The Spack Package Manager: Bringing Order to HPC Software Chaos

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http://bit.ly/spack-git

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.

HPC software is becoming increasingly complex

- Not much standardization in HPC: every machine/app has a different software stack

- Sites share unique hardware among teams with *very* different requirements
  - Users want to experiment with many exotic architectures, compilers, MPI versions
  - All of this is necessary to get the best ***performance***

- 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

We want an easy way to quickly sample the space, to build configurations on demand!

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.

How do HPC sites deal with combinatorial builds?

- HPC software is typically installed manually in a directory hierarchy.
  - Hierarchy often doesn't give all needed information about a build.
  - Sites can run out of unique directory names quickly.

Site	Naming Convention
LLNL	`/ usr / global / tools / $arch / $package / $version` `/ usr / local  / tools / $package-$compiler-$build-$version`
Oak Ridge	`/ $arch / $package / $version / $build`
TACC	`/ $compiler-$comp_version / $mpi / $mpi_version / $package / $version`

Environment modules can help, but are hard to get right.

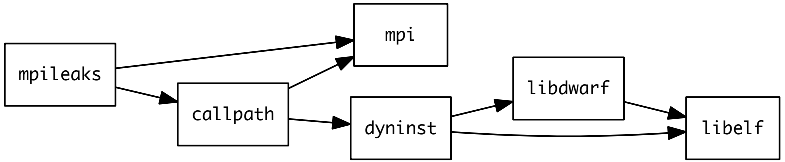
```
$ module avail

--------------------------- /opt/modules/modulefiles ----------------------------
acml-gnu/4.4              intel/12.0               mvapich2-pgi-ofa/1.7
acml-gnu_mp/4.4           intel/13.0               mvapich2-pgi-psm/1.7
acml-intel/4.4            intel/14.0(default)      mvapich2-pgi-shmem/1.7...

$ module load intel/13.0
$ module load mvapich2-pgi-shmem/1.7
```

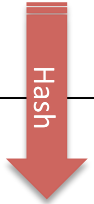
- **Advantages:**
  - Swap different library versions dynamically, in a shell.
  - Abstracts a lot of environment complexity from the user.

- **Disadvantages:**
  - Users must typically remember to load the same module that they built with.
    - Easy to load wrong module and break code.
  - Many sites and vendors deploy extremely brittle, inconsistent modules.
  - Module systems do not build software; they only change the environment.

Spack handles combinatorial software complexity.

Dependency DAG





Installation Layout

```
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 list` shows what packages are available

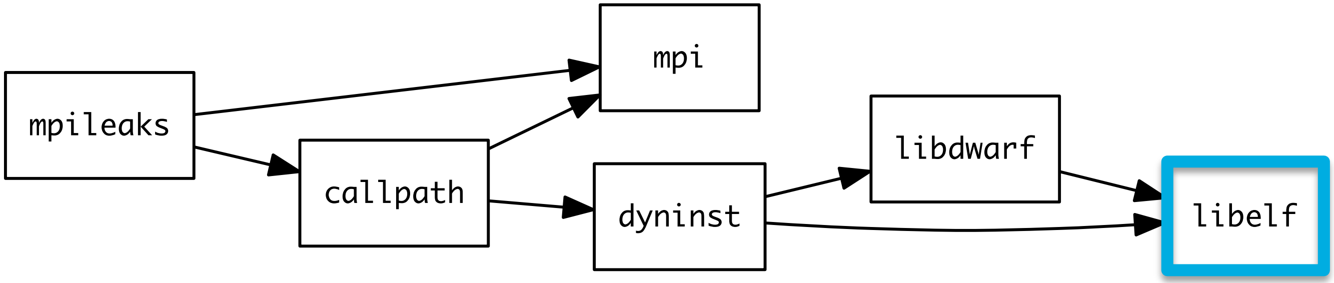
```
$ spack list
==> 243 packages.
activeharmony  coreutils        ghostscript  leveldb        libxslt   netcdf           ppl             py-pychecker         qt                   thrift
adept-utils    cppcheck         git          libarchive     llvm      netgauge         protobuf        py-pycparser         qthreads             tk
apex           cram             glib         libcircle      llvm-lld  netlib-blas      py-basemap      py-pyelftools        R                    tmux
arpack         cscope           glm          libdrm         lmdb      netlib-lapack    py-biopython    py-pygments          ravel                tmuxinator
asciidoc       cube             global       libdwarf       lua       nettle           py-cffi         py-pylint            readline             trilinos
atk            czmq             glog         libelf         lwgrp     ompss            py-cython       py-pypar             rose                 uncrustify
atlas          dbus             gmp          libevent       lwm2      ompt-openmp      py-dateutil     py-pyparsing         ruby                 util-linux
autoconf       docbook-xml      gnutls       libffi         matio     opari2           py-epydoc       py-pyqt              SAMRAI               vim
automaded      doxygen          gperf        libgcrypt      memaxes   openmpi          py-genders      py-pyside            samtools             vtk
automake       dri2proto        gperftools   libgpg-error   mesa      openssl          py-gnuplot      py-python-daemon     scalasca             wget
bear           dtcmp            graphlib     libjpeg-turbo  metis     otf              py-h5py         py-pytz              scorep               wx
bib2xhtml      dyninst          graphviz     libjson-c      Mitos     otf2             py-ipython      py-rpy2              scotch               wxpropgrid
binutils       elfutils         gtkplus      libmng         mpc       pango            py-libxml2      py-scientificpython  scr                  xcb-proto
bison          extrae           harfbuzz     libmonitor     mpe2      papi             py-lockfile     py-scikit-learn      silo                 xz
boost          exuberant-ctags  hdf5         libNBC         mpfr      paraver          py-mako         py-scipy             snappy               yasm
bowtie2        fish             hwloc        libpciaccess   mpibash   paraview         py-matplotlib   py-setuptools        spindle              zeromq
boxlib         flex             hypre        libpng         mpich     parmetis         py-mock         py-shiboken          sqlite               zlib
bzip2          flux             icu          libsodium      mpileaks  parpack          py-mpi4py       py-sip               stat                 zsh
cairo          fontconfig       icu4c        libtiff        mrnet     pcre             py-mx           py-six               sundials
callpath       freetype         ImageMagick  libtool        munge     petsc            py-nose         py-sphinx            swig
cblas          gasnet           isl          libunwind      muster    pidx             py-numpy        py-sympy             task
cgm            gcc              jdk          libuuid        mvapich2  pixman           py-pandas       py-virtualenv        taskd
clang          gdk-pixbuf       jpeg         libxcb         nasm      pkg-config       py-pexpect      py-yapf              tau
cloog          geos             launchmon    libxml2        ncdu      pmgr_collective  py-pil          python               tcl
cmake          gflags           lcms         libxshmfence   ncurses   postgresql       py-pmw          qhull                the_silver_searcher
```

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 =bgq                         = cross-compile
```

- 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!
- Syntax abstracts details in the common case
  - Makes parameterization by version, compiler, and options easy when necessary

Spack Specs can constrain versions of dependencies

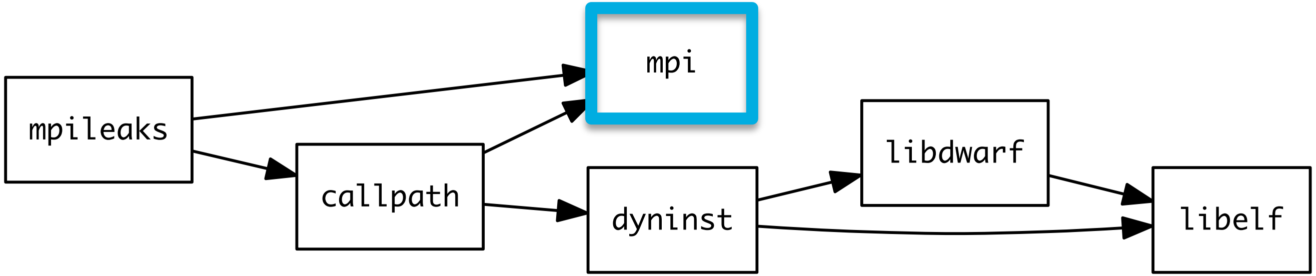



```
$ spack install mpileaks %intel@12.1 ^libelf@0.8.12
```

- 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 version, as long as it provides MPI 2 interface:

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

Spack packages are simple Python scripts.

```
from spack import *

class Dyninst(Package):
    """API for dynamic binary instrumentation."""

    homepage = "https://paradyn.org"

    version('8.2.1', 'abf60b7faabe7a2e', url="http://www.paradyn.org/release8.2/DyninstAPI-8.2.1.tgz")
    version('8.1.2', 'bf03b33375afa66f', url="http://www.paradyn.org/release8.1.2/DyninstAPI-8.1.2.tgz")
    version('8.1.1', 'd1a04e995b7aa709', url="http://www.paradyn.org/release8.1/DyninstAPI-8.1.1.tgz")

    depends_on("libelf")
    depends_on("libdwarf")
    depends_on("boost@1.42:")

    def install(self, spec, prefix):
        libelf = spec['libelf'].prefix
        libdwarf = spec['libdwarf'].prefix

        with working_dir('spack-build', create=True):
            cmake('..',
                  '-DBoost_INCLUDE_DIR=%s' % spec['boost'].prefix.include,
                  '-DBoost_LIBRARY_DIR=%s' % spec['boost'].prefix.lib,
                  '-DBoost_NO_SYSTEM_PATHS=TRUE'
                  *std_cmake_args)
            make()
            make("install")

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

Metadata

Versions and URLs

Dependencies

Patches, variants (not shown)

Commands for installation

Access build config through the *spec* parameter.

Dependencies in Spack may be optional.

- The user can define named *variants*:

```
variant("python", default=False, “Build with python support”)
depends_on("python", when="+python")
```

- And use them to install:

```
$ spack install vim +python
$ spack install vim –python
```

- Dependencies may be optional according to other conditions:
  e.g., gcc dependency on `mpc` from 4.5 on:

```
depends_on("mpc", when="@4.5:")
```

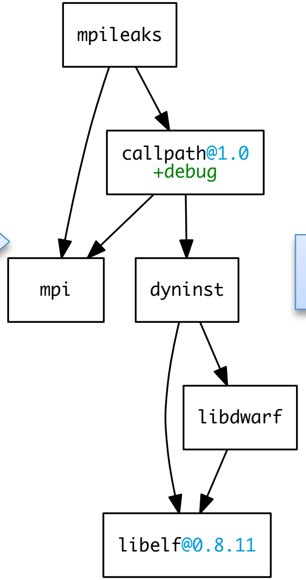
- DAG is not always complete before concretization!

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

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

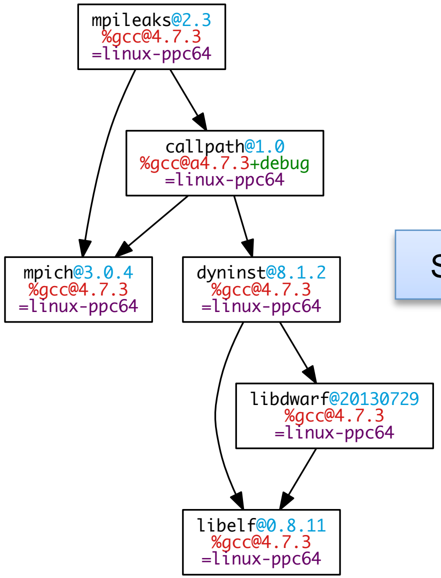
User input: *abstract* spec with some constraints

Normalize



Abstract, normalized spec with some dependencies.

Concretize



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

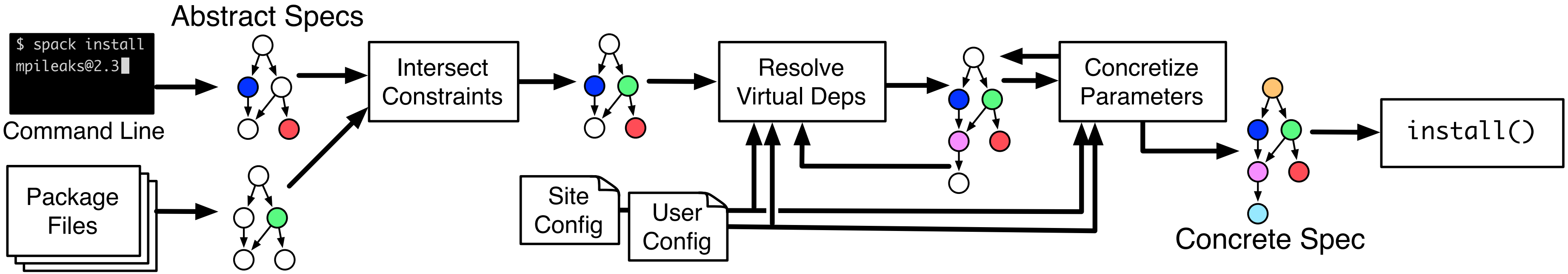
Store

spec.yaml


```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
...
```

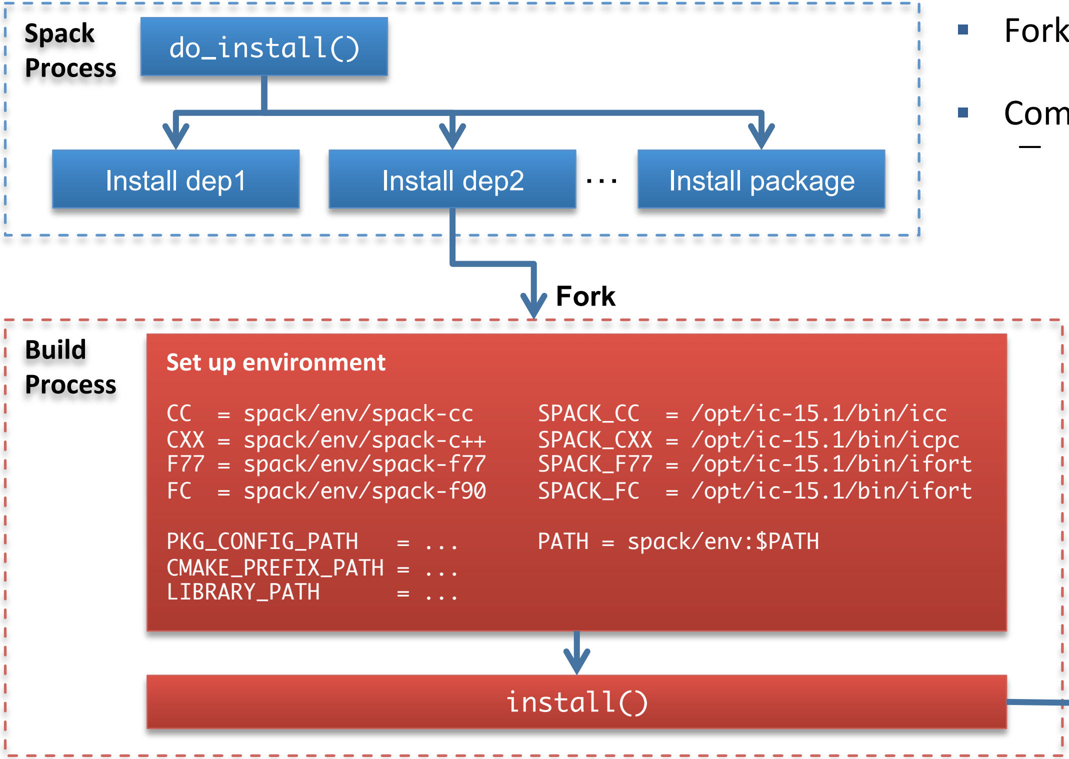

Detailed provenance is stored with the installed package

Concretization algorithm iterates until the DAG does not change.

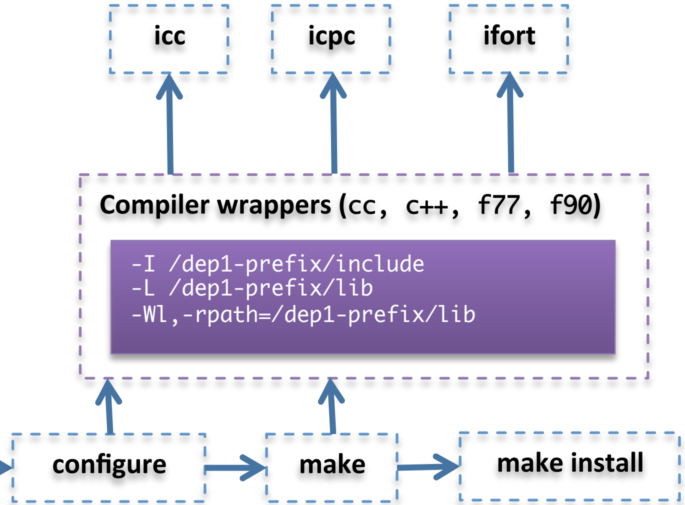


- When underspecified, concretization chooses a value based on user/site preferences.
- Concretization must add new dependencies in response to constraint updates.
- Current algorithm is greedy, will not backtrack once a decision is made.
  - Can fail to find a build that satisfies a query, but has not happened for current packages.
  - Really needs a full constraint solver (coming soon!)

Spack builds each package in its own compilation environment

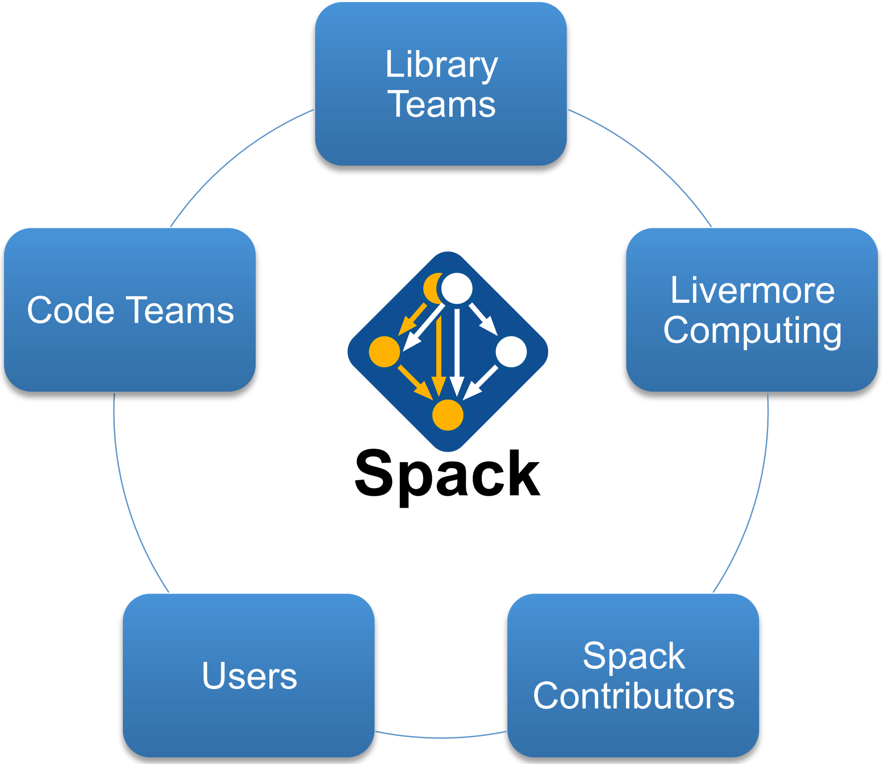


- Forking build process isolates environment for each build.
- Compiler wrappers add include, lib, and RPATH flags
  - Ensure that dependencies are found automatically



Build automation allows tedious work to be leveraged.

- Spack enables teams to share work.
  - Archives common library build recipes.
  - Prevents duplication of build effort.
  - We can share builds among LC, code teams, and users
- Patches allow rapid deployment of bug fixes
  - App team porting a library may not own its repo.
  - Library teams may not have time to fix issues quickly.
  - Code teams can fix quickly, then feed back changes.
- Python allowed quick adoption by code teams.
  - Many app developers already know Python
  - Spec syntax provides extra expressiveness.



Use Case 1: Managing combinatorial installations

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

-- linux-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-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
```

- spack find shows all installed configurations
  - Multiple versions of same package are ok.
- Packages are divided by architecture/compiler.
- Spack also generates module files.
  - Don't *have* to use them.

Using the Spec syntax, Spack can restrict queries

```
$ spack find mpich
==> 5 installed packages.
-- linux-x86_64 / gcc@4.4.7 --------------------------------
mpich@3.0.4

-- linux-x86_64 / gcc@4.8.2 --------------------------------
mpich@3.0.4

-- linux-x86_64 / intel@14.0.2 -----------------------------
mpich@3.0.4

-- linux-x86_64 / intel@15.0.0 -----------------------------
mpich@3.0.4

-- linux-x86_64 / intel@15.0.1 -----------------------------
mpich@3.0.4
```

- Querying by package name retrieves a subset

The Spec syntax doubles as a query language to allow refinement of searches.

```
$ spack find libelf
==> 5 installed packages.
-- linux-x86_64 / gcc@4.4.7 ---------
libelf@0.8.12  libelf@0.8.13

-- linux-x86_64 / gcc@4.8.2 ---------
libelf@0.8.13

-- linux-x86_64 / intel@15.0.0 ------
libelf@0.8.13

-- linux-x86_64 / intel@15.0.1 ------
libelf@0.8.13
```

Query versions of `libelf` package

List only those built with Intel compiler.

```
$ spack find libelf %intel
-- linux-x86_64 / intel@15.0.0 ------
libelf@0.8.13

-- linux-x86_64 / intel@15.0.1 ------
libelf@0.8.13
```

```
$ spack find libelf %intel@15.0.1
-- linux-x86_64 / intel@15.0.1 ------
libelf@0.8.13
```

Restrict to specific compiler version

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, and dependency versions may differ between builds.

Use Case 2: Package Views for HPC Center Installs

```
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/
    ...
```

```
/software/
    linux-x86_64/
        gcc-4.7.2/
            mvapich-1.9/
                mpileaks-1.1/
        intel-14.1/
            mvapich-1.9/
                hdf5-1.8.15/
    bgq/
        xl-12.1/
            ibm-mpi/
                hdf5-1-8.16/
    ...
```

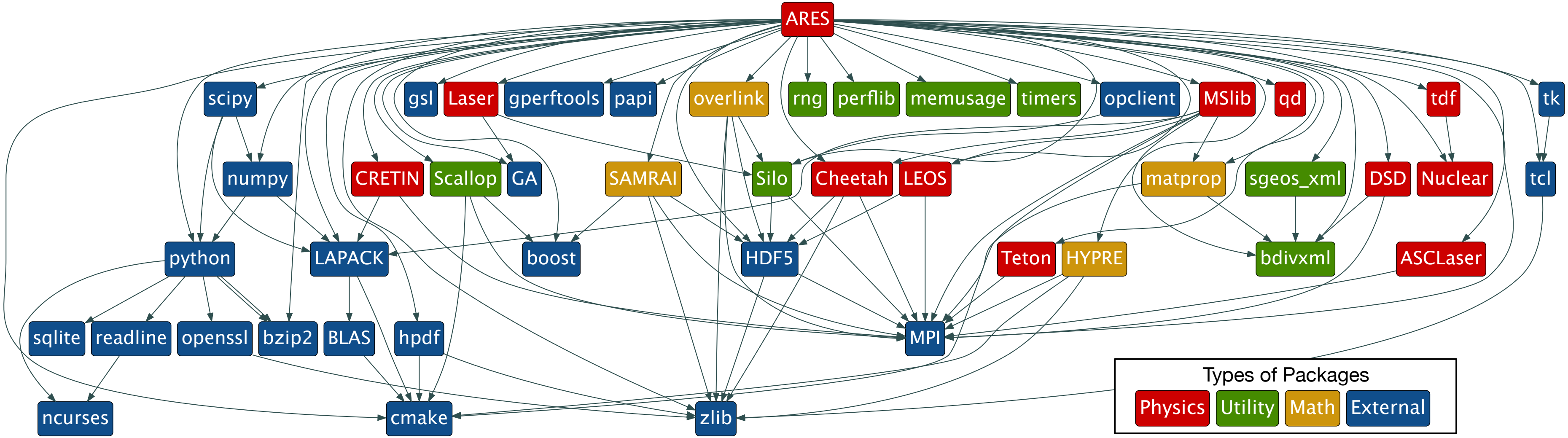
- Many users like to navigate a readable directory hierarchy
  - Spack's combinatorial package space is large and can be hard to navigate
- Spack can generate a coarser tree *view* of symbolic links
  - View is a projection from the higher-dimensional Spack space
  - Some names may conflict, but spec syntax allows us to express *preferences* to guide view creation.

Use case 3: Python and other interpreted languages

```
$ spack install python@2.7.10
==> Building python.
==> Successfully installed python.
  Fetch: 5.01s.  Build: 97.16s.  Total: 103.17s.
[+] /home/gamblin2/spack/opt/spack/linux-x86_64/gcc-4.9.2/python-2.7.10-y2zr767

$ spack extensions python@2.7.10
==> python@2.7.10%gcc@4.9.2=linux-x86_64-y2zr767
==> 49 extensions:
geos          py-h5py       py-numpy      py-pypar              py-setuptools
libxml2       py-ipython    py-pandas     py-pyparsing          py-shiboken
py-basemap    py-libxml2    py-pexpect    py-pyqt               py-sip
py-biopython  py-lockfile   py-pil        py-pyside             py-six
py-cffi       py-mako       py-pmw        py-python-daemon      py-sphinx
py-cython     py-matplotlib py-pychecker  py-pytz               py-sympy
py-dateutil   py-mock       py-pycparser  py-rpy2               py-virtualenv
py-epydoc     py-mpi4py     py-pyelftools py-scientificpython   py-yapf
py-genders    py-mx         py-pygments   py-scikit-learn       thrift
py-gnuplot    py-nose       py-pylint     py-scipy

==> 3 installed:
-- linux-x86_64 / gcc@4.9.2 -----------------------------------
py-nose@1.3.6  py-numpy@1.9.2  py-setuptools@18.1

==> None currently activated.

$ spack activate py-numpy
==> Activated extension py-setuptools-18.1-gcc-4.9.2-ru7w3lx
==> Activated extension py-nose-1.3.6-gcc-4.9.2-vudjpwc
==> Activated extension py-numpy-1.9.2-gcc@4.9.2-45hjazt

$ spack deactivate -a py-numpy
==> Deactivated extension py-numpy-1.9.2-gcc@4.9.2-45hjazt
==> Deactivated extension py-nose-1.3.6-gcc-4.9.2-vudjpwc
==> Deactivated extension py-setuptools-18.1-gcc-4.9.2-ru7w3lx
```

- Many interpreted languages have their own mechanisms for modules, e.g.:
  - Require installation into interpreter prefix
  - Breaks combinatorial versioning
- Spack installs each Python package in its own prefix
- “Activating” links an extension into the interpreter directory on demand
  - Supports .egg, merging .pth files
  - Mechanism is extensible to other languages
  - Similar to virtualenv, but Spack allows much more build customization.

Use case 4: Spack is being adopted by LLNL code teams



- ARES is a 1, 2, and 3-D radiation hydrodynamics code
- Spack automates the build of ARES and all of its dependencies
  - The ARES configuration shown above has 47 dependencies

ARES has used Spack to test 36 different configurations

- Nightly builds of ARES are shown at right.

  4 code versions:
  - **(C)**urrent Production
  - **(P)**revious Production
  - **(L)**ite
  - **(D)**evelopment

	Linux			*BG/Q*	*Cray XE6*
	MVAPICH	*MVAPICH2*	*OpenMPI*	*BG/Q MPI*	*Cray MPI*
GCC	C P L D			C P L D	
Intel 14	C P L D				
Intel 15	C P L D	D			
PGI		D	C P L D		C L D
Clang	C P L D			C L D	
XL				C P L D	

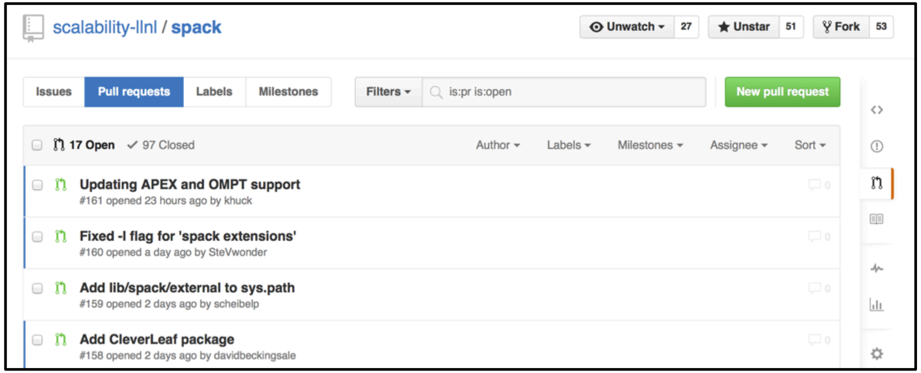
- Learning Spack and porting all libraries took a single developer 2 months, half-time.
- Previously, the team was only able to automate its development Linux builds.
  - Spack enabled thorough testing of many more configurations
  - Testing with Spack helped find compilation issues when using Clang compiler.
- Spack is helping the team port to LANL's new Trinity (Cray XC-40) machine

Related work

- **OS package managers**
  - Don’t handle combinatorial builds
  - Single compiler; single stable version of pkg.
  - Allow smooth upgrades and predictable user experience.
- **Gentoo Prefix**
  - Based on Gentoo Linux: builds from source, installs into common prefix
  - Common prefix limits multi-compiler and multi-version support.
- **Nix (from NixOS)**
  - Allows many separate configurations
  - Packages are cryptographically hashed.
  - Multi-compiler, version support is limited
  - No virtual dependencies
  - No syntax for parameterization.
- **EasyBuild** (HPC U. Ghent)
  - Requires a file per configuration of software
    - 3300 config files for 600 packages (!)
  - Limited command line interface
  - Limited DAG and dependency analysis
- **Hashdist**
  - No spec syntax, more package file and profile editing required, less composable.
  - Compiler/architecture support is limited
- **Smithy** (ORNL), **Maali** (Pawsey)
  - No dependency management; only install automation

Many new feature developments are in progress

- Current:
  - Lmod hierarchy integration
  - External dependencies
    - Autodetect system MPI and other packages
  - Custom compiler flag injection
  - XML Test output (JUnit)
    - Each dependency exposed as test case
  - Better Cray environment integration



http://bit.ly/spack-git

- Planned:
  - Use compiler wrappers to apply tools to large codes
    - Klocwork, thread sanitizers, etc.
  - Dependencies on compiler features (C++11, lambdas, OpenMP versions)
  - Automatic ABI checking & upgrading

The Spack project is growing rapidly.

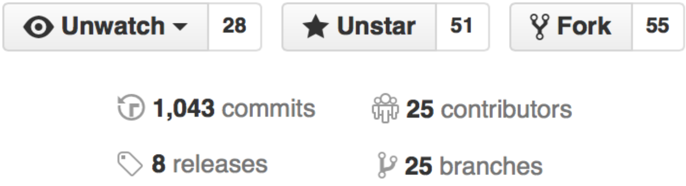
- Spack is flexible enough for HPC needs
  - From single users of small clusters, to
    large code teams on top-10 supercomputers.

- Spack is starting to be used in production at LLNL
  - Build, test, and deployment by code teams.
  - Tools, libraries, and Python at Livermore Computing.
  - Build research projects for students, postdocs.

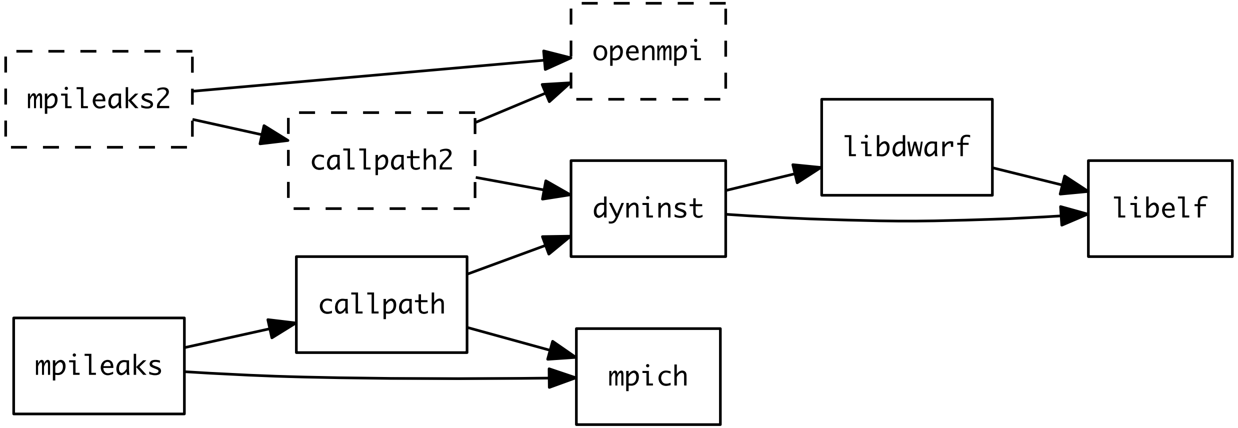
- Spack has a rapidly growing external community.
  - NERSC is working with LLNL on Cray support for Cori.
  - Argonne/IIT cluster challenge project.
  - Kitware contributing ParaView builds & features.
  - INRIA using Spack to package MORSE numerical software
  - Users and contributors at EPFL, U. Oregon, Sandia, LANL.

Get Spack!

https://bit.ly/spack-git

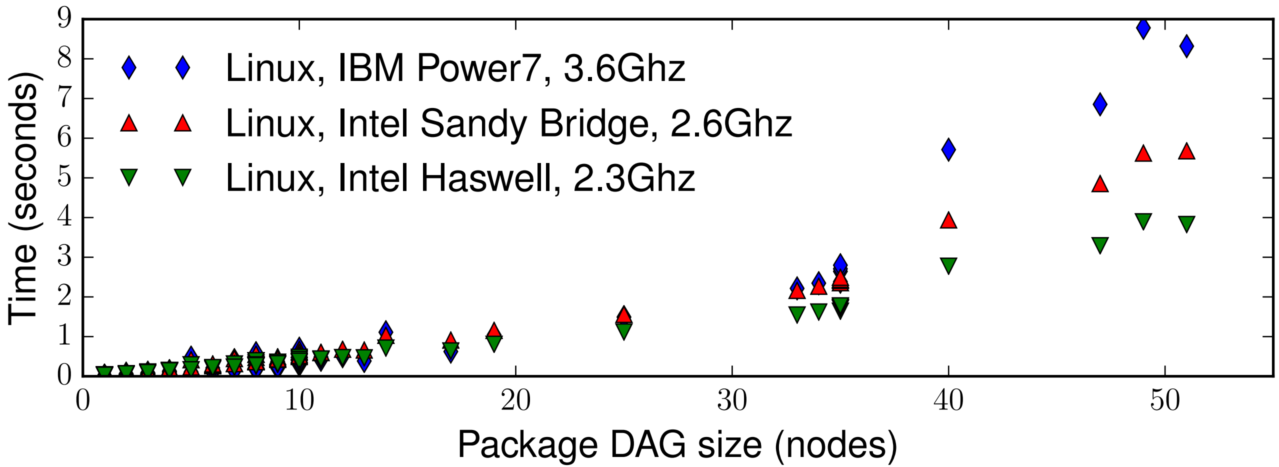


Builds share as many dependencies as possible



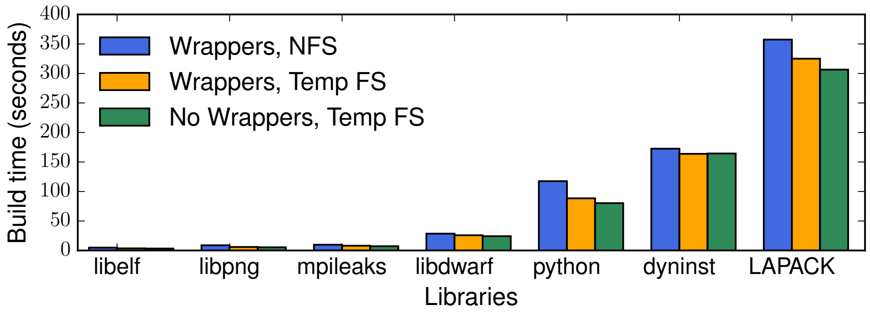
- May add space overhead compared to an LD_LIBRARY_PATH based system
- Safer than modules or LD_LIBRARY_PATH since the user cannot get deps wrong
  - Installations always run they way they are built.
- Above shows mpileaks built with mpich, then openmpi
  - Dotted packages must be rebuilt.

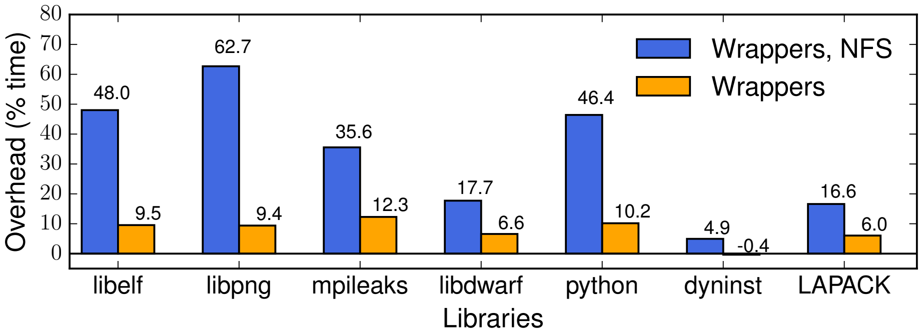
Concretization time is reasonable even for large packages.



- Fixed-point concretization algorithm scales quadratically
- Spack graphs are small, even for the largest packages
  - Thousands of dependencies are unlikely, even in multi-million line code bases.
  - Using a proper constraint solver will speed this up.

Compiler wrappers incur some overhead





- Extra script layer requires some overhead
- Spack's decision to build in tmp filesystem improves more than script overhead hurts.

Future direction: Dependencies on compiler features

- Profusion of new compiler features frequently causes build confusion:
  - C++11 feature support
  - OpenMP language levels
  - CUDA compute capabilities

- Spack could allow packages to request compiler features like dependencies:

```
require('cxx11-lambda')
require('openmp@4:')
```

- Spack could:
  1. Ensure that a compiler with these features is used
  2. Ensure consistency among compiler runtimes in the same DAG.

Future direction: Compiler wrappers for tools

- **Automatically adding source instrumentation to large codes is difficult**
  - Usually requires a lot of effort, especially if libraries need to be instrumented as well.

- **Spack could expose Klocwork, Scalasca, TAU, etc. as "secondary" compiler wrappers.**
  - Allow user to build many instrumented versions of large codes, with many different compilers:

```
spack install application@3.3 %gcc@4.7.3 +tau
```

- **Spack packages provide a general interface to build details.**

- **LLNL PRUNER debugging tool is looking into this.**
  - Uses LLVM for instrumentation; needs to cover all libraries.

Future direction: Automatic ABI checking

- **We're starting to add the ability to link to external packages**
  - Vendor MPI
  - OS-provided packages that are costly to rebuild

- **External packages are already built, so:**
  - Can't always match compiler exactly
  - Can't always match dependency versions exactly

- **Need to guarantee that the RPATH'd version of a library is compatible with one that an external package was built with**
  - Allows more builds to succeed
  - Potentially violates ABI compatibility

- **Looking into using `libabigail` from RedHat to do some checking at install time.**