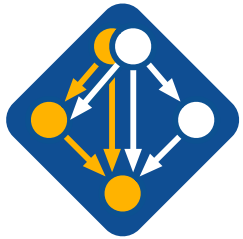

Managing HPC Software Complexity with Spack

Invited Tutorial
RIKEN R-CCS
April 23, 2019
Kobe, Japan

The most recent version of these slides can be found at:
https://spack.readthedocs.io/en/latest/tutorial.html

LLNL-PRES-806064

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Lawrence Livermore National Security, LLC

github.com/spack/spack

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.

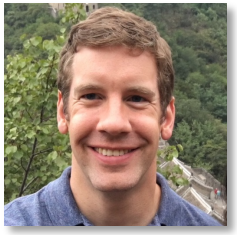
- Spack GitHub repository: **http://github.com/spack/spack**
- Spack Documentation: **http://spack.readthedocs.io**

Tweet at us!

@spackpm

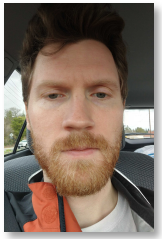
Tutorial Presenters

Lawrence Livermore National Laboratory



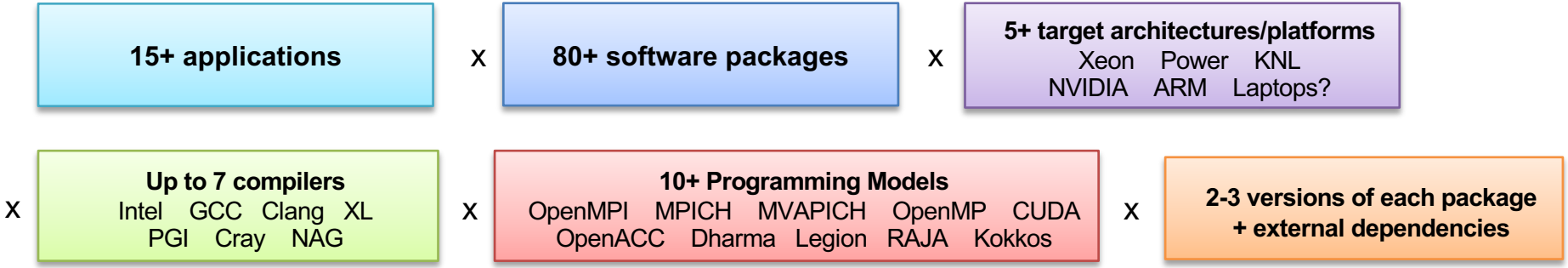
Todd Gamblin

Greg Becker



Peter Scheibel

The complexity of the exascale ecosystem threatens productivity.



= up to **1,260,000** combinations!

- Every application has its own stack of dependencies.
- Developers, users, and facilities dedicate (many) FTEs to building & porting.
- Often trade reuse and usability for performance.

We must make it easier to rely on others' software!

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.

Spack is a flexible package manager for HPC

- How to install Spack:

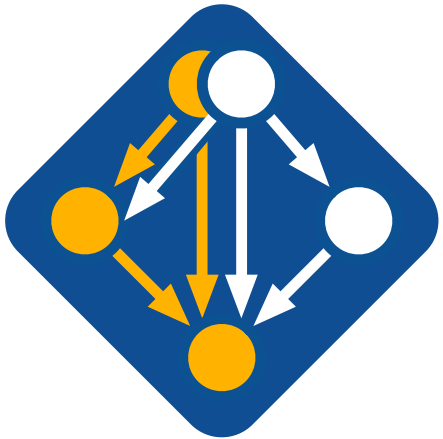
```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
```

- 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/spack/spack

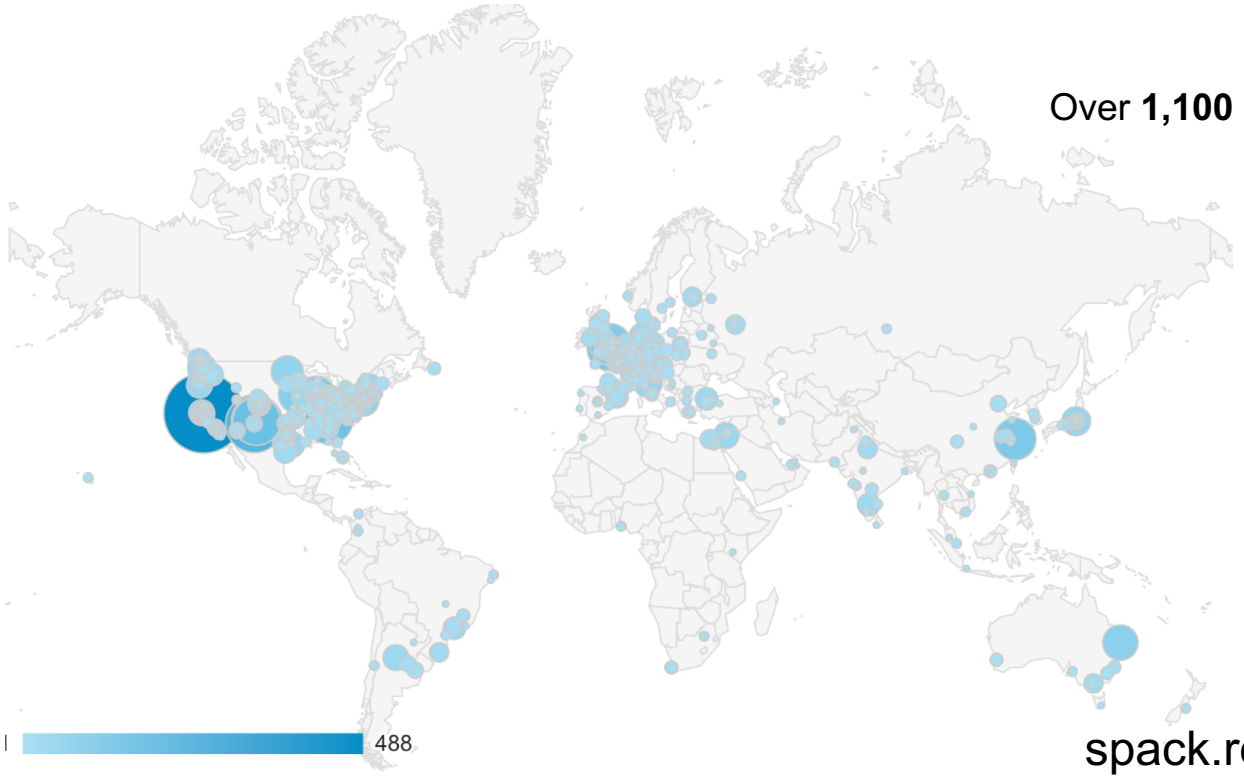
@spackpm

Who can use Spack?

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

Spack is used worldwide!

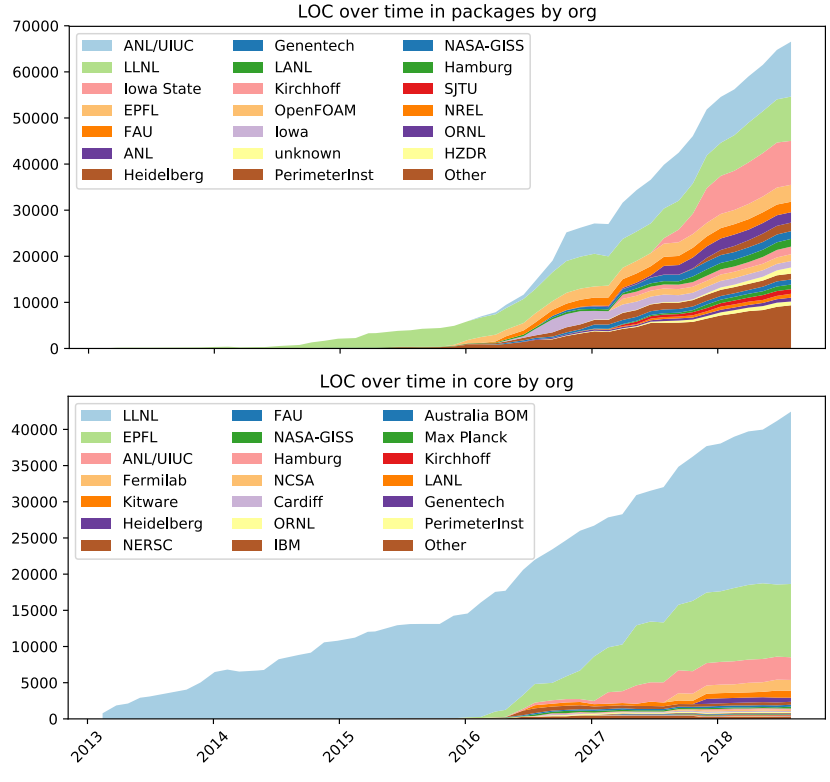


Over **3,100** software packages
Over **1,100** monthly active users (on docs site)

Over **380** contributors
from labs, academia, industry

Plot shows sessions on
spack.readthedocs.io for one month

Contributions to Spack continue to grow!



- In November 2015, LLNL provided most of the contributions to Spack
- Since then, we've gone from 300 to over 3,100 packages
- Most packages are from external contributors!
- Many contributions in core, as well.
- We are committed to sustaining Spack's open source ecosystem!

Spack v0.12.1 is the latest release

- **New stuff:**
  1. Spack environments (covered today)
  2. `spack.yaml` and `spack.lock` files for tracking dependencies (covered today)
  3. Custom configurations via command line (covered today)
  4. Better support for linking Python packages into view directories (pip in views)
  5. Support for uploading build logs to CDash
  6. Packages have more control over compiler flags via flag handlers
  7. Better support for module file generation
  8. Better support for Intel compilers, Intel MPI, etc.
  9. Many performance improvements, improved startup time

- Spack is now permissively licensed under **Apache-2.0 or MIT**
  - previously LGPL

- Over 2,900 packages (800 added since last year)
  - This is from November; over 3,100 in latest develop branch

What's on the road map?

- **Spack Stacks:** better support for facility deployment
  - Extension of environments to better support facility workflows
  - Ability to easily specify full facility software stack and module configuration
  - Build all of it at once with a single command!

- **Architecture-specific binaries**
  - Better provenance for builds
  - Better support for matching optimized binary packages to machines

- **Better concretization**
  - Spack's dependency resolution can hit snags
  - We need better support to enable features above

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

- **Conda** — https://conda.io
  - Very popular binary package manager for data science
  - Not targeted at HPC; generally unoptimized binaries

Tutorial Overview (times are estimates)

1.	For everyone:	**Welcome & Overview Talk**	9:00 - 9:50
		-- Break --	9:50 - 10:10
2.	For everyone:	**Spack Basics (hands on)**	10:10 - 10:55
3.	For everyone:	**Core Spack Concepts**	10:55 - 11:10
4.	For everyone:	**Configuration (hands-on)**	11:10 - 11:40
		-- Lunch --	11:40 - 1:30
5.	For packagers:	**Basics of Building and Linking**	1:30 – 1:40
6.	For packagers:	**Making your own Packages (hands on)**	1:40 - 2:40
7.	For everyone:	**Spack environments, spack.yaml/spack.lock (hands-on)**	2:40 - 3:00
		-- Break --	3:00 - 3:30
8.	For HPC centers:	**Generating Module Files with Spack (hands-on)**	3:30 - 4:15
9.	For packagers:	**Advanced Packaging (build systems)**	4:15 - 4:30
10.	For packagers:	**Advanced Packaging (virtual dependencies: BLAS/LAPACK/MPI)**	4:30 - 5:00

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 -g3"       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 2,900 packages now.

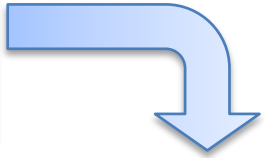
`spack find` shows what is installed

```
$ spack find
==> 103 installed packages.
-- linux-rhel6-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-rhel6-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-rhel6-x86_64 / intel@14.0.2 ---------------------------
hwloc@1.9  mpich@3.0.4  starpu@1.1.4

-- linux-rhel6-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-rhel6-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-rhel6-x86_64 / clang@3.4 --     -- linux-rhel6-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-rhel6-x86_64 / clang@3.4 -----      -- linux-rhel6-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:
    ...
```

Core Spack Concepts

Most existing tools do not support combinatorial versioning

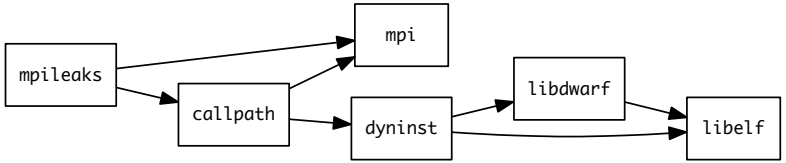
- Traditional binary package managers
  - RPM, yum, APT, yast, etc.
  - Designed to manage a single stack.
  - Install *one* version of each package in a single prefix (`/usr`).
  - Seamless upgrades to a *stable, well tested* stack

- 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



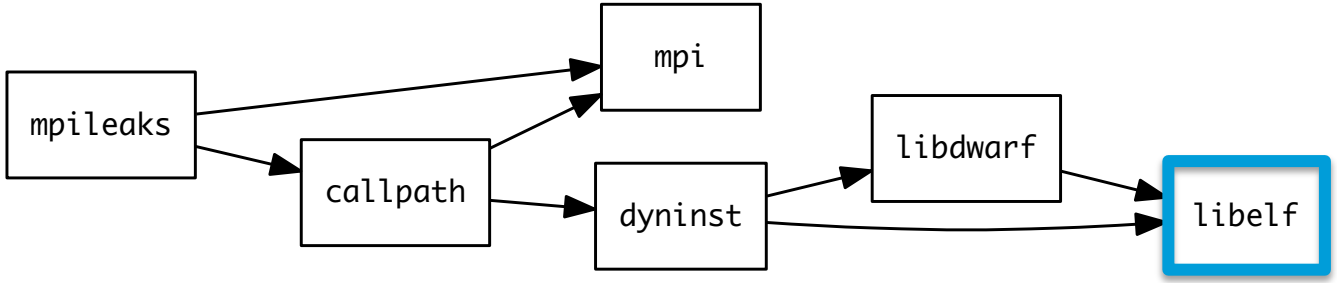
Installation Layout

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*

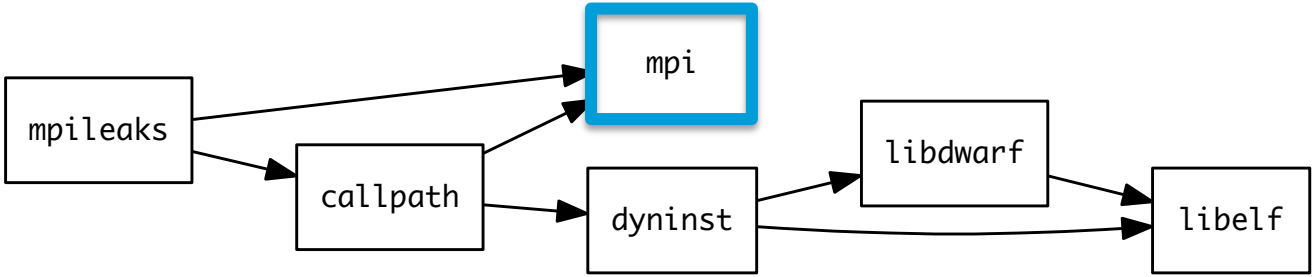
Spack Specs can constrain versions of dependencies




```
$ 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:
```

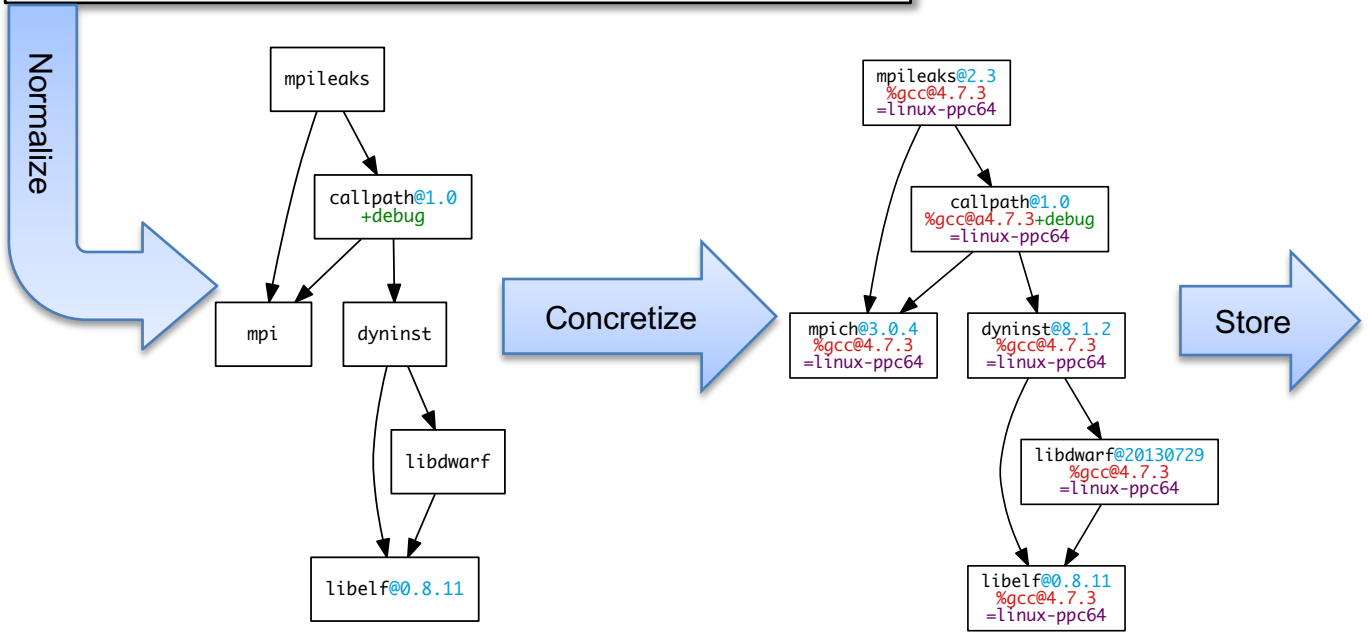
- Let Spack choose MPI implementation, as long as it provides MPI 2 interface:

```
$ 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

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
```

Extensions and Python Support

- Spack installs each package in its 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))
```

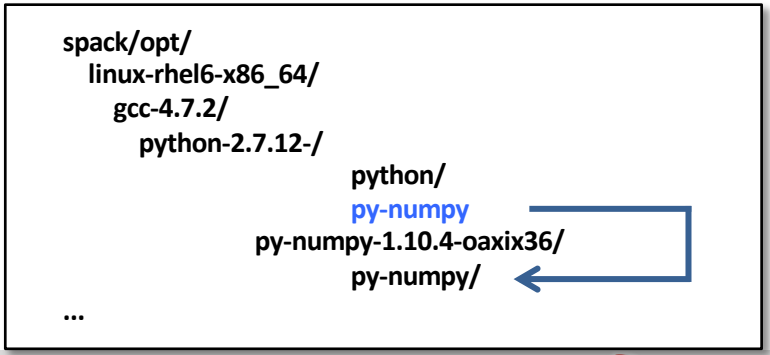
Spack extensions

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

```
spack/opt/
  linux-rhel6-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



Extensions must be activated into extendee

```
$ spack extensions python
==> python@2.7.12% gcc@4.9.3 ~tk~ucs4 arch=linux-rhel7-x86_64-i25k4oi
==> 118 extensions:
…
py-autopep8      py-docutils        py-mako            py-numpy        py-py2neo
…

==> 3 installed:
-- linux-rhel7-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-rhel7-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-rhel7-x86_64-i25k4oi
…
==> 1 currently activated:
-- linux-rhel7-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
```

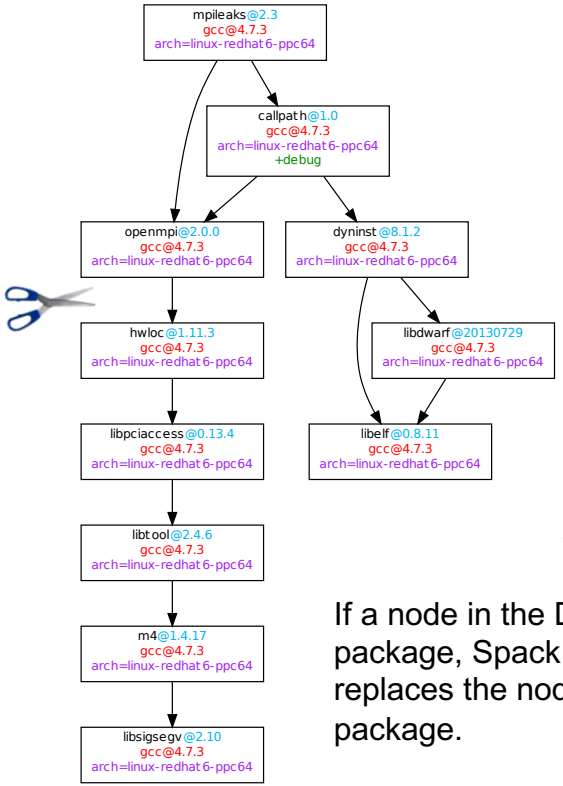
Building against externally installed software

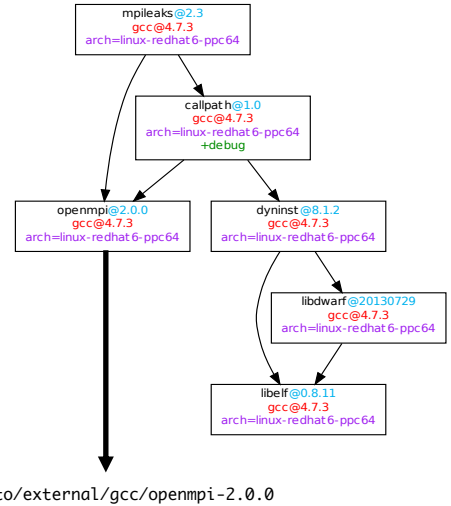
```
mpileaks ^callpath@1.0+debug
    ^openmpi ^libelf@0.8.11
```

packages.yaml

```
packages:
  mpi:
    buildable: False
  openmpi:
    buildable: False
    paths:
      openmpi@2.0.0 %gcc@4.7.3 arch=linux-rhel6-ppc64:
        /path/to/external/gcc/openmpi-2.0.0
      openmpi@1.10.3 %gcc@4.7.3 arch=linux-rhel6-ppc64:
        /path/to/external/gcc/openmpi-1.10.3
      openmpi@2.0.0 %intel@16.0.0 arch=linux-rhel6-ppc64:
        /path/to/external/intel/openmpi-2.0.0
      openmpi@1.10.3 %intel@16.0.0 arch=linux-rhel6-ppc64:
        /path/to/external/intel/openmpi-1.10.3
...
```

A user registers external packages with Spack.

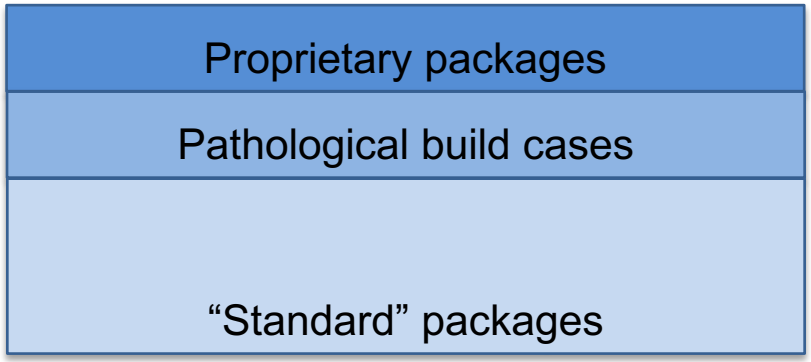




If a node in the DAG matches an registered external package, Spack prunes the DAG at that node and replaces the node with a reference to the external package.

Spack package repositories

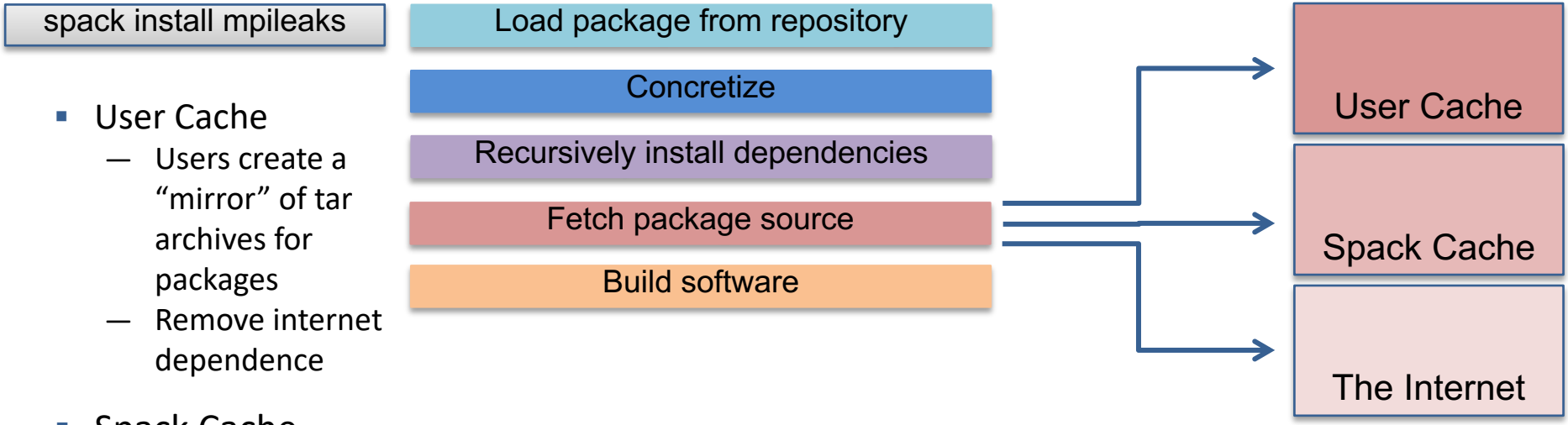
- Some packages can not be released publicly
- Some users have use cases that require ~~bizarre~~ custom builds
- Packaging issues should not prevent users from updating Spack
  - Solution: separate repositories
  - A repository is simply a directory of package files
- Spack supports external repositories that can be layered on top of the built-in packages
- Custom packages can depend on built-in packages (or packages in other repositories)



`my_repo`

`var/spack/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 custom compiler flags

```
$ spack install hdf5 cflags='-O3 –g –fast –fpack-struct'
```

- This installs HDF5 with the specified flags
  - Flags are injected via Spack's compiler wrappers (discussed later).
- Flags are propagated to dependencies automatically
  - Flags are included in the **DAG hash**
  - Each build with different flags 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

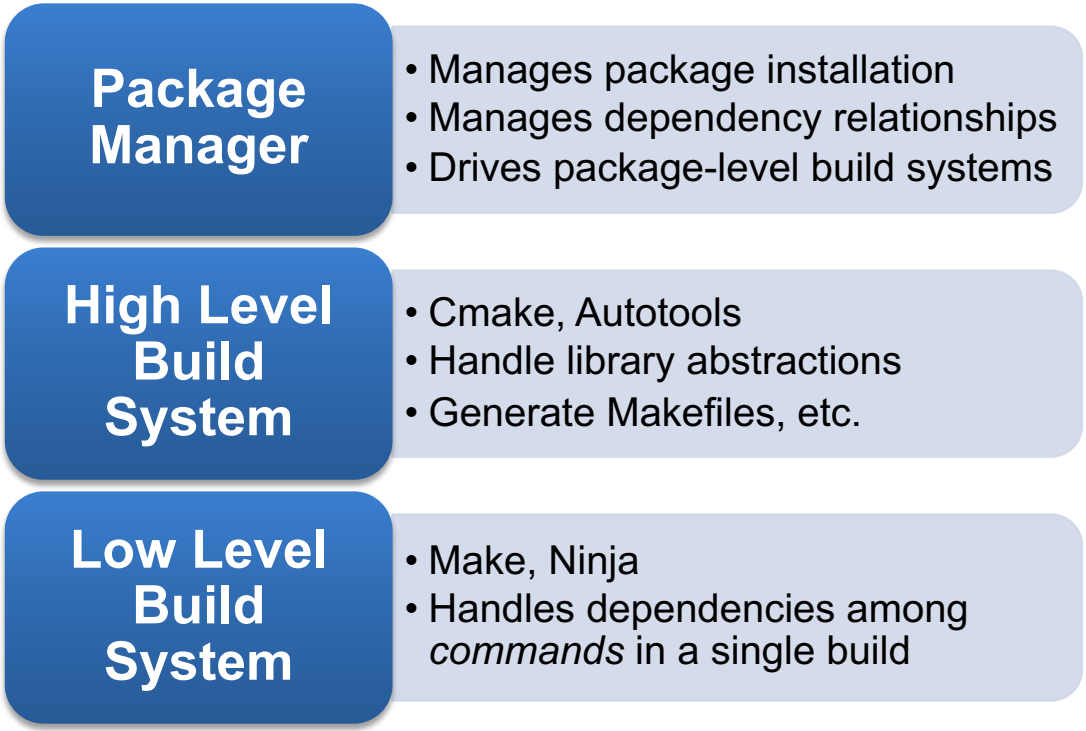
Hands-on Time: Configuration

Follow script at http://spack.rtfd.io
Under “Tutorial: Spack 101"

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

Spack has built-in support for these plus Waf, Perl, Python, and R

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		

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
```

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 source”
  - 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
```

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 **`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')
```

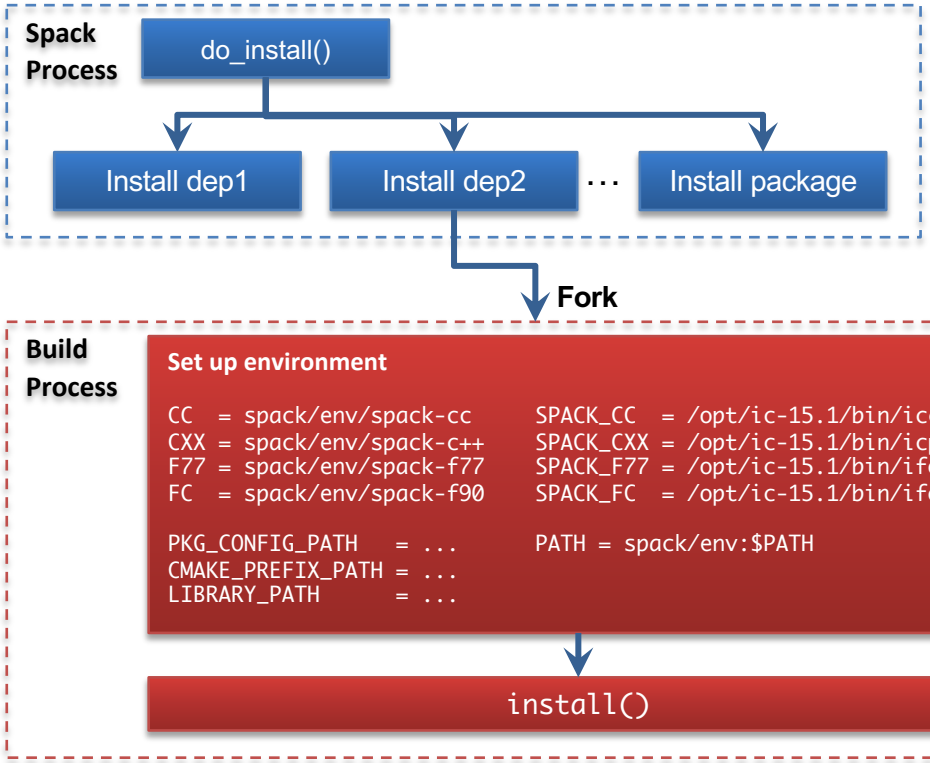
Spack packages are *templates* for builds

- Each package has one class
  - zlib for Intel compiler and zlib for GCC compiler are built with the same recipe.
- Can add conditional logic using spec syntax
  - Think of package as *translating* a concrete DAG to build instructions.
  - Dependencies are already built
  - No searching or testing; just do what the DAG says
- 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.

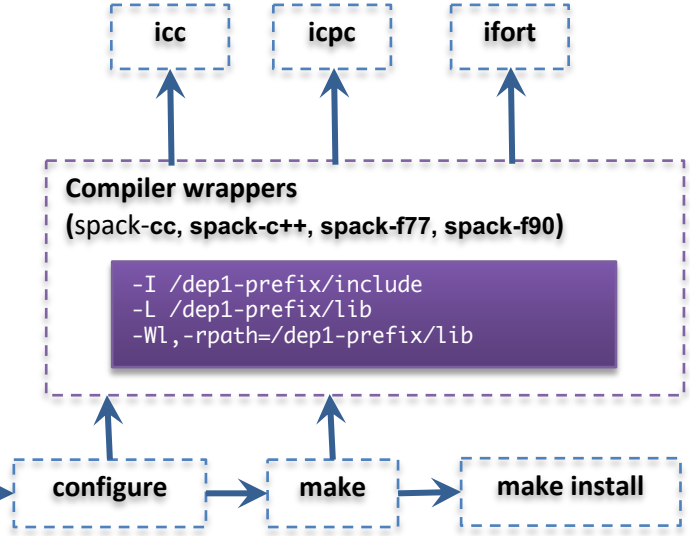
package.py

```
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/mvapich2/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')
```

- Package downloads are hashed with SHA-256 by default
  - Also supports SHA-512
  - Many packages still have legacy md5 checksums
- 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

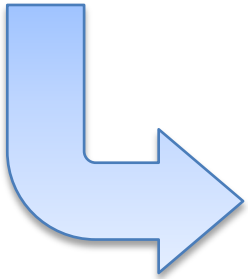
- Functions wrap common ops
  - cmake, configure, patch, make, …
  - **Executable** and **which** for new wrappers.
- Commands executed in clean environment
- Full Python functionality
  - Patch up source code
  - Make files and directories
  - Calculate flags
  - …

$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.
  - Generates boilerplate for Cmake, Makefile, autotools, Python, R, Waf, Perl
    - Not intended to completely write the package, but gets you 80% of the way there.
- spack edit <package> for subsequent changes

Hands-on Time: Creating Packages

Follow script at http://spack.rtfd.io
Under “Tutorial: Spack 101"

Hands-on Time: Environments

Follow script at http://spack.rtfd.io
Under “Tutorial: Spack 101"

Hands-on Time: Module Files

Follow script at http://spack.rtfd.io
Under “Tutorial: Spack 101"

Hands-on Time: Build Systems

Follow script at http://spack.rtfd.io
Under “Tutorial: Spack 101"

Build Systems

- Repeated patterns in packages
- Build System Subclasses
  - Provide convenience methods for ease of writing package files
  - Better control over the install phases
  - Sensible defaults
- Build Systems
  - Autotools
  - Cmake
  - Python
  - R
  - QMake
  - Waf
  - Scons
  - Octave
  - Intel
  - Perl
  - Aspell Dict
  - Cuda
  - Makefile

Optimize for the Common Case

CP2K

```
def install(self, spec, prefix):
      # Construct a proper filename for the architecture file
      cp2k_arch= '{0}-{1}'.format(spec.arch, spec.compiler)
      cp2k_ver = 'sopt' if '~mpi' in spec else 'popt'
      makefile_basename = '.'.join([cp2k_arch, cp2k_ver])
      makefile = join_path('arch', makefile_basename)

      # Write the custom makefile
      with open(makefile, 'w') as mkf:

          # Special Optimization flags
          optflags = {
               'gcc': [
                  '-O2',
                  '-mtune=native',
                  '-funroll-loops',
                  '-ffast-math',
                  '-ftree-vectorize',
                      ], 'intel': [
                        '-O2',
                        '-pc64',


      ...
```

mpileaks

```
def install(self, spec, prefix):
   configure("--prefix=" + prefix,
             "--with-adept-utils=" + spec['adeptutils'].prefix,
             "--with-callpath=" + spec['callpath'].prefix)
   make()
   make("install")
```

cups

```
def install(self, spec, prefix):
    configure("—prefix=" + prefix,
              "—enable-gnutls",
              "—with-components=core")
    make()
    make("install")
```

github.com/spack/spack

Common Build Patterns

gmp (Autotools)

```
./configure
make
make install
```

openJPEG (CMake)

```
cmake ..
make
make install
```

BSGenome (R)

```
R CMD INSTALL –l lib pkgs
```

pandas (setuptools)

```
python setup.py build
python setup.py install
```

Spack Build Systems Implement Common Patterns

```
class AutotoolsPackage(Package):

    def configure(self, spec, prefix):
        options = get_configure_options()
        with working_dir(self.build_directory):
            inspect.getmodule(self).configure(*options)

    def build(self, spec, prefix):
        with working_dir(self.build_directory):
            inspect.getmodule(self).make(*self.build_targets)

    def install(self, spec, prefix):
        with working_dir(self.build_directory):
            inspect.getmodule(self).make(*self.install_targets)
```

```
./configure [options]

make

make install
```

Spack Build Systems Implement Common Patterns

```
class CmakePackage(Package):

    def cmake(self, spec, prefix):
        options = get_cmake_args()
        with working_dir(self.build_directory):
            inspect.getmodule(self).cmake(*options)

    def build(self, spec, prefix):
        with working_dir(self.build_directory):
            inspect.getmodule(self).make(*self.build_targets)

    def install(self, spec, prefix):
        with working_dir(self.build_directory, create=True):
            inspect.getmodule(self).make(*self.install_targets)
```

```
cmake [options]

make

make install
```

Spack Build Systems Implement Common Patterns

```
class PythonPackage(Package):

    def build(self, spec, prefix):
        args = get_build_args()
        self.setup_py('build', *args)


    def install(self, spec, prefix):
       args = get_install_args()
       self.setup_py('install', *args)
```

```
python setup.py build
```

```
python setup.py install
```

Packagers Provide Minimal Details

- Spack provides sensible defaults to the build system and takes care of common patterns.
- Packagers only need to provide arguments (if any).

cups/package.py

```
class Cups(AutotoolsPackage):

    def configure_args(self):
        return ['--enable-gnutls', '--with-components=core']
```

hpx/package.py

```
class Hpx(CMakePackage):

def cmake_args(self):
    return ['-DHPX_BUILD_EXAMPLES=OFF', '-DHPX_MALLOC=system']
```

Example: AutotoolsPackage

```
from spack import *

class Gmp(Package):
   """GMP is a free library for arbitrary precision arithmetic"""

   homepage = "https://gmplib.org"
   url      = "https://gmplib.org/download/gmp/gmp-6.0.0a.tar.bz"

   version("6.1.1", '4c175f86e11eb32d8bf9872ca3a8e11d' )
   version("6.1.0", ''86ee6e54ebfc4a90b643a65e402c4048')
   version("6.0.0a", 'b7ff2d88cae7f8085bd5006096eed470')

   # dependencies ...

   def install(self, spec, prefix):
       configure("--prefix={0}".format(prefix),
                 "—enable-cxx")
       make()
       make("install")
```

```
from spack import *

class Gmp(AutotoolsPackage):
    """GMP is a free library for arbitrary precision arithmetic"""

    homepage = "https://gmplib.org"
    url      = "https://ftp.gnu.org/gnu/gmp/gmp-6.1.2.tar.bz2"

    version('6.1.1',  '4c175f86e11eb32d8bf9872ca3a8e11d')
    version('6.1.0',  '86ee6e54ebfc4a90b643a65e402c4048')
    version('6.0.0a', 'b7ff2d88cae7f8085bd5006096eed470')

    # dependencies ...

    def configure_args(self):
        return ['--enable-cxx']
```

Example: CMakePackage

```
from spack import *

class Openjpeg(Package):
    """OpenJPEG is an open-source JPEG 2000 codec."""

    homepage = "https://github.com/uclouvain/openjpeg"
    url = "https://github.com/uclouvain/version.2.1.tar.gz"

    version("2.1.0", '3e1c451c087f8462955426da38aa3b3d')
    version("2.0.1", '105876ed43ff7dbb2f90b41b5a43cfa5')
    version("2.0.0", 'cdf266530fee8af87454f15feb619609')

    def install(self, spec, prefix):
        cmake(".", "-DCMAKE_BUILD_TYPE=RelWithDebInfo")
        make()
        make("install")
```

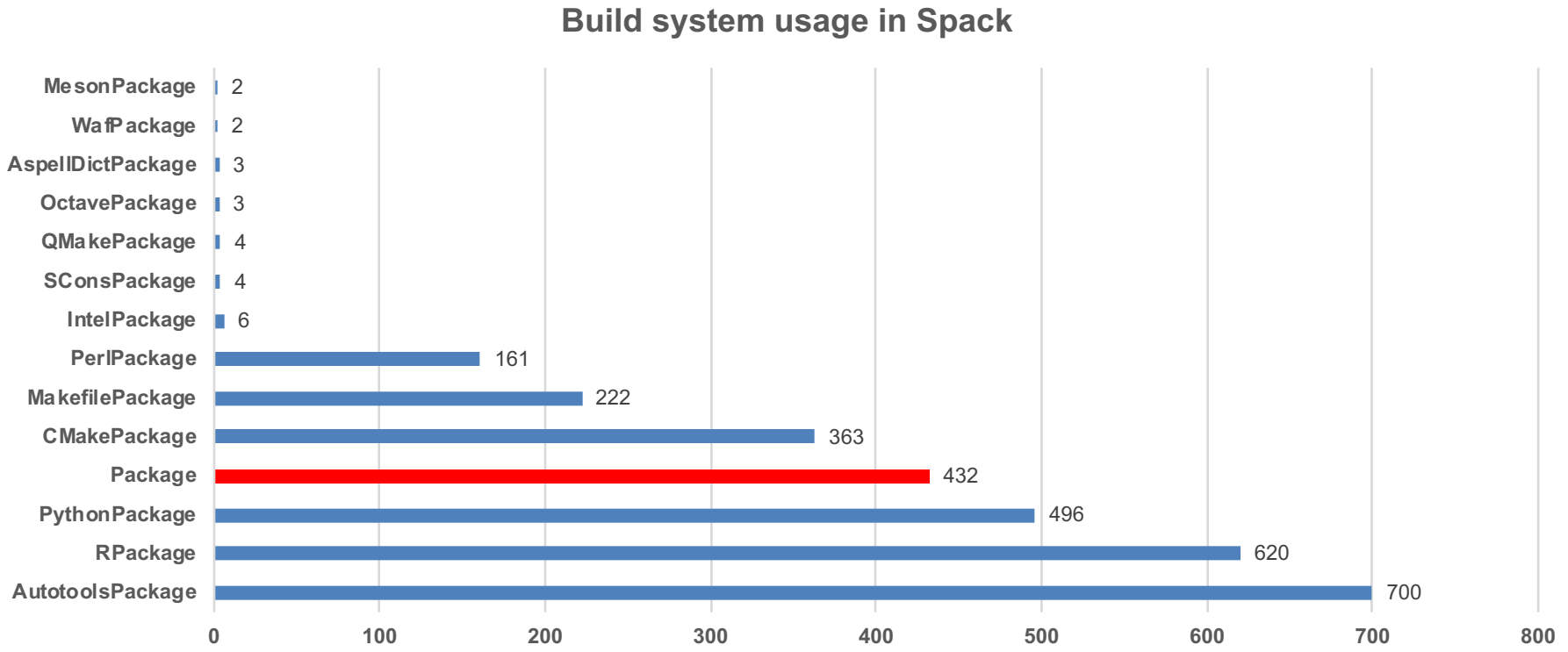
```
from spack import *

class Openjpeg(CMakePackage):
    """OpenJPEG is an open-source JPEG 2000 codec."""

    homepage = "https://github.com/uclouvain/openjpeg"
    url = "https://github.com/uclouvain/version.2.1.tar.gz

    version('2.1.0', '3e1c451c087f8462955426da38aa3b3d')
    version('2.0.1', '105876ed43ff7dbb2f90b41b5a43cfa5')
    version('2.0.0', ''cdf266530fee8af87454f15feb619609')

    def cmake_args(self):
        return ["-DCMAKE_BUILD_TYPE=RelWithDebInfo"]
```

Example: PythonPackage

```
from spack import *

class PyPandas(Package):
    """pandas is a Python package providing fast, flexible, and
      expressive data structures."""

    homepage = "http://pandas.pydata.org"
    url = "https://pypi.python.org/pandas-0.16.0.tar.gz"

    version('0.16.0', 'bfe311f05dc0c351f8955fbd1e296e73')
    version('0.16.1', 'fac4f25748f9610a3e00e765474bdea8')

    depends_on("py-dateutil", type=("build", "run")
    depends_on("py-numpy", type=("build", "run")
    depends_on("py-setuptools", type=("build", "run"))
    depends_on("py-cython", type=("build", "run"))
    depends_on("py-pytz", type=("build", "run"))
    depends_on("py-numexpr", type=("build", "run"))
    depends_on("py-bottleneck", type=("build", "run"))

    def install(self, spec, prefix):
        python("setup.py", "install", "--prefix=%s" % prefix)
```

```
from spack import *

class PyPandas(PythonPackage):
  """pandas is a Python package providing fast, flexible, and
    expressive data structures."""

    homepage = "http://pandas.pydata.org"
    url = "https://pypi.python.org/pandas-0.16.0.tar.gz"

    version('0.16.1', 'fac4f25748f9610a3e00e765474bdea8')
    version('0.16.0', 'bfe311f05dc0c351f8955fbd1e296e73')

    depends_on('py-dateutil', type=('build', 'run'))
    depends_on('py-numpy', type=('build', 'run'))
    depends_on('py-setuptools', type='build')
    depends_on('py-cython', type='build')
    depends_on('py-pytz', type=('build', 'run'))
    depends_on('py-numexpr', type=('build', 'run'))
    depends_on('py-bottleneck', type=('build', 'run'))
```

Total Packages: 3,018



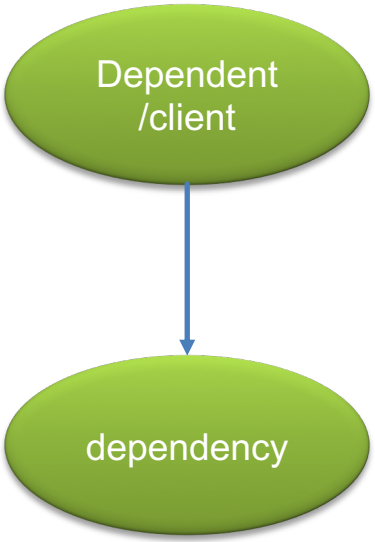
Simplified Package Writing

- Only need to provide arguments to configure, cmake, etc
- Reduce boilerplate code
- Can easily extend classes and add more behavior
- Can control install phases with finer granularity
  - spack configure
  - spack build
  - spack install

Advanced Packaging

Advanced Topics in Packaging

- Spack tries to automatically configure packages with information from dependencies
  - But there are many special cases. Often you need to retrieve details about dependencies to configure properly
- The goal is to answer the following questions that come up when writing package files:
  - How do I retrieve dependency libraries/headers when configuring my package?
  - How does spack help me configure my build-time environment?
- We'll start with a client view and then look at how we add functionality to packages to make it easier for dependents



Accessing Dependency Libraries

- Although Spack performs some work to help a build find libraries, you may need to explicitly specify dependency libraries during configuration
- Specs provide a ".libs" property which retrieves the individual library files provided by the package
- Accessing ".libs" for a virtual package will retrieve the libraries provided by the chosen implementation

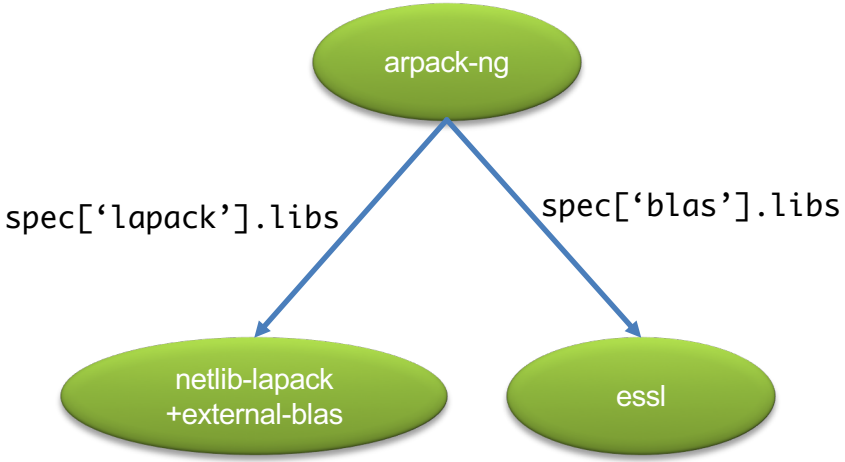
```
class ArpackNg(Package):
    depends_on('blas')
    depends_on('lapack')

    def install(self, spec, prefix):
        lapack_libs = spec['lapack'].libs.joined(';')
        blas_libs = spec['blas'].libs.joined(';')

        cmake(*[
            '-DLAPACK_LIBRARIES={0}'.format(lapack_libs),
            '-DBLAS_LIBRARIES={0}'.format(blas_libs)
        ], '.')
```

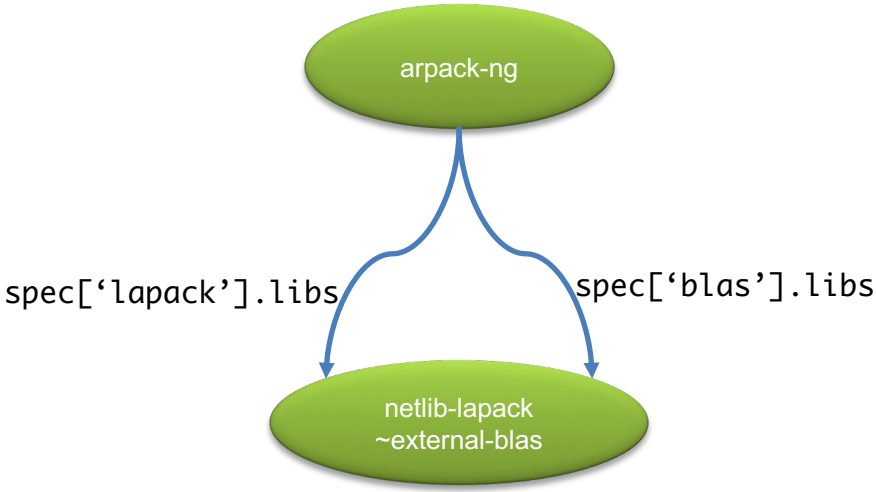
.libs.joined() expresses the list of libraries as a single string like "/…/lib1.so;/…/lib2.so" (e.g. for cmake)

.libs.search_flags expresses the libraries as linker arguments like "-L/…/libdir1/ -L/…/libdir2/" (e.g. as an argument to the compiler)

Accessing Dependency Libraries: Virtuals

- The client side code for accessing ".libs" is the same regardless of which implementation of blas is used
- As a client, you don't have to care whether 'blas' and 'lapack' are provided by the same implementation





Accessing Dependency Libraries: Subsets

- HDF5 builds many libraries, what if you just want the libraries for the high-level interface?
- You can qualify spec queries with additional parameters to specify a subset of libraries from a package

```
class Netcdf(AutotoolsPackage):
    depends_on('hdf5@1.8.9:+hl')

    def configure_args(self):
        LDFLAGS = []

        # Starting version 4.1.3, --with-hdf5= and other such configure options
        # are removed. Variables CPPFLAGS, LDFLAGS, and LD_LIBRARY_PATH must be
        # used instead.
        hdf5_hl = self.spec['hdf5:hl']
        LDFLAGS.append(hdf5_hl.libs.search_flags)
```

Since the hdf5 query was qualified with “hl”, only the libraries for hdf5’s high level interface will be retrieved

Accessing Dependency Headers

- Just like Spack tries to help build systems find libraries, it also tries to automate finding headers
- When that doesn't work and you need to explicitly configure dependency headers, the ".headers" property provides them

```
class Netcdf(AutotoolsPackage):
    depends_on('hdf5@1.8.9:+hl')

    def configure_args(self):
        LDFLAGS = []
        CPPFLAGS = []

        # Starting version 4.1.3, --with-hdf5= and other such configure options
        # are removed. Variables CPPFLAGS, LDFLAGS, and LD_LIBRARY_PATH must be
        # used instead.
        hdf5_hl = self.spec['hdf5:hl']
        CPPFLAGS.append(hdf5_hl.headers.cpp_flags)
        LDFLAGS.append(hdf5_hl.libs.search_flags)
```

headers.cpp_flags gives
`'-I/dir1 -I/dir2 -DMACRO_DEF_EXAMPLE'`

headers.include_flags gives
`'-I/dir1 -I/dir2' (e.g. for CFLAGS)`

Accessing Dependency Command

```
class Openbabel(CMakePackage):
    variant('python', default=True, description='Build Python bindings')
    extends('python', when='+python')
    depends_on('python', type=('build', 'run'), when='+python')

    def cmake_args(self):
        spec = self.spec
        args = []

        if '+python' in spec:
            args.extend([
                '-DPYTHON_BINDINGS=ON',
                '-DPYTHON_EXECUTABLE={0}'.format(spec['python'].command.path),
            ])
        else:
            args.append('-DPYTHON_BINDINGS=OFF')

        return args
```

- Some packages have a single well-known binary to run
- The ".command" spec property can retrieve it

Convenience Methods/Attributes from Dependencies

- Dependencies may provide shortcuts for invoking binaries
- For example: the Python package provides a globally-defined “python” function to run the python exe:

```
class PyScipy(PythonPackage):
    def install_test(self):
        python('-c', 'import scipy; scipy.test("full", verbose=2)')
```

- For example: all mpi implementations set the .mpicc attribute on their associated spec

```
class Elemental(CMakePackage):
    depends_on('mpi')

    def cmake_args(self):
        spec = self.spec
        args = [
            '-DCMAKE_C_COMPILER=%s' % spec['mpi'].mpicc
            ]
```

Environment Setup from Dependencies

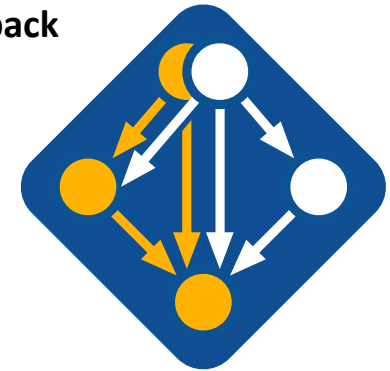
- If your package uses a python extension to build (e.g. setuptools), the Python package makes it available at build time with PYTHONPATH
- All MPI implementation packages make MPICC available in the environment at build for their dependents

Hands-on Time: Advanced Packaging

Follow script at http://spack.rtfd.io
Under “Tutorial: Spack 101"

Join the Spack community!

- There are lots of ways to get involved!
  - Contribute packages, documentation, or features at **github.com/spack/spack**
  - Contribute your configurations to **github.com/spack/spack-configs**
- Talk to us!
  - Join our **Google Group** (see GitHub repo for info)
  - Join our **Slack channel** (see GitHub repo for info)
  - Submit GitHub issues and talk to us!



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