:

- key: anonymous spec
- value: suffix to be added (if key matches)
- concatenate multiple matches

Change the naming of module files: set the naming scheme

```
modules:
  tcl:
    # In this directive you can use
    # either literals or tokens that
    # are understood by `Spec.format`
    naming_scheme: '${PACKAGE}/${VERSION}-
${COMPILERNAME}-${COMPILERVER}'
    all:
      # The same applies to the
      # list of conflicts
      conflict:
        - '${PACKAGE}'
```

```
--- /modules/linux-Ubuntu14-x86_64 ---
autoconf/2.69-gcc-4.8-eud4m3w
ghostscript/9.18-gcc-4.8-5n627qp
    libedit/3.1-gcc-6.1.0-hzefu25
...
```

naming_scheme:

- sets the layout for module files
- TCL / Non-hierarchical modules only

conflict:

- sets a conflict directive in the module file
- behavior varies depending on the tool

Add custom environment modifications

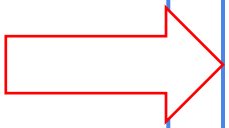
```
modules:
 tcl:
   all:
     environment:
       set: # Variable pointing to package prefix
         '${PACKAGE}_ROOT': '${PREFIX}'
   intel: # Customize intel package
     environment:
       set:
         'CC': icc
              ...
       prepend_path:
         'PATH': '<paths-to-be-prepended>'
         ...
```

environment:

- gathers all directives for env modifications
- key-value: *set, prepend_path, append_path*
- key only: *unset*
- tokens from `Spec.format` accepted in sub-directives

Autoloading dependencies in module files

```
modules:
  tcl:
    all:
      # Add code to load dependencies
      # automatically. Either 'direct'
      # or 'all' are allowed values.
      autoload: 'direct'
      # Load "literal" modules
      load:
        - 'intel'
```



```
...
if ![ is-loaded openmpi-2.0.0-gcc-4.8-r2nqvn ]
    puts stderr "Autoloading openmpi-2.0.0-gcc-4.8-r2nqvn"
    module load openmpi-2.0.0-gcc-4.8-r2nqvn
}

if ![ is-loaded intel ] {
    puts stderr "Autoloading intel"
    module load intel
}

conflict hdf5
conflict foo
```

Lua - Hierarchical module files: Core/Compiler/MPI hierarchy

```
modules:
  # Double colon is intentional:
  # it overrides the same keyword
  # when merging configuration files
  # at different scopes
  enable::
    - lmod
  lmod:
    # Specify which compilers are to be
    # considered Core compilers in the
    # hierarchy
    core_compilers:
      - 'gcc@4.8'
```

```
# Unuse the default TCL / Non-hierarchical modules
$ module unuse ${SPACK_ROOT}/share/spack/modules/<arch>

# Use the Core part of the Hierarchy
$ module use ${SPACK_ROOT}/share/spack/lmod/<arch>/Core
```

core_compilers:

- accepts a list of compilers
- anything '%gcc@4.8' generates a module in the Core part of the hierarchy
- usually only utilities and compilers in Core

Extend the hierarchy to other virtual providers [experimental]

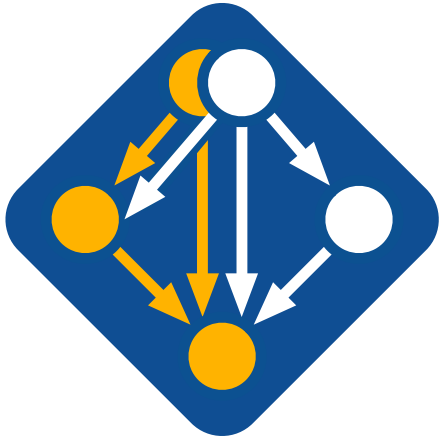
```
modules:
  enable::
    - lmod
  lmod:
    core_compilers:
      - 'gcc@4.8'
    # Any virtual package in principle
    # can be used. It will be treated
    # as MPI in the usual hierarchy
    hierarchical_scheme:
      - lapack
```

hierarchical_scheme:

- accepts a list of virtual packages
- added at the same level as MPI
- handles multiple virtual dependencies

Join the Spack community!

- Contributing packages to Spack is simple
  - Make packages on your own system
  - Send a pull request to Spack to let others use them
  - GitHub guide to pull requests: https://help.github.com/articles/creating-a-pull-request/
  - See contributor guide in the Spack repository
  - Spack is licensed under **LGPLv2.1**
- We want more than just packages
  - New features
  - New documentation
  - Any contribution can help the community
- Spack has a helpful online community
  - Typically happy to respond to GitHub issues
  - Active mailing list on Google Groups: https://groups.google.com/d/forum/spack
- We hope to make distributing & using HPC software easy.



http://github.com/LLNL/spack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