Spack: A Package Manager for HPC

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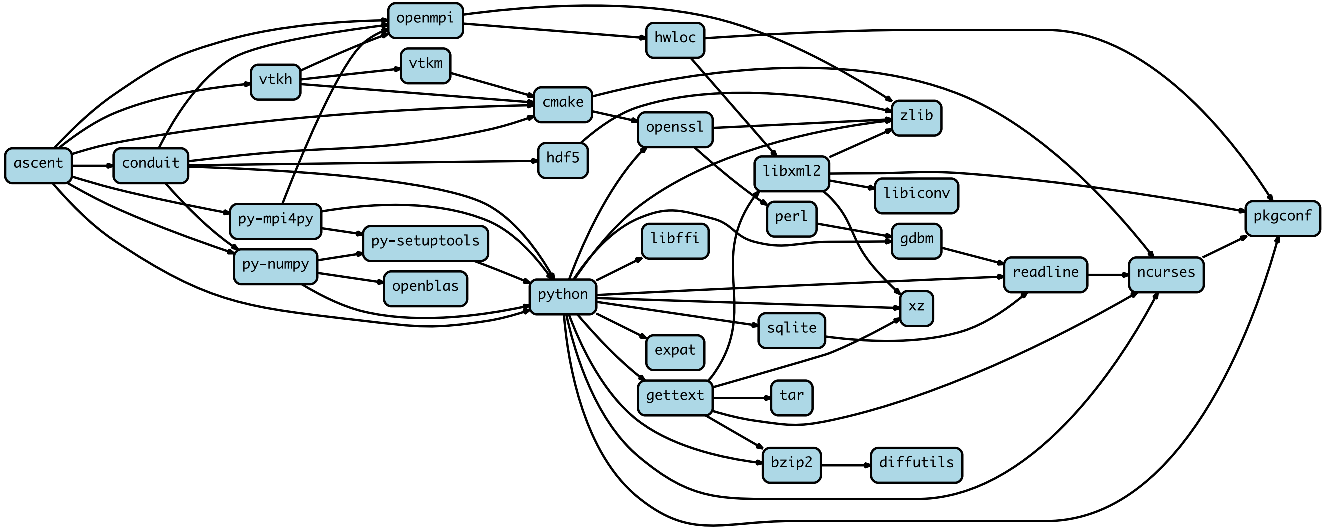
github.com/spack/spack

Software complexity in HPC is growing



Ascent: Lightweight, in-situ, many-core visualization and analysis

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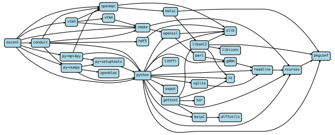

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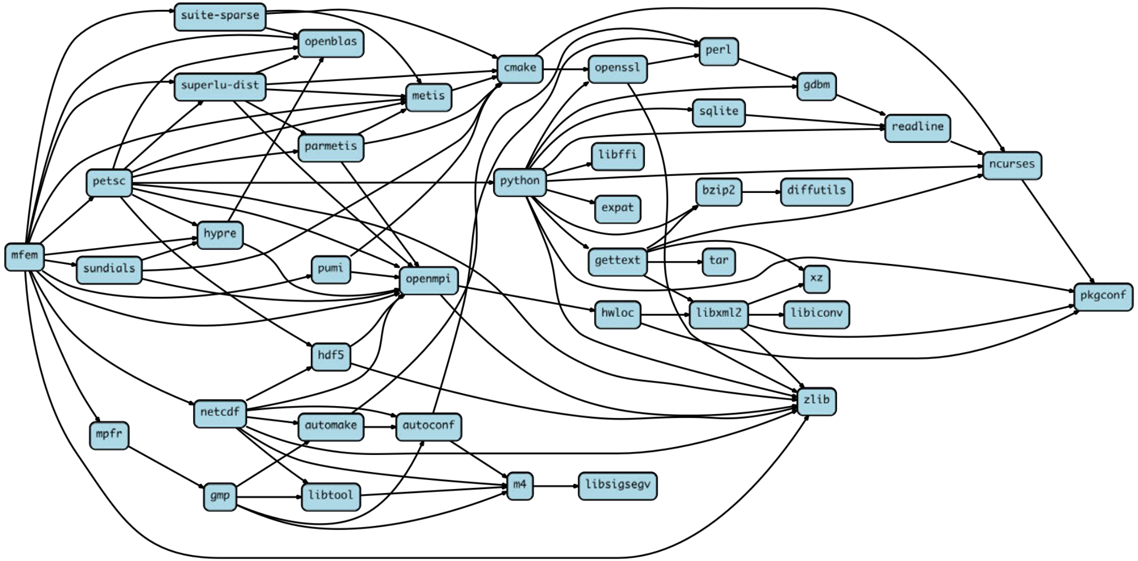

MFEM: Arbitrary high-order finite elements

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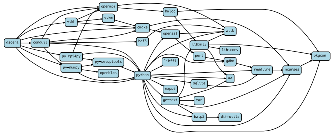

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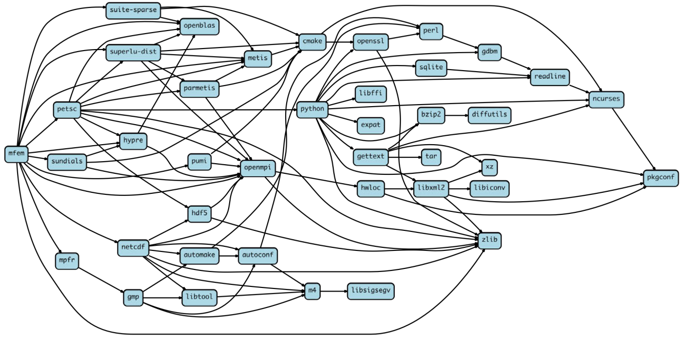
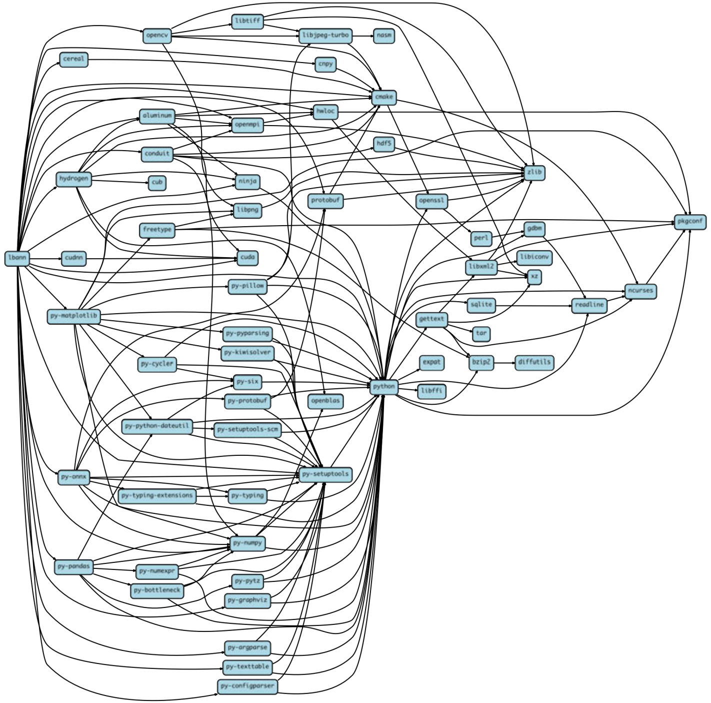


MFEM: Arbitrary high-order finite elements



LBANN: Artificial Neural Nets for HPC

The complexity of the exascale ecosystem threatens productivity.

15+ applications x **80+ software packages** x **5+ target architectures/platforms**
Xeon Power ~~KNL~~
NVIDIA ARM Laptops?

x **Up to 7 compilers**
Intel GCC Clang XL
PGI Cray NAG

x **10+ Programming Models**
OpenMPI MPICH MVAPICH OpenMP CUDA
OpenACC Dharma Legion RAJA Kokkos

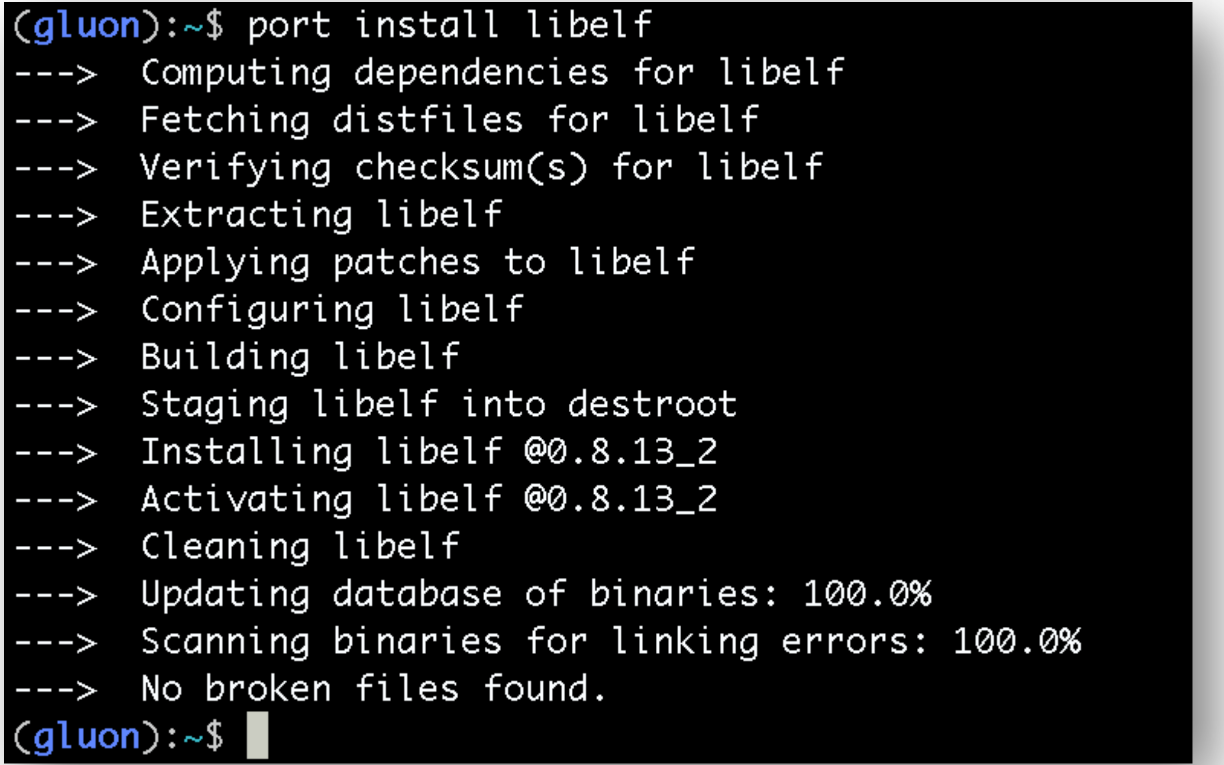
x **2-3 versions of each package + external dependencies**

= 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!

How to install software on a Mac laptop, circa 2013



```
(gluon):~$ port install libelf
--->  Computing dependencies for libelf
--->  Fetching distfiles for libelf
--->  Verifying checksum(s) for libelf
--->  Extracting libelf
--->  Applying patches to libelf
--->  Configuring libelf
--->  Building libelf
--->  Staging libelf into destroot
--->  Installing libelf @0.8.13_2
--->  Activating libelf @0.8.13_2
--->  Cleaning libelf
--->  Updating database of binaries: 100.0%
--->  Scanning binaries for linking errors: 100.0%
--->  No broken files found.
(gluon):~$ 
```

How to install software on a supercomputer

1. Download all 16 tarballs you need
2. Start building!

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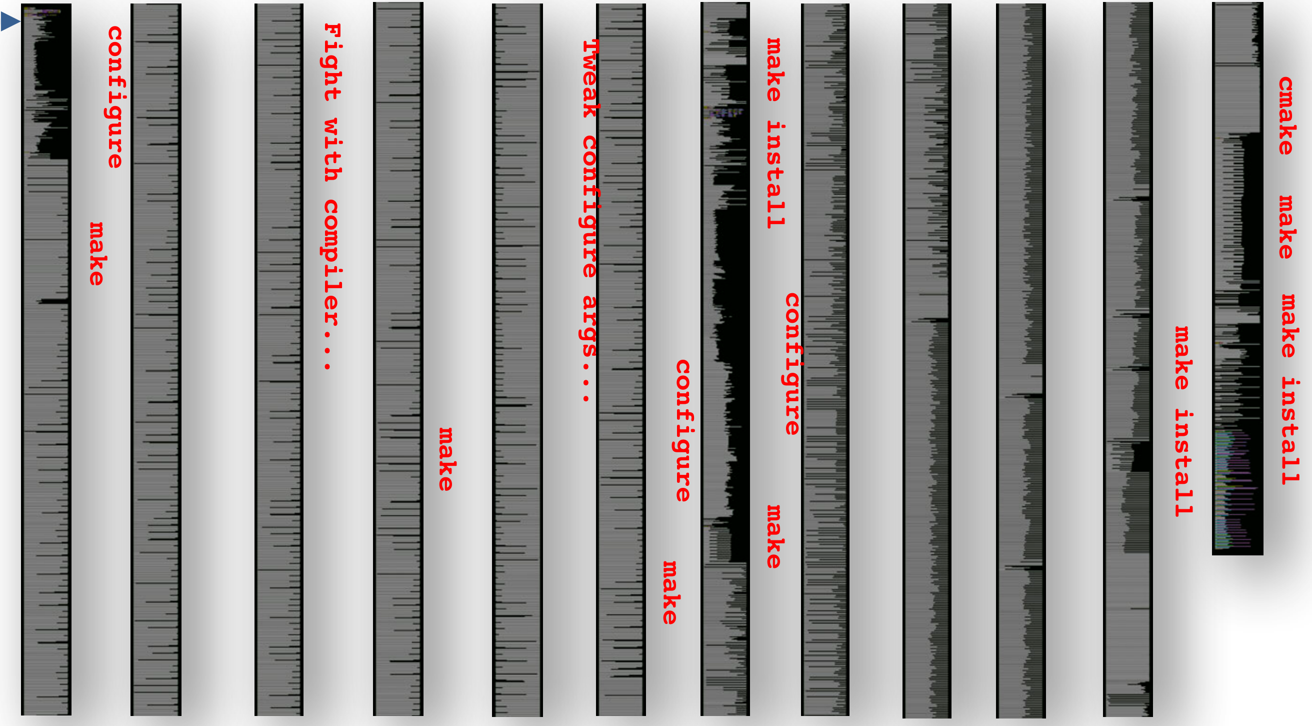
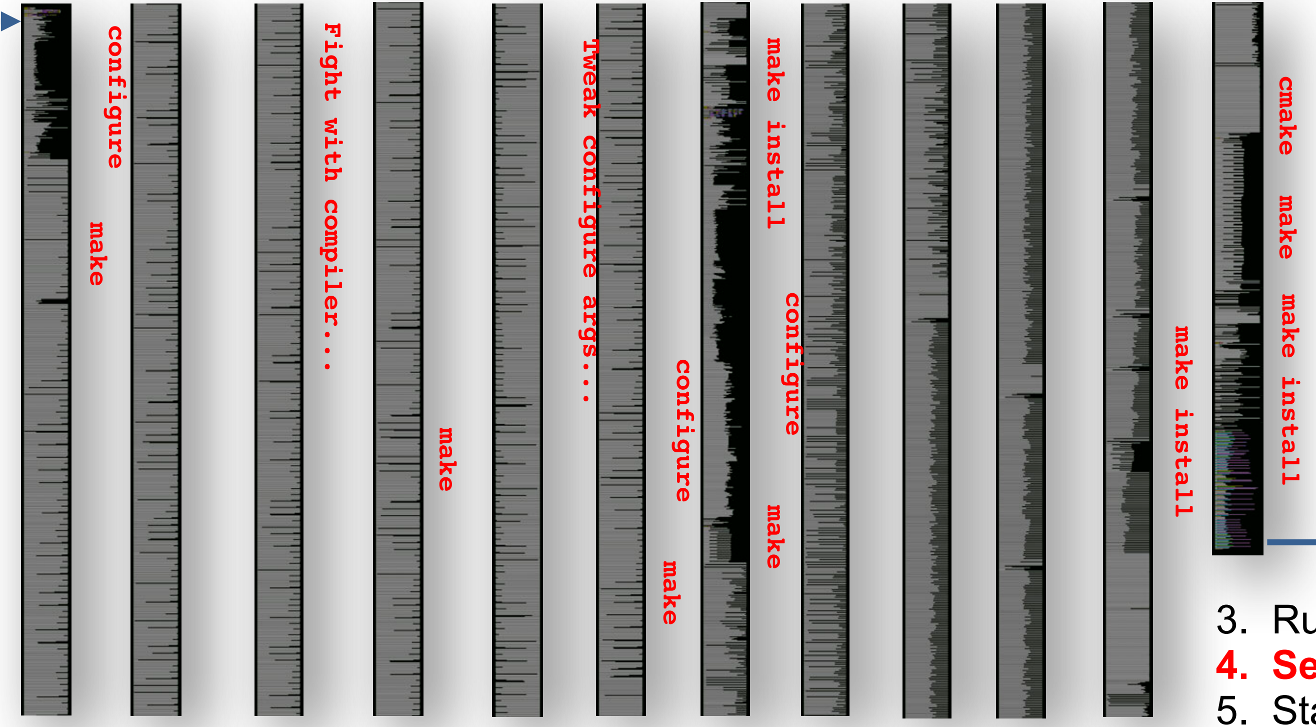


How to install software on a supercomputer

1. Download all 16 tarballs you need
2. Start building!



3. Run code
4. **Segfault!?**
5. Start over…

What about modules?

- Most supercomputers deploy some form of *environment modules*
  - TCL modules (dates back to 1995) and Lmod (from TACC) are the most popular

```
$ gcc
-bash: gcc: command not found

$ module load gcc/7.0.1
$ gcc –dumpversion
7.0.1
```

- Modules don’t handle installation!
  - They only modify your environment (things like PATH, LD_LIBRARY_PATH, etc.)

- Someone (likely a team of people) has already installed gcc for you!
  - Also, you can *only* `module load` the things they’ve installed

What about containers?

- **Containers provide a great way to reproduce and distribute an already-built software stack**

- **Someone needs to build the container!**
  - This isn’t trivial
  - Containerized applications still have hundreds of dependencies

- **Using the OS package manager inside a container is insufficient**
  - Most binaries are built unoptimized
  - Generic binaries, not optimized for specific architectures

- **HPC containers may need to be *rebuilt* to support many different hosts, anyway.**
  - Not clear that we can ever build one container for all facilities
  - Containers likely won’t solve the N-platforms problem in HPC

We need something more flexible to **build** the containers

Spack is a flexible package manager for HPC

- Spack automates the build and installation of scientific software
- Packages are *templated,* so that users can easily tune for the host environment

No installation required: clone and go

```
$ git clone https://github.com/spack/spack
$ spack install hdf5
```

Simple syntax enables complex installs

```
$ spack install hdf5@1.10.5                          $ spack install hdf5@1.10.5 cppflags="-O3 –g3"
$ spack install hdf5@1.10.5 %clang@6.0               $ spack install hdf5@1.10.5 target=haswell
$ spack install hdf5@1.10.5 +threadssafe             $ spack install hdf5@1.10.5 +mpi ^mpich@3.2
```

github.com/spack/spack

- Ease of use of mainstream tools, with flexibility needed for HPC tuning

- Major victories:
  - ARES porting time on a new platform was reduced from **2 weeks to 3 hours**
  - Deployment time for 1,300-package stack on Summit supercomputer reduced from **2 weeks to a 12-hour overnight build**
  - Used by teams across ECP to **accelerate development**

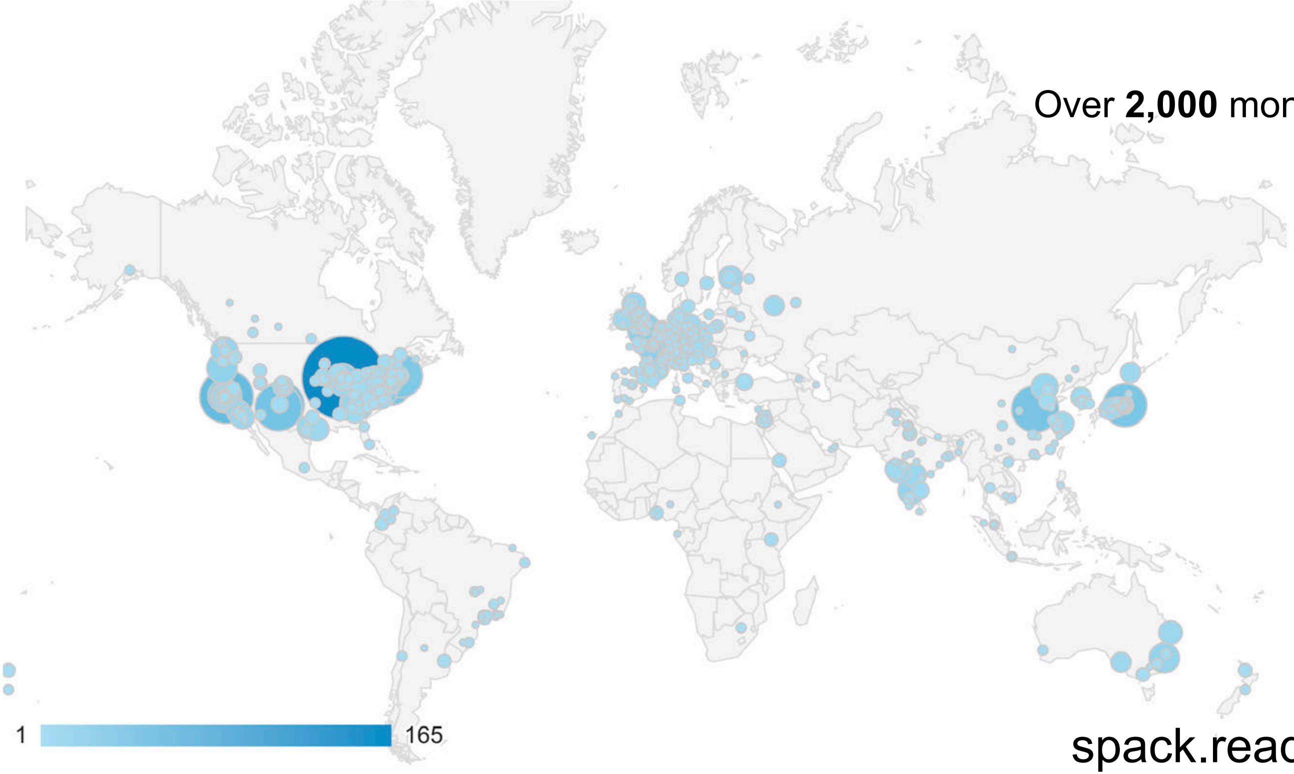
  github.com/spack/spack

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!

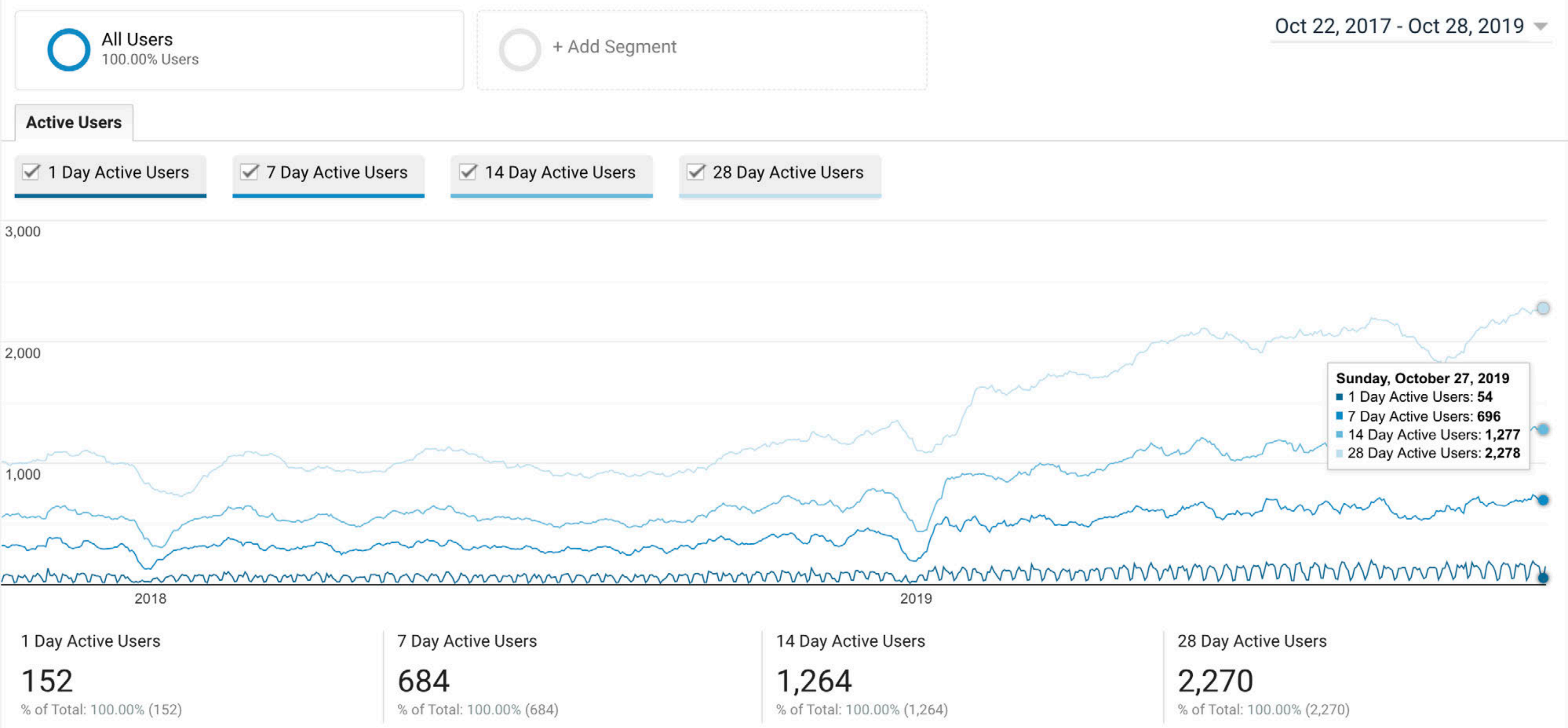


Over **3,500** software packages
Over **2,000** monthly active users (on docs site)

Over **450** contributors
from labs, academia, industry

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

Active Users on the spack.readthedocs.io



All Users
100.00% Users

+ Add Segment

Oct 22, 2017 - Oct 28, 2019

Active Users

☑ 1 Day Active Users ☑ 7 Day Active Users ☑ 14 Day Active Users ☑ 28 Day Active Users

Sunday, October 27, 2019
- 1 Day Active Users: **54**
- 7 Day Active Users: **696**
- 14 Day Active Users: **1,277**
- 28 Day Active Users: **2,278**

1 Day Active Users	7 Day Active Users	14 Day Active Users	28 Day Active Users
152	684	1,264	2,270
% of Total: 100.00% (152)	% of Total: 100.00% (684)	% of Total: 100.00% (1,264)	% of Total: 100.00% (2,270)

Spack is being used on many of the top HPC systems

- Official deployment tool for the U.S. Exascale Computing Project
- 7 of the top 10 supercomputers
- High Energy Physics community
  - Fermilab, CERN, collaborators
- Astra (Sandia)
- Fugaku (Japanese National Supercomputer Project)

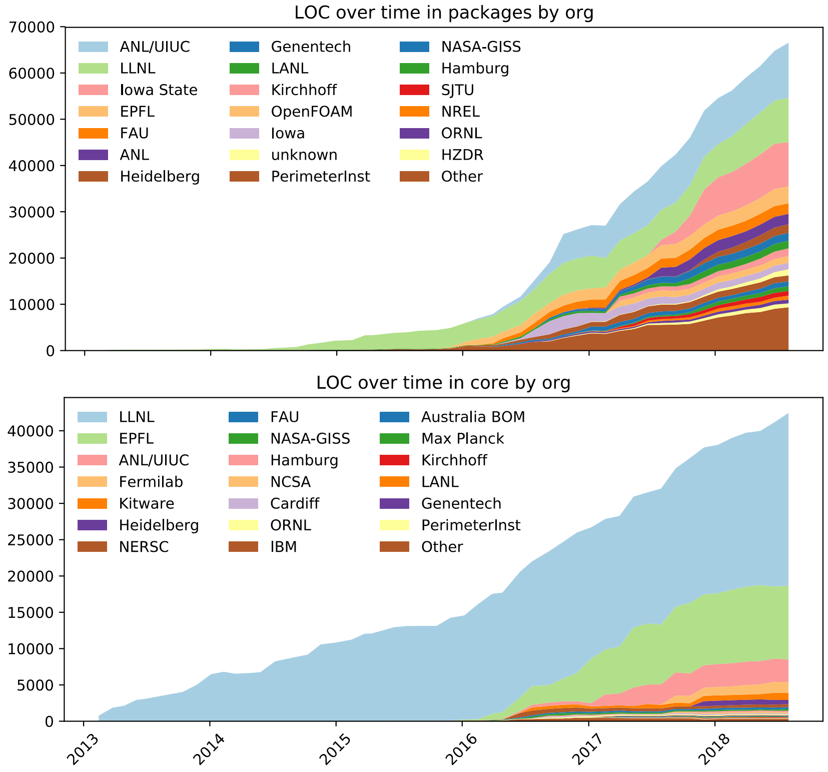
Fugaku coming to RIKEN in 2021
DOE/MEXT collaboration

Summit (ORNL), Sierra (LLNL)

SuperMUC-NG (LRZ, Germany)

Edison, Cori, Perlmutter (NERSC)

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 3,500 packages
- Most packages are from external contributors!
- Many contributions in core, as well.
- We are committed to sustaining Spack’s open source ecosystem!

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

Spack Basics

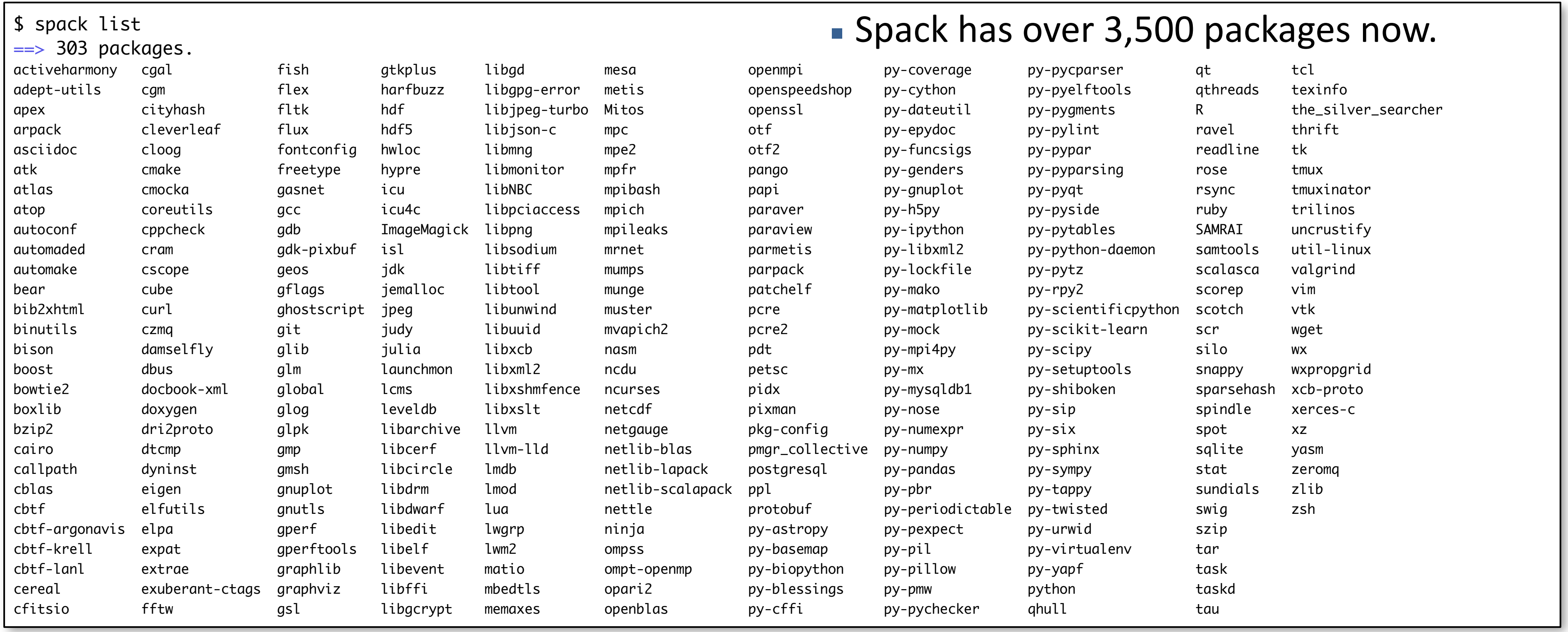
Spack provides a *spec* syntax to describe customized DAG configurations

```
$ 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"       set compiler flags
$ spack install mpileaks@3.3 target=skylake           set target microarchitecture
$ 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

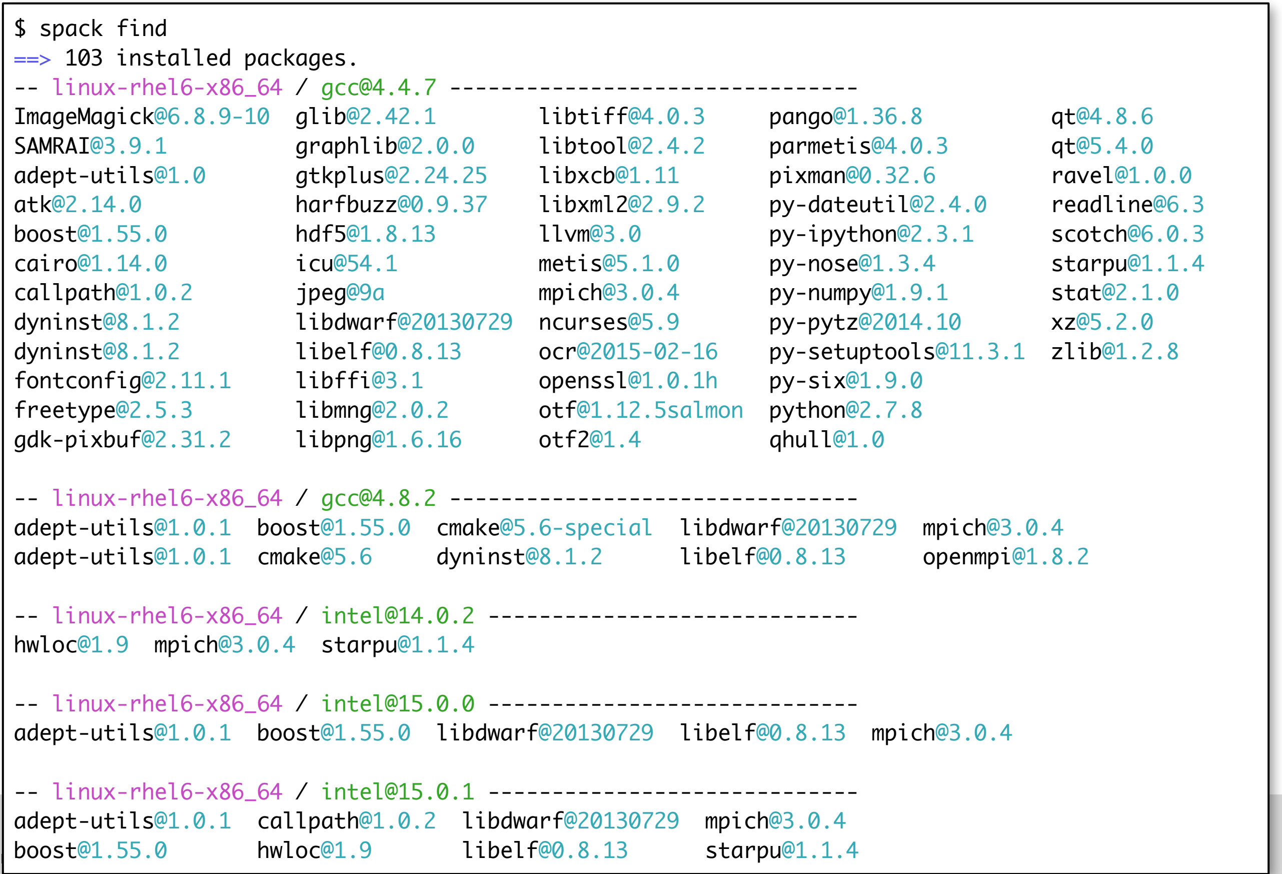


```
$ spack list
==> 303 packages.
activeharmony   cgal             fish         gtkplus      libgd          mesa              openmpi          py-coverage       py-pycparser         qt          tcl
adept-utils     cgm              flex         harfbuzz     libgpg-error   metis             openspeedshop    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 3,500 packages now.

github.com/spack/spack

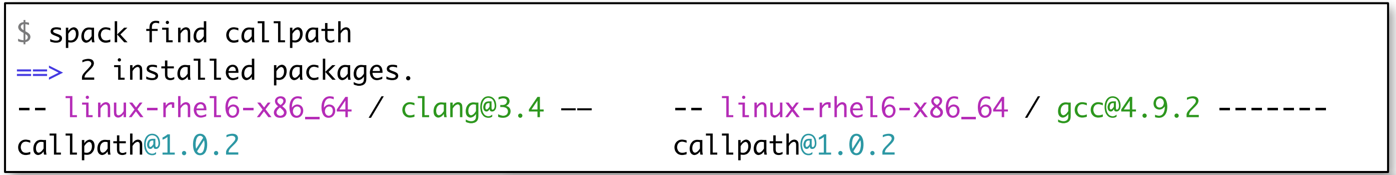
`spack find` shows what is installed



```
$ 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.

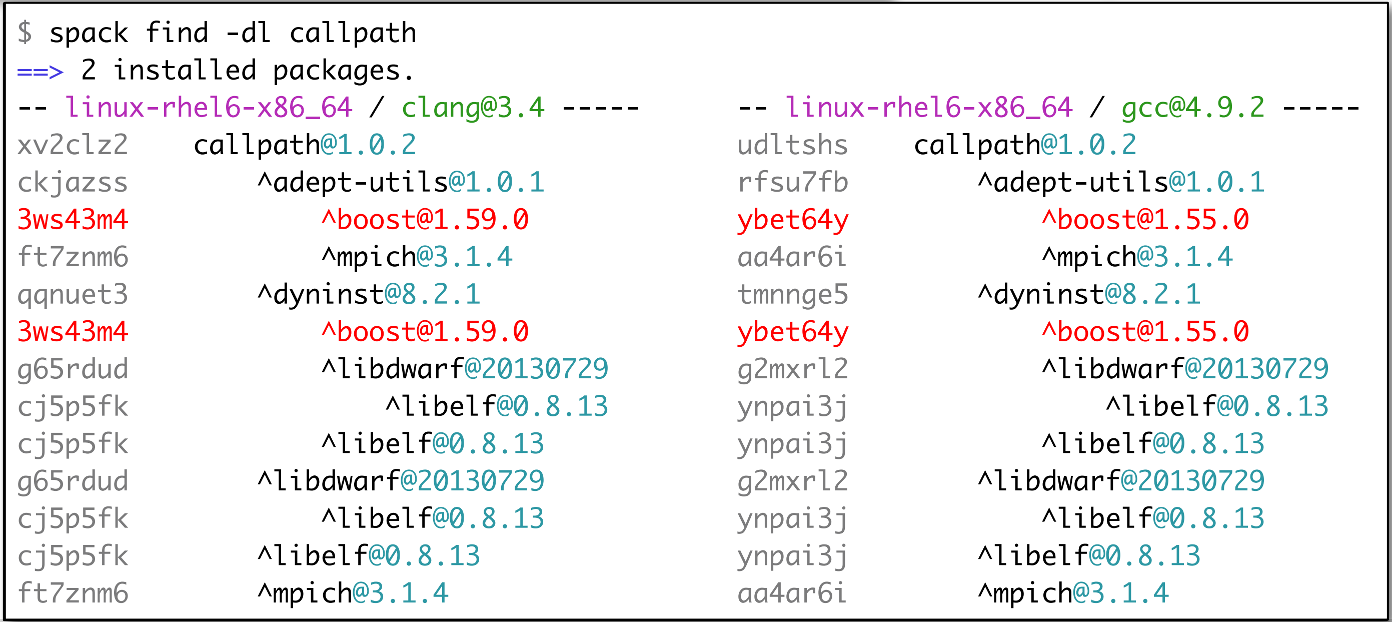
Users can query the full dependency configuration of installed packages.



```
$ 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`

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



```
$ 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
```

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

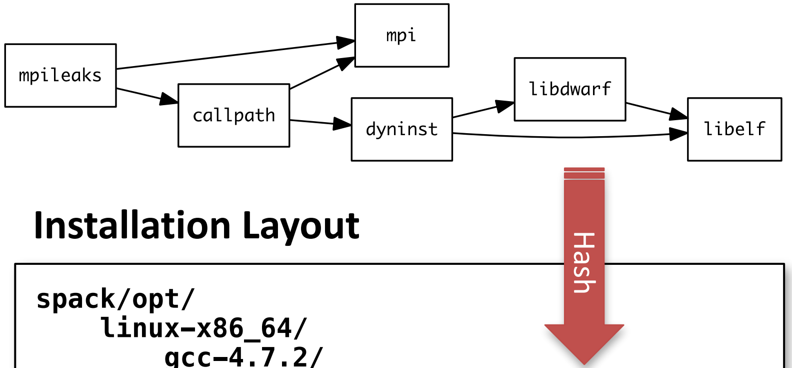
- Traditional binary package managers
  - RPM, yum, APT, yast, etc.
  - Designed to manage a single stack.
  - Install *one* version of each package in a single prefix (`/usr`).
  - Seamless upgrades to a *stable, well tested* stack

- 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

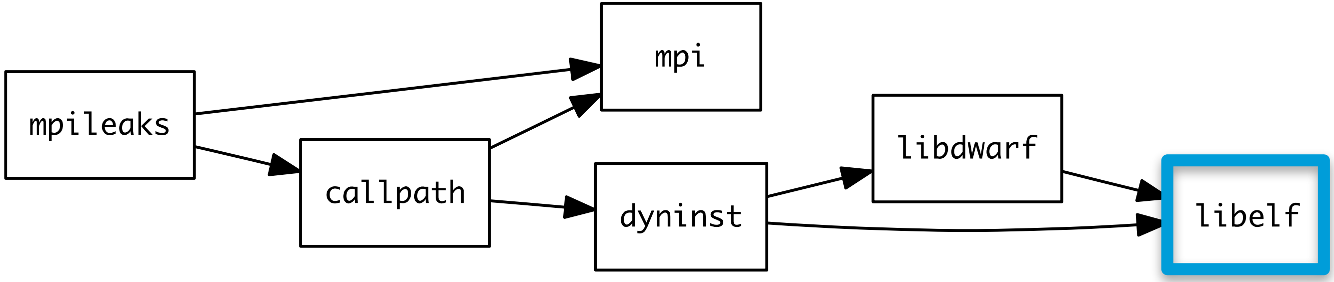


Installation Layout

```
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

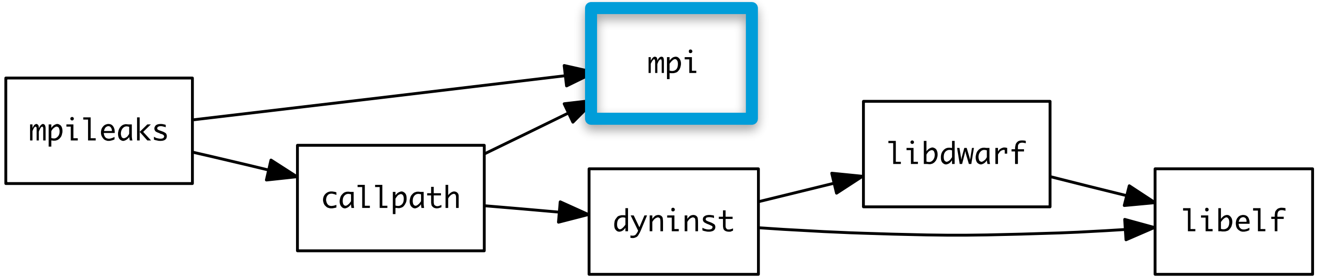


```
$ spack install mpileaks %intel@12.1 ^libelf@0.8.12
```

- 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:
```

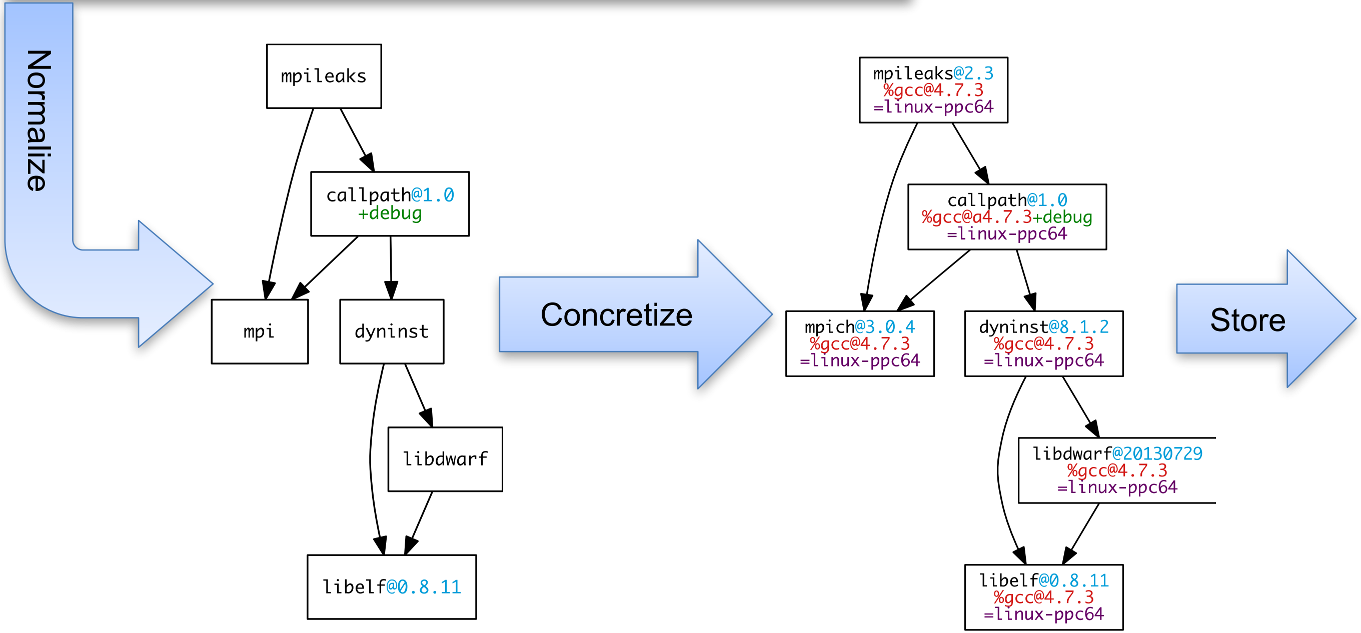
- Let Spack choose MPI implementation, as long as it provides MPI 2 interface:

```
$ 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.

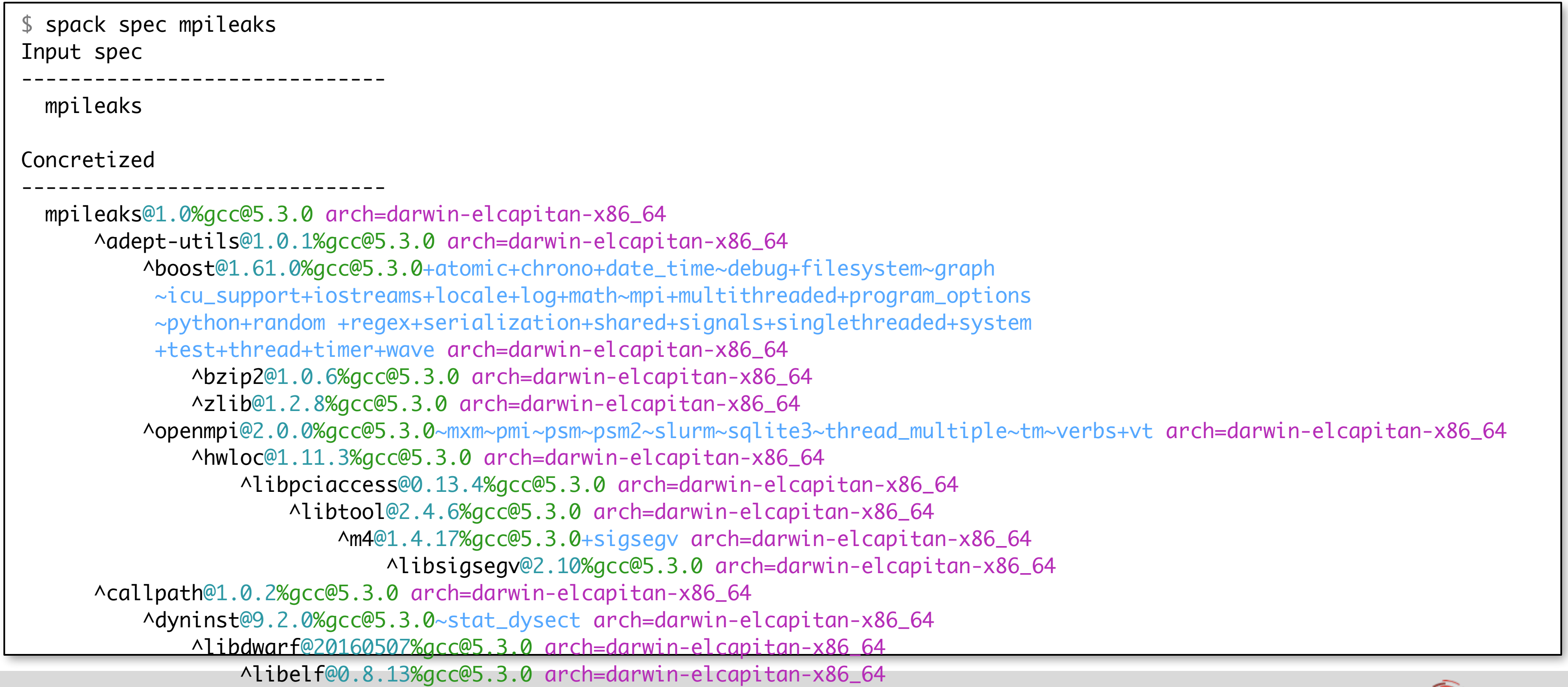
Concrete spec is fully constrained and can be passed to install.

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
```

Not shown: patches, **resources**, **conflicts**,
other directives.

Spack packages are *templates*
They use a simple Python DSL to define how to build

```
from spack import *

class Kripke(CMakePackage):
    """Kripke is a simple, scalable, 3D Sn deterministic particle
       transport proxy/mini app.
    """

    homepage = "https://computation.llnl.gov/projects/co-design/kripke"
    url      = "https://computation.llnl.gov/projects/co-design/download/kripke-openmp-1.1.tar.gz"

    version(‘1.2.3’, sha256='3f7f2eef0d1ba5825780d626741eb0b3f026a096048d7ec4794d2a7dfbe2b8a6’)
    version(‘1.2.2’, sha256='eaf9ddf562416974157b34d00c3a1c880fc5296fce2aa2efa039a86e0976f3a3’)
    version('1.1’, sha256='232d74072fc7b848fa2adc8a1bc839ae8fb5f96d50224186601f55554a25f64a’)

    variant('mpi',    default=True, description='Build with MPI.’)
    variant('openmp', default=True, description='Build with OpenMP enabled.’)

    depends_on('mpi', when='+mpi’)
    depends_on('cmake@3.0:', type='build’)

    def cmake_args(self):
        return [
            '-DENABLE_OPENMP=%s’ % ('+openmp’ in self.spec),
            '-DENABLE_MPI=%s' % ('+mpi’ in self.spec),
        ]

    def install(self, spec, prefix):
        # Kripke does not provide install target, so we have to copy
        # things into place.
        mkdirp(prefix.bin)
        install('../spack-build/kripke', prefix.bin)
```

Base package
(CMake support)

Metadata at the class level

Versions

Variants (build options)

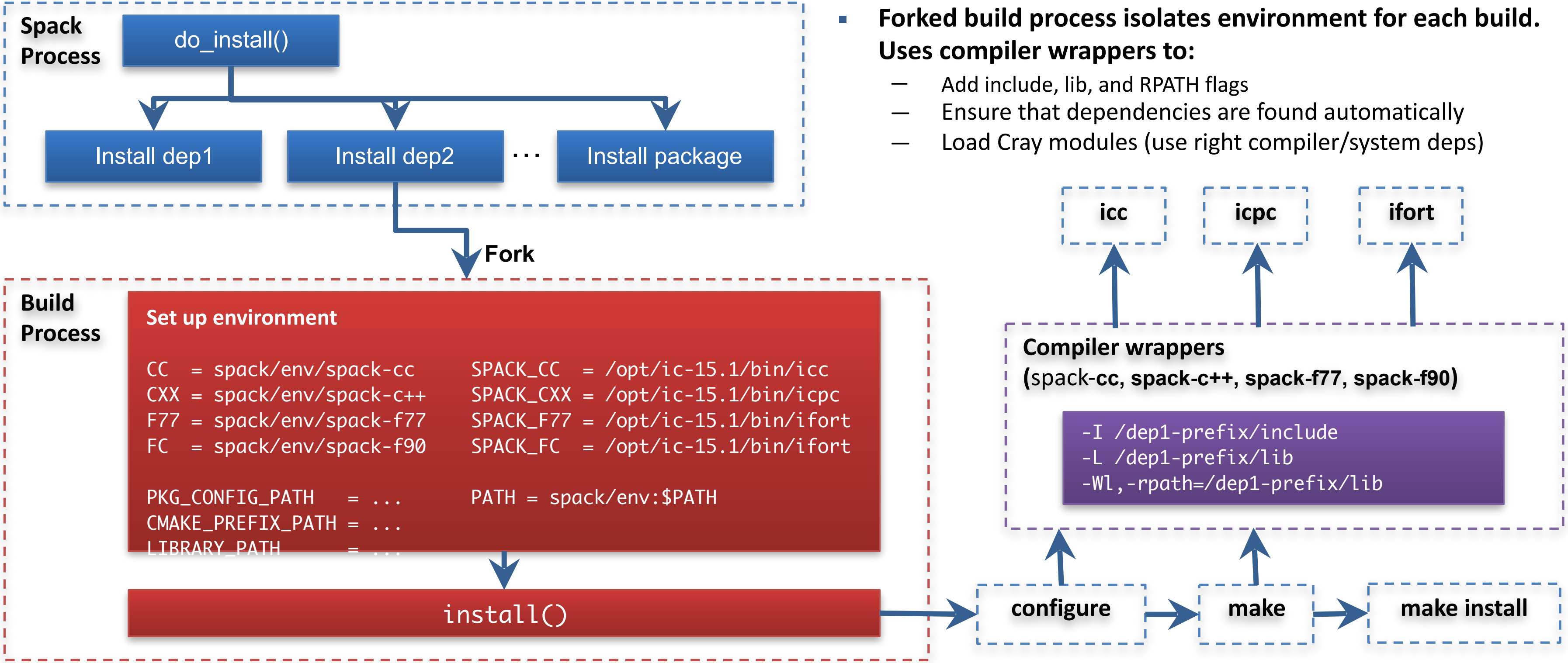
Dependencies
(note: same spec syntax)

Install logic
in instance methods

Don’t typically need `install()` for `CMakePackage`, but we can work around codes that don’t have it.

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)



Spack Process

do_install()

Install dep1

Install dep2

. . .

Install package

Fork

Build Process

Set up environment

```
CC  = spack/env/spack-cc      SPACK_CC  = /opt/ic-15.1/bin/icc
CXX = spack/env/spack-c++     SPACK_CXX = /opt/ic-15.1/bin/icpc
F77 = spack/env/spack-f77     SPACK_F77 = /opt/ic-15.1/bin/ifort
FC  = spack/env/spack-f90     SPACK_FC  = /opt/ic-15.1/bin/ifort

PKG_CONFIG_PATH   = ...       PATH = spack/env:$PATH
CMAKE_PREFIX_PATH = ...
LIBRARY_PATH      = ...
```

install()

configure

make

make install

Compiler wrappers
(spack-**cc**, **spack-c++**, **spack-f77**, **spack-f90)**

```
-I /dep1-prefix/include
-L /dep1-prefix/lib
-Wl,-rpath=/dep1-prefix/lib
```

icc

icpc

ifort

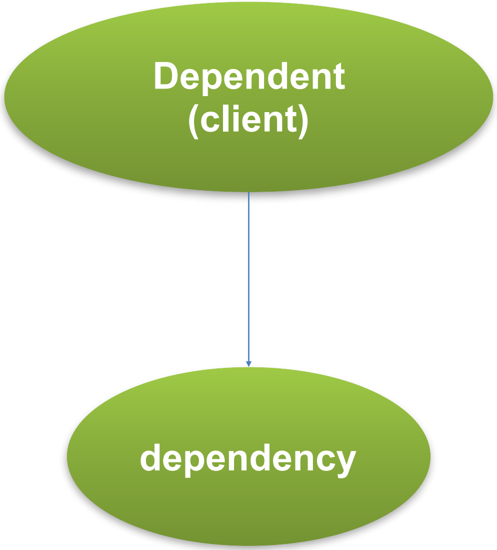
Some advanced features

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

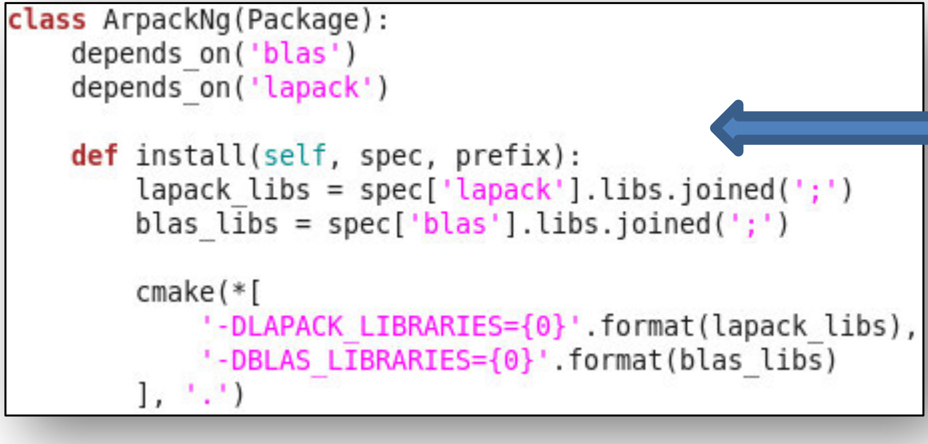
- The goal is to answer the following questions that come up when writing package files:
  - How do I retrieve dependency libraries/headers when configuring my package?
  - How does spack help me configure my build-time environment?

- 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:

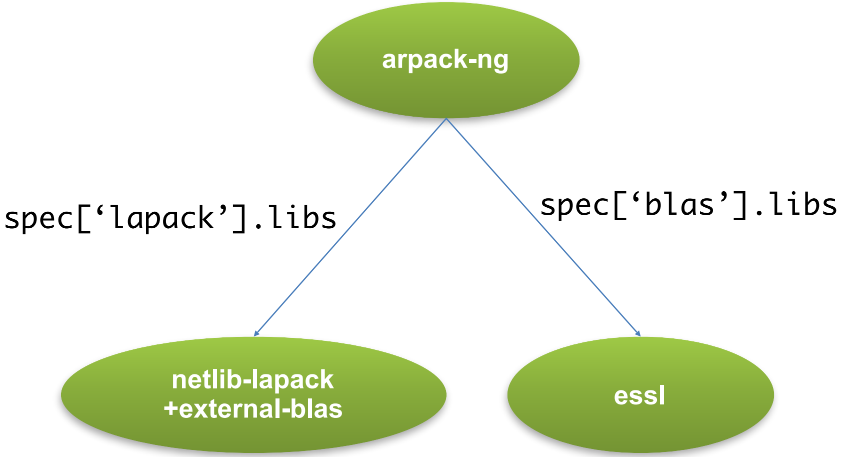
`"-L/…/libdir1/ -L/…/libdir2/"`

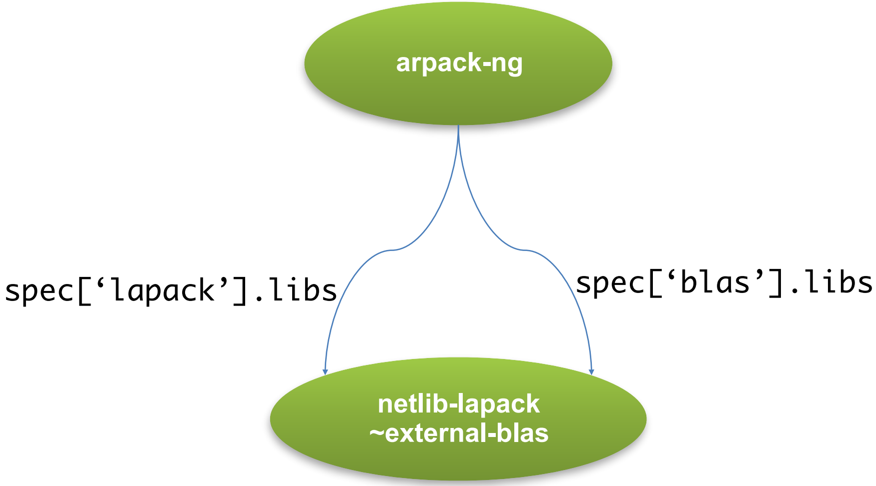
(e.g. as an argument to the compiler)

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





What's New?
What's on the Road Map?

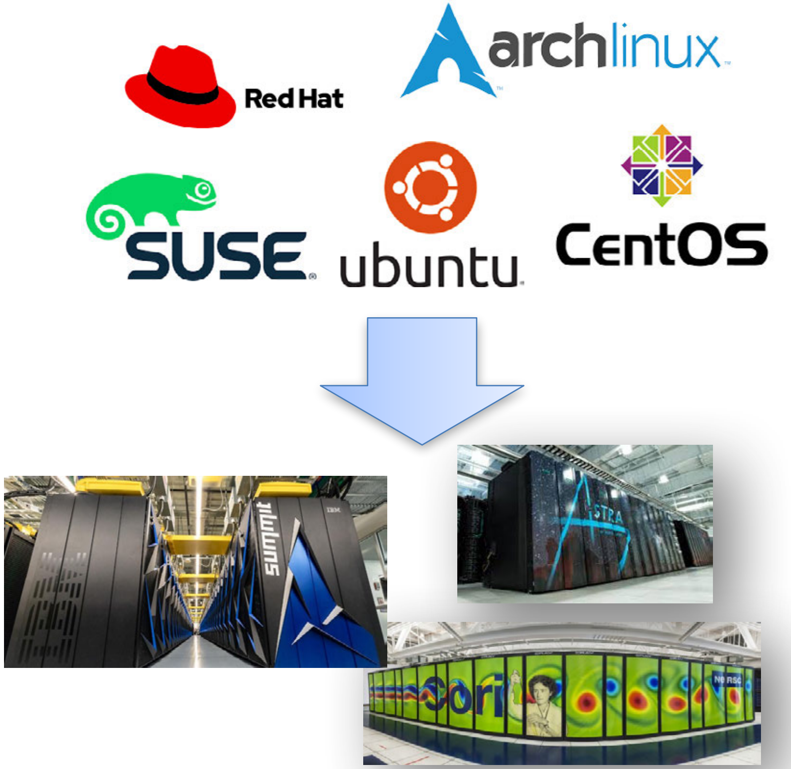
We are working to enable optimized software distribution for HPC

- Distribution effort required is similar to efforts like Red Hat, Debian, Ubuntu, etc.
  - Curation and vetting of software
  - Packaging, building
  - Wide distribution

- HPC community is not as mainstream, not as widespread as these distributions

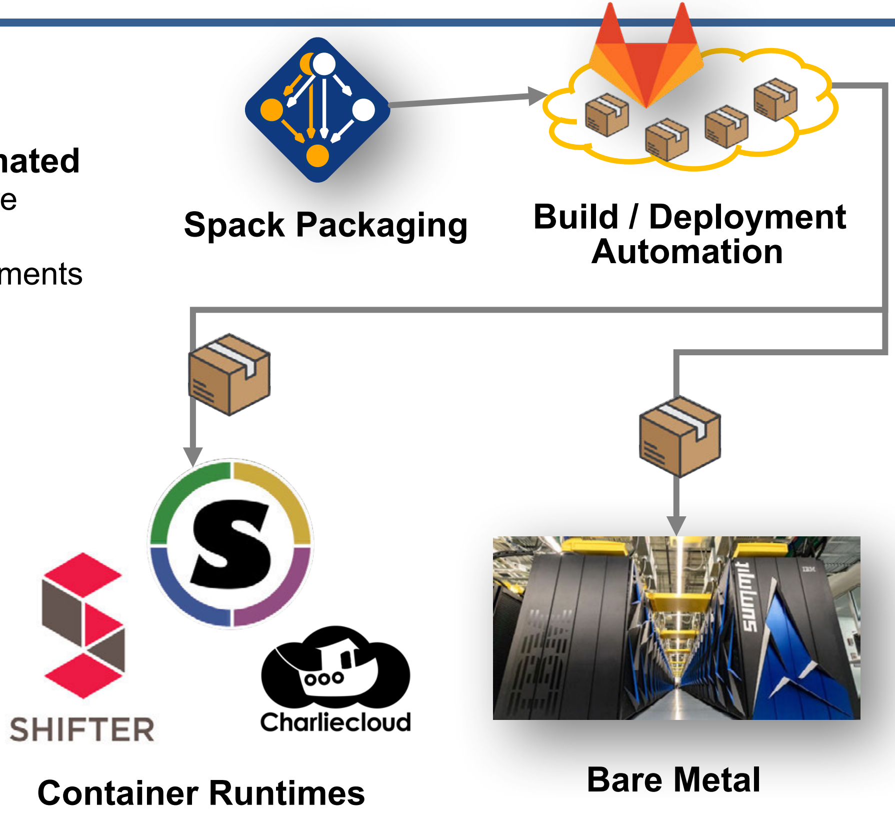
- HPC platform complexity poses challenges
  - Many (often unique) platforms
  - Many software ecosystems
  - From-source distribution
  - Must support Optimization, GPUs, fast networks

- Much more automation is required to practically support our ecosystem!



Our strategy is to enable exascale software distribution on *both* bare metal and containers

- **New capabilities to make HPC packaging easy and automated**
  - Optimized builds and package binaries that exploit the hardware
  - Workflow automation for facilities, developers, and users
  - Strong integration with containers as well as bare metal deployments
- **Work with ECP and other partners to harden packages**
  - Build pipelines at facilities
  - Coordination on multi-site testing
  - Security integration
- **Outreach to users**
  - Tutorials, workshops, BOFs



Spack Packaging

Build / Deployment Automation

Container Runtimes

Bare Metal

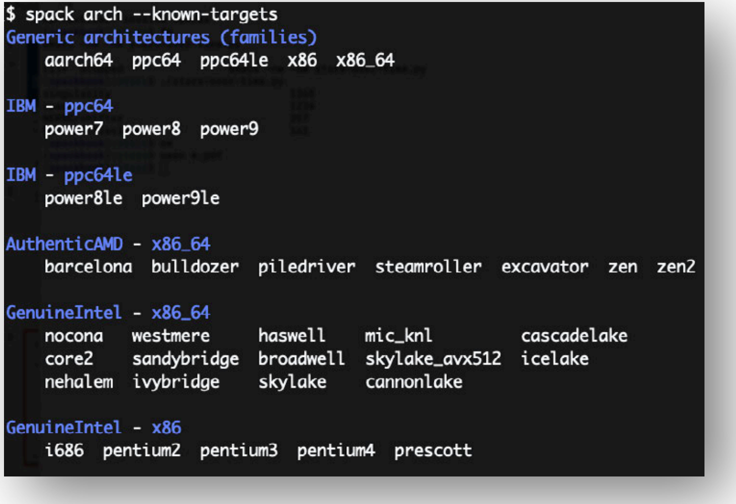
Spack now understands specific target microarchitectures

- We have developed a cross-platform library to detect and compare microarchitecture metadata
  - Detects based on /proc/cpuinfo (Linux), sysctl (Mac)
  - Allows comparisons for compatibility, e.g.:

```
skylake > broadwell
zen2 > x86_64
```

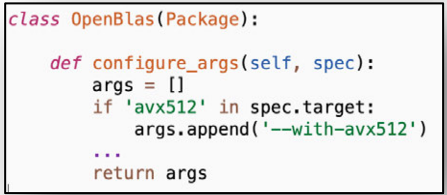
- Key features:
  - Know which compilers support which chips/which flags
  - Determine compatibility
  - Enable creation and reuse of optimized binary packages
  - Easily query available architecture features for portable build recipes

- We will be extracting this as a standalone library for other tools & languages
  - Hope to make this standard!



```
$ spack arch --known-targets
Generic architectures (families)
    aarch64  ppc64  ppc64le  x86  x86_64

IBM - ppc64
    power7  power8  power9

IBM - ppc64le
    power8le  power9le

AuthenticAMD - x86_64
    barcelona  bulldozer  piledriver  steamroller  excavator  zen  zen2

GenuineIntel - x86_64
    nocona   westmere     haswell    mic_knl         cascadelake
    core2    sandybridge  broadwell  skylake_avx512  icelake
    nehalem  ivybridge    skylake    cannonlake

GenuineIntel - x86
    i686  pentium2  pentium3  pentium4  prescott
```

Extensive microarchitecture knowledge



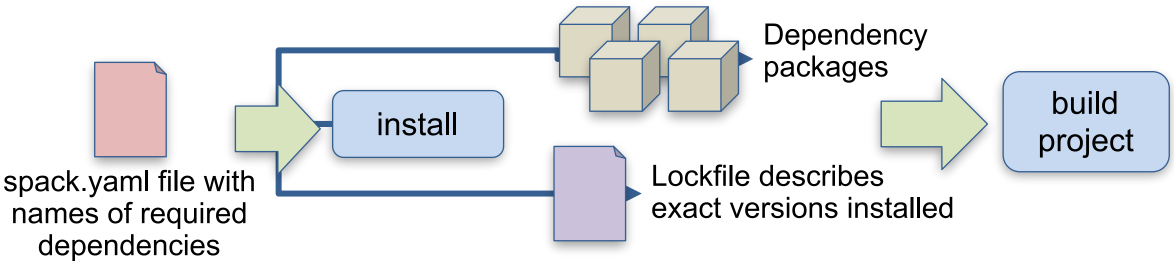
```
class OpenBlas(Package):

    def configure_args(self, spec):
        args = []
        if 'avx512' in spec.target:
            args.append('--with-avx512')
        ...
        return args
```

Simple feature query

```
$ spack install lbann target=cascadelake

$ spack install petsc target=zen2
```

Specialized installations

Spack environments enable users to build customized stacks from an abstract description



spack.yaml file with names of required dependencies

install

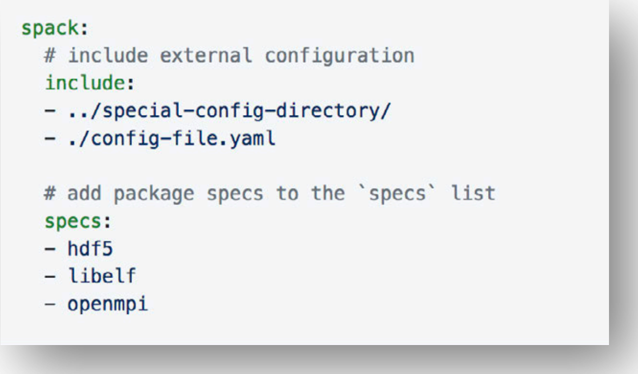
Dependency packages

Lockfile describes exact versions installed

build project

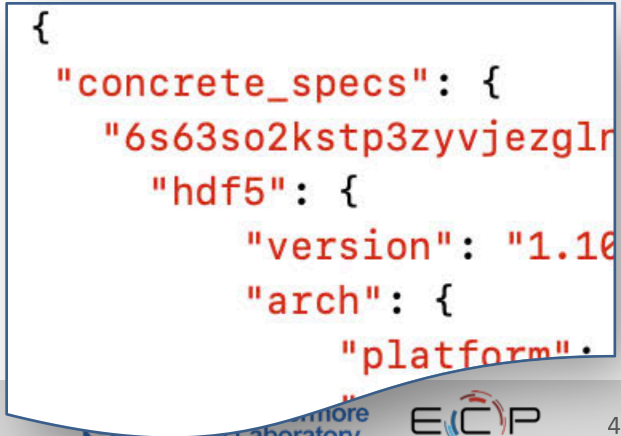
- Allows developers to bundle Spack configuration with their repository
- Can also be used to maintain configuration together with Spack packages.
  - E.g., versioning your own local software stack with consistent compilers/ MPI implementations
- Manifest / Lockfile model pioneered by Bundler is becoming standard
  - spack.yaml describes project requirements
  - spack.lock describes exactly what versions/configurations were installed, allows them to be reproduced.

Simple spack.yaml file



```
spack:
  # include external configuration
  include:
  - ../special-config-directory/
  - ./config-file.yaml

  # add package specs to the `specs` list
  specs:
  - hdf5
  - libelf
  - openmpi
```

Concrete spack.lock file (generated)

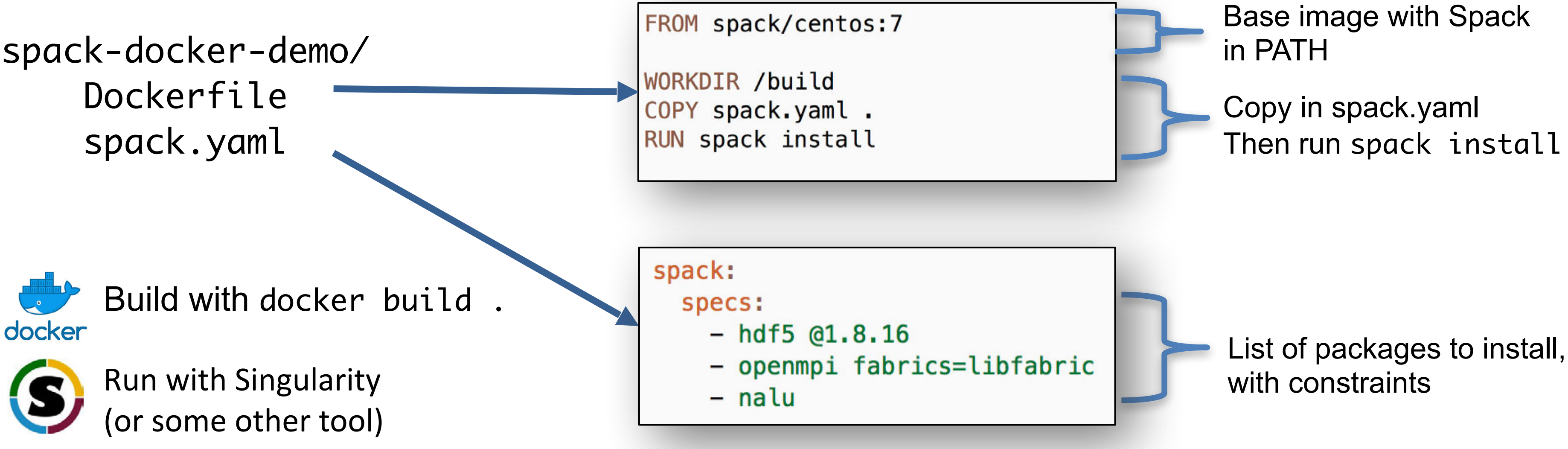


```
{
 "concrete_specs": {
   "6s63so2kstp3zyvjezglr
     "hdf5": {
       "version": "1.10
       "arch": {
         "platform":
```

We have simplified container deployments using Spack Environments

- We recently started providing base images on DockerHub with Spack preinstalled.

- **Very** easy to build a container with some Spack packages in it:



```
spack-docker-demo/
    Dockerfile
    spack.yaml
```

```
FROM spack/centos:7

WORKDIR /build
COPY spack.yaml .
RUN spack install
```

Base image with Spack in PATH

Copy in spack.yaml
Then run `spack install`

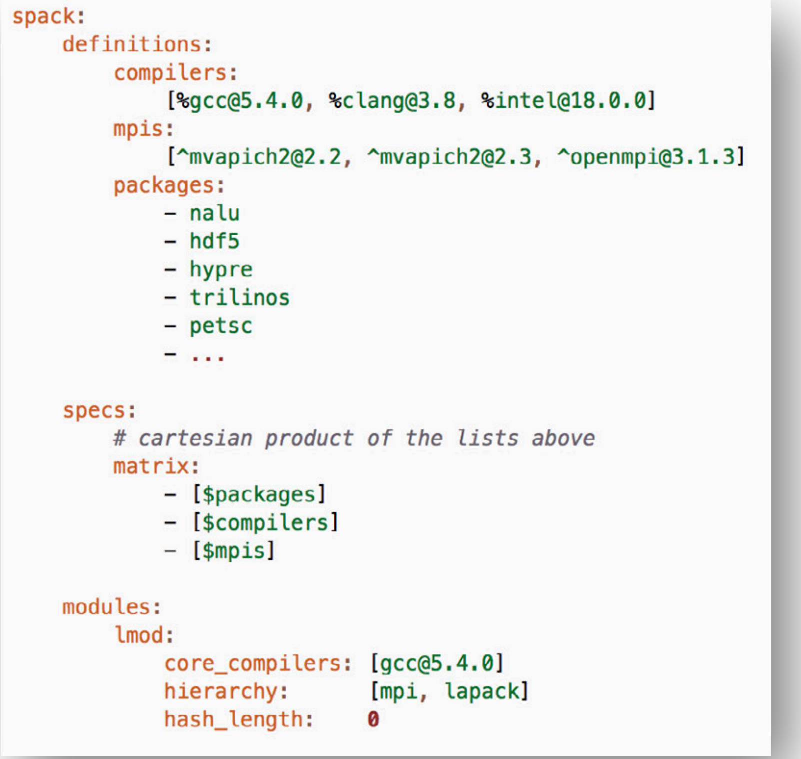
```
spack:
  specs:
    - hdf5 @1.8.16
    - openmpi fabrics=libfabric
    - nalu
```

List of packages to install, with constraints

Build with `docker build .`

Run with Singularity (or some other tool)

We have developed Spack stacks: combinatorial environments for entire facility deployments



```
spack:
    definitions:
        compilers:
            [%gcc@5.4.0, %clang@3.8, %intel@18.0.0]
        mpis:
            [^mvapich2@2.2, ^mvapich2@2.3, ^openmpi@3.1.3]
        packages:
            - nalu
            - hdf5
            - hypre
            - trilinos
            - petsc
            - ...

    specs:
        # cartesian product of the lists above
        matrix:
            - [$packages]
            - [$compilers]
            - [$mpis]

    modules:
        lmod:
            core_compilers: [gcc@5.4.0]
            hierarchy:      [mpi, lapack]
            hash_length:    0
```

- Allow users to easily express a huge cross-product of specs
  - All the packages needed for a facility
  - Generate modules tailored to the site
  - Generate a directory layout to browse the packages

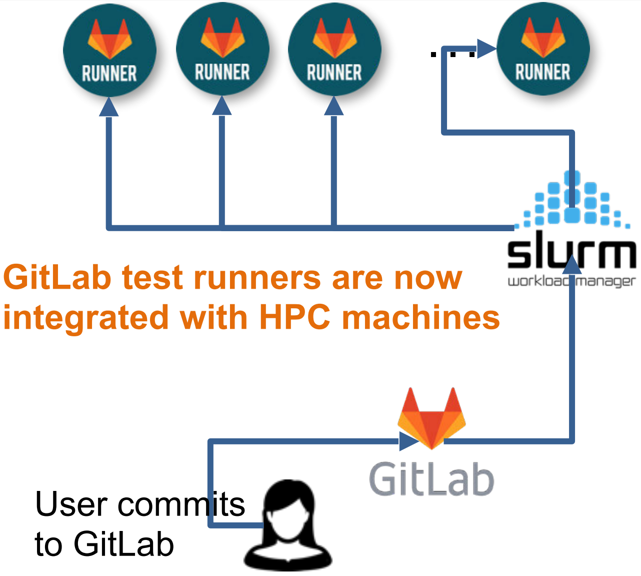
- Build on the environments workflow
  - Manifest + lockfile
  - Lockfile enables reproducibility

- Relocatable binaries allow the same binary to be used in a stack, regular install, or container build.
  - Difference is how the user interacts with the stack
  - Single-PATH stack vs. modules.

We have been heavily involved in the ECP CI project.

OnyxPoint ECP EXASCALE COMPUTING PROJECT GitLab

- We have added security features to the open source GitLab product.
  - Integration with center identity management
  - Integration with schedulers like SLURM, LSF
- We are democratizing testing at Livermore Computing
  - Users can run tests across 30+ machines by editing a file
  - Previously, each team had to administer own servers
- ECP sites are deploying GitLab CI for users
  - All HPC centers can leverage these improvements
  - NNSA labs plan to deploy common high-side CI infrastructure
  - We are developing new security policies to allow external open source code to be tested safely on key machines

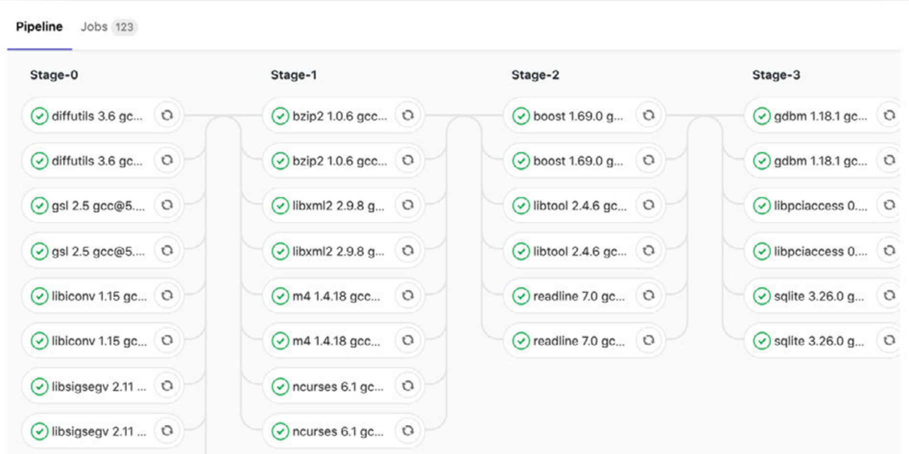


GitLab test runners are now integrated with HPC machines

User commits to GitLab

Spack has added GitLab CI integration to automate package build pipelines

- Builds on Spack environments
  - Support auto-generating GitLab CI jobs
  - Can run in a Kube cluster or on bare metal runners at an HPC site
  - Sends progress to CDash

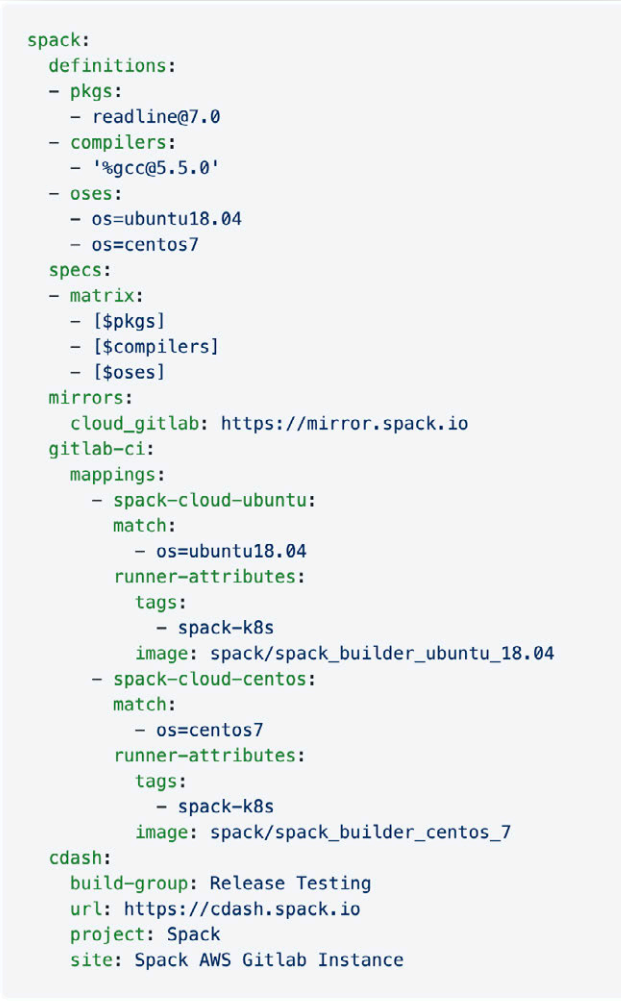


Stage-0
- diffutils 3.6 gc...
- diffutils 3.6 gc...
- gsl 2.5 gcc@5....
- gsl 2.5 gcc@5....
- libiconv 1.15 gc...
- libiconv 1.15 gc...
- libsigsegv 2.11 ...
- libsigsegv 2.11 ...

Stage-1
- bzip2 1.0.6 gcc...
- bzip2 1.0.6 gcc...
- libxml2 2.9.8 g...
- libxml2 2.9.8 g...
- m4 1.4.18 gcc...
- m4 1.4.18 gcc...
- ncurses 6.1 gc...
- ncurses 6.1 gc...

Stage-2
- boost 1.69.0 g...
- boost 1.69.0 g...
- libtool 2.4.6 gc...
- libtool 2.4.6 gc...
- readline 7.0 gc...
- readline 7.0 gc...

Stage-3
- gdbm 1.18.1 gc...
- gdbm 1.18.1 gc...
- libpciaccess 0....
- libpciaccess 0....
- sqlite 3.26.0 g...
- sqlite 3.26.0 g...



```
spack:
  definitions:
  - pkgs:
    - readline@7.0
  - compilers:
    - '%gcc@5.5.0'
  - oses:
    - os=ubuntu18.04
    - os=centos7
  specs:
  - matrix:
    - [$pkgs]
    - [$compilers]
    - [$oses]
  mirrors:
    cloud_gitlab: https://mirror.spack.io
  gitlab-ci:
    mappings:
      - spack-cloud-ubuntu:
        match:
          - os=ubuntu18.04
        runner-attributes:
          tags:
            - spack-k8s
          image: spack/spack_builder_ubuntu_18.04
      - spack-cloud-centos:
        match:
          - os=centos7
        runner-attributes:
          tags:
            - spack-k8s
          image: spack/spack_builder_centos_7
  cdash:
    build-group: Release Testing
    url: https://cdash.spack.io
    project: Spack
    site: Spack AWS Gitlab Instance
```

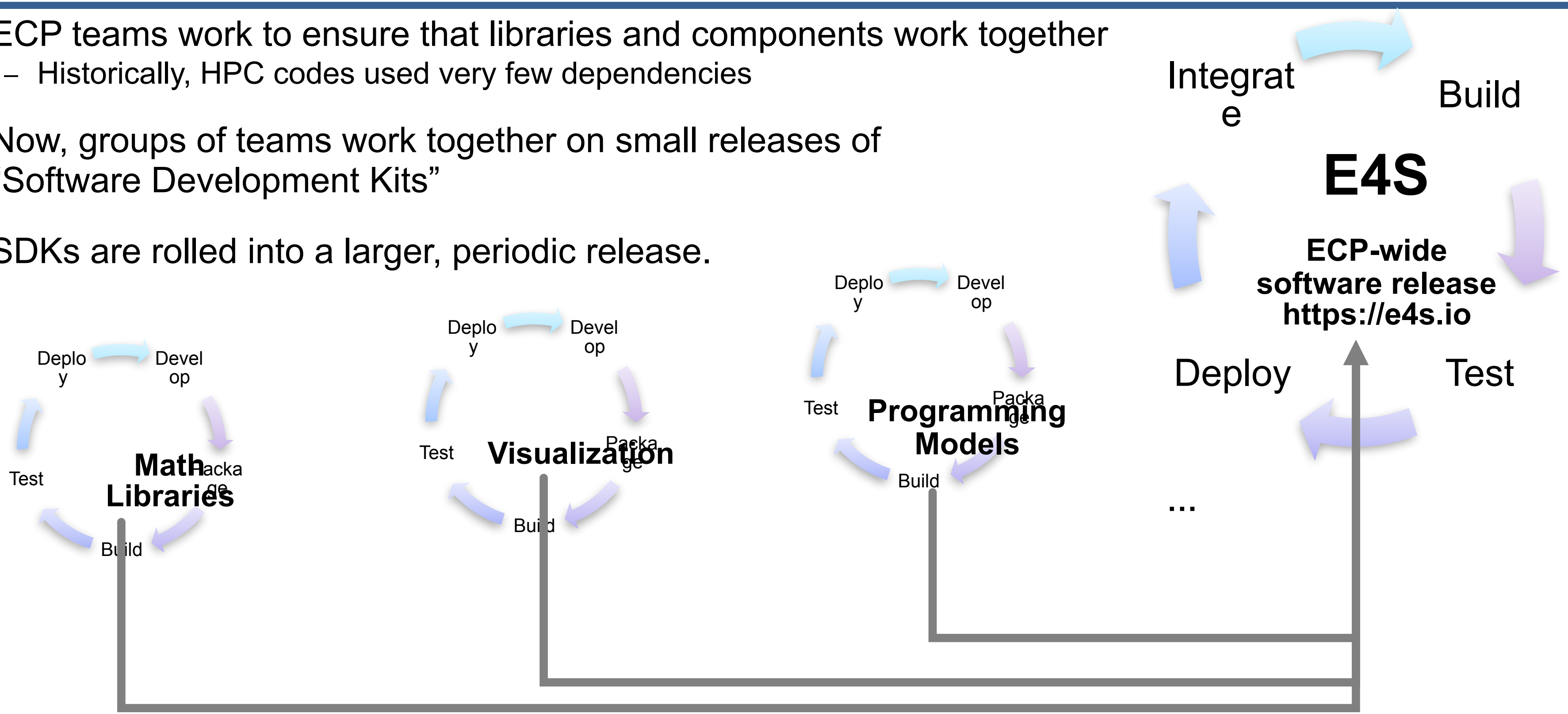
github.com/spack/spack

ECP is working towards a periodic, hierarchical release process

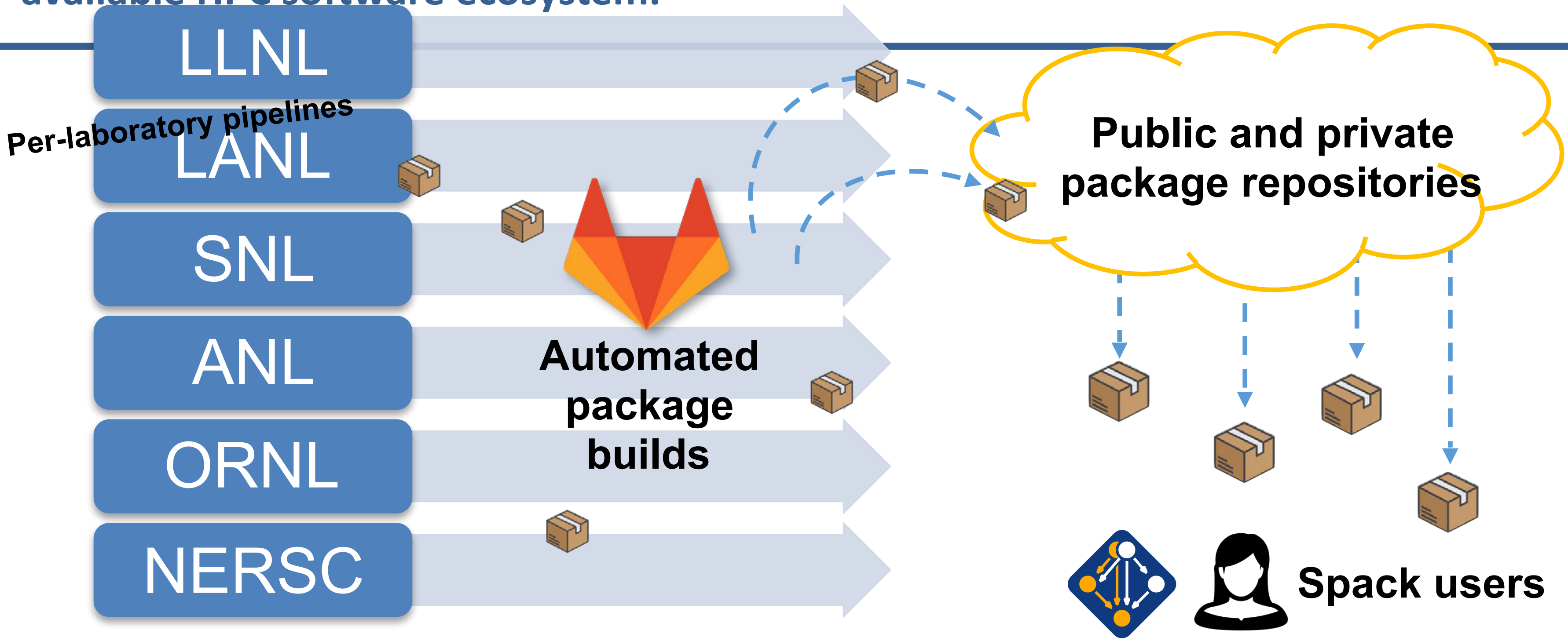
- ECP teams work to ensure that libraries and components work together
  - Historically, HPC codes used very few dependencies

- Now, groups of teams work together on small releases of “Software Development Kits”

- SDKs are rolled into a larger, periodic release.



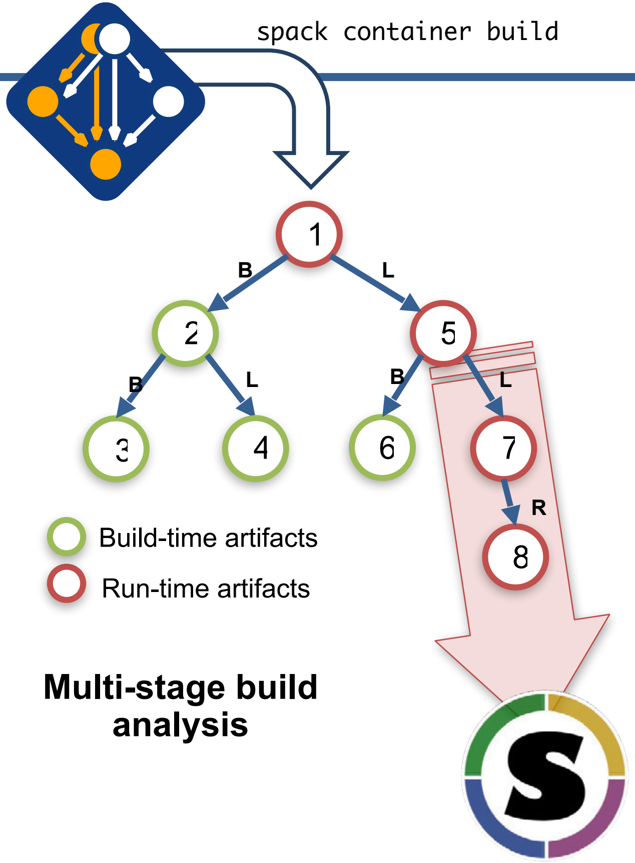
Automated builds using ECP CI will enable a robust, widely available HPC software ecosystem.



With pipeline efforts at E6 labs, users will no longer need to *build* their own software for high performance.

Spack focus areas in FY20

- **Multi-stage container generation with Spack**
  - Add support to Spack to generate *multi-stage* container builds that exclude build dependencies from artifacts automatically
- **Build Hardening with Spack Pipelines**
  - Continue working with E4S team to harden container builds
- **Parallel builds**
  - “`srun spack install`” will use the entire allocation to build
- **New concretizer based on fast ASP/SAT solvers**
- **Improved dependency models for compilers**
  - icpc depends on g++ for its libstdc++, and other ABI nightmares



Multi-stage build analysis

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 **Slack channel** (see GitHub repo for info)
  - Join our **Google Group** (see GitHub repo for info)
  - Submit GitHub issues and pull requests!

- **Docs and a full day tutorial are available at:**

  spack.readthedocs.io

spack.io

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