Managing HPC Software Complexity with Spack

SC22 Full Day Tutorial
November 13, 2022

The most recent versionof these slides can be found at:
https://spack-tutorial.readthedocs.io

Tutorial Materials

Find these slides and associated scripts here:

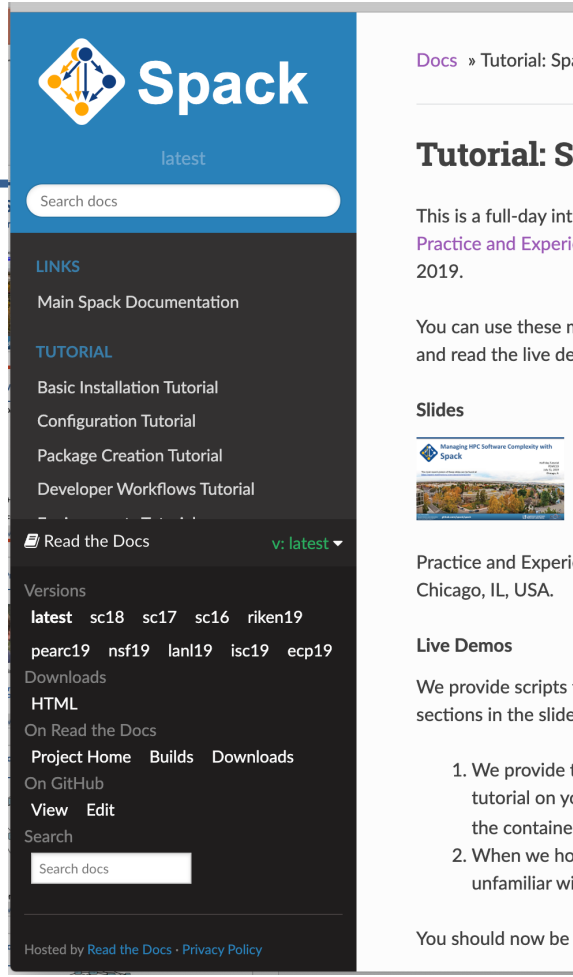
spack-tutorial.rtfd.io

We also have a chat room on Spack slack.
You can join here:

slack.spack.io

Join the **#tutorial** channel!

You can ask questions here after the conference is over.
Over **2,000 people** can help you on Slack!



Tutorial Presenters

Greg Becker
LLNL

Adam Stewart
UIUC

Todd Gamblin
LLNL

Agenda (approximate)

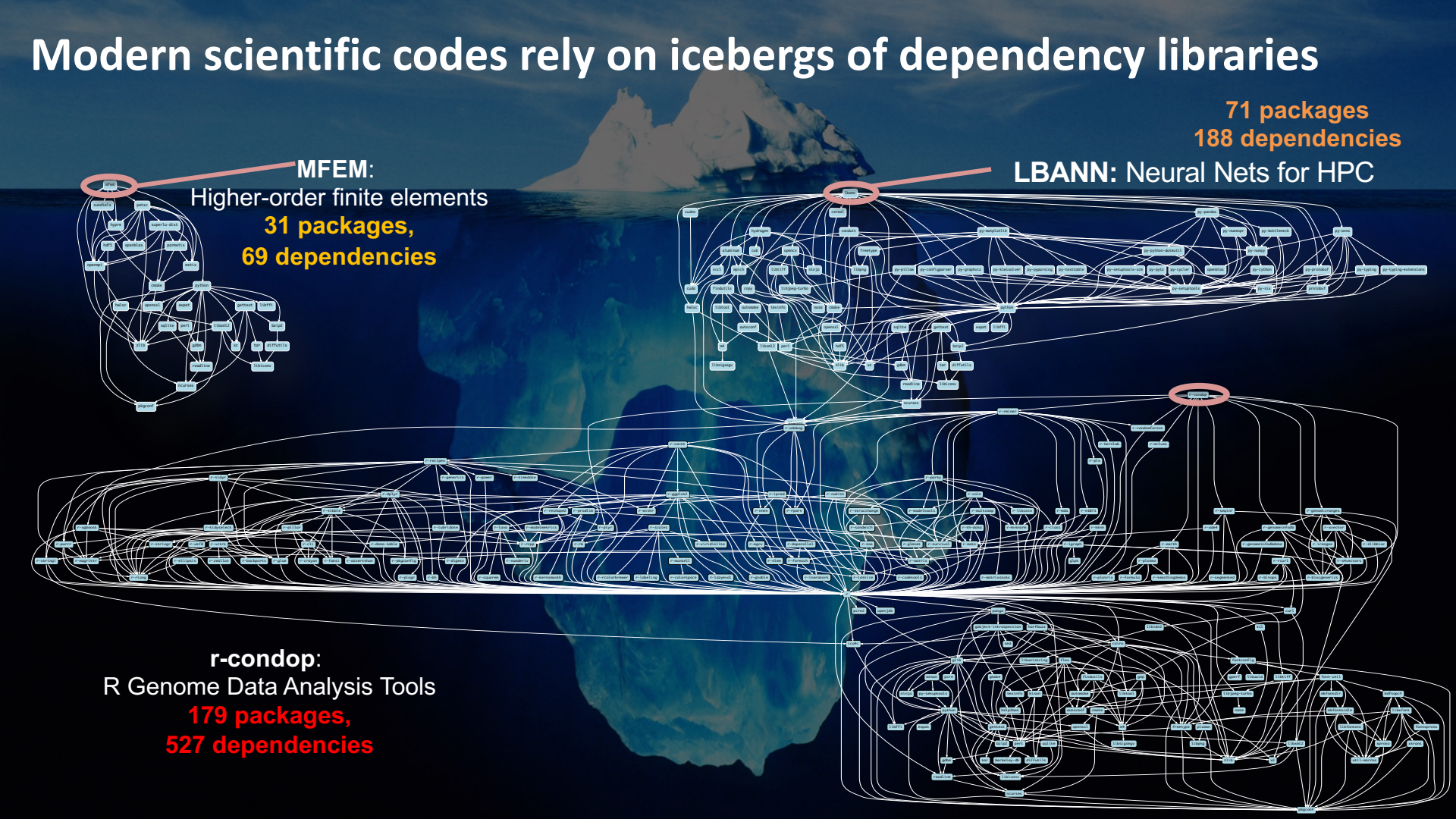
Morning

Intro	8:30 am
Basics	8:45 am
Concepts	9:30 am
Break	10:00 am
Environments	10:30 am
Configuration	11:15 am
Lunch	12:00 pm

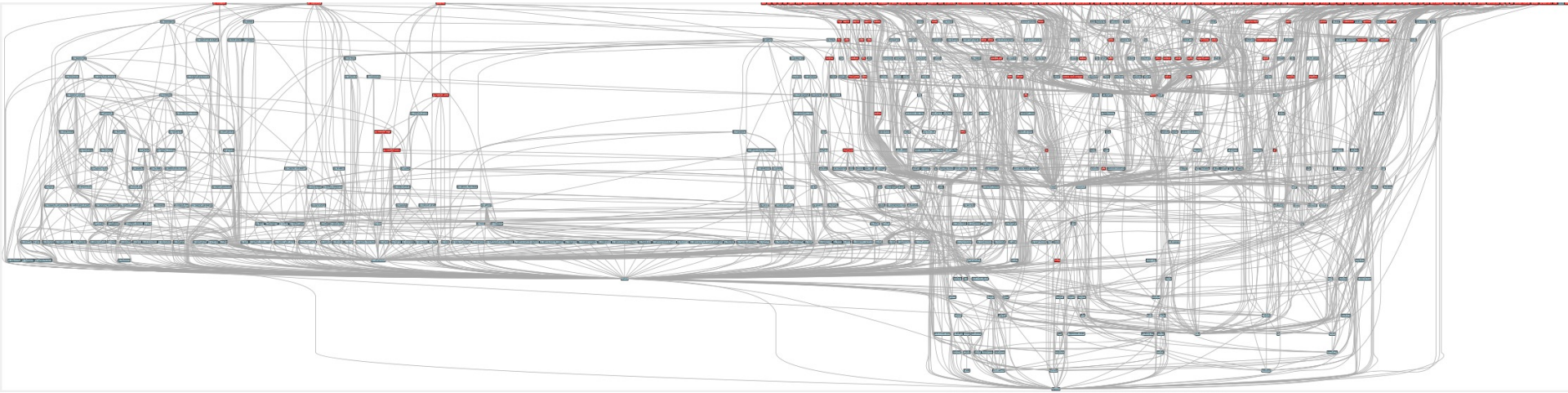
Afternoon

Stacks	1:30 pm
Packaging	2:00 pm
Break	3:00 pm
Developer Workflows	3:30 pm
Mirrors & Binary Caches	4:00 pm
Scripting	4:20 pm
Roadmap / Questions	4:35 pm
End	5:00 pm

Modern scientific codes rely on icebergs of dependency libraries



ECP's E4S stack is even larger than these codes



- Red boxes are the packages in it (about 100)
- Blue boxes are what *else* you need to build it (about 600)
- It's infeasible to build and integrate all of this manually

Some fairly common (but questionable) assumptions made by package managers (conda, pip, apt, etc.)

- **1:1 relationship between source code and binary (per platform)**
  - Good for reproducibility (e.g., Debian)
  - Bad for performance optimization
- **Binaries should be as portable as possible**
  - What most distributions do
  - Again, bad for performance
- **Toolchain is the same across the ecosystem**
  - One compiler, one set of runtime libraries
  - Or, no compiler (for interpreted languages)

Outside these boundaries, users are typically on their own

High Performance Computing (HPC) violates many of these assumptions

- **Code is typically distributed as source**
  - With exception of vendor libraries, compilers
- **Often build many variants of the same package**
  - Developers' builds may be very different
  - Many first-time builds when machines are new
- **Code is optimized for the processor and GPU**
  - Must make effective use of the hardware
  - Can make 10-100x perf difference
- **Rely heavily on system packages**
  - Need to use optimized libraries that come with machines
  - Need to use host GPU libraries and network
- **Multi-language**
  - C, C++, Fortran, Python, others all in the same ecosystem

Some Supercomputers

Current

Oak Ridge National Lab
Power9 / NVIDIA

RIKEN
Fujitsu/ARM a64fx

Upcoming

Lawrence Berkeley National Lab
AMD Zen / NVIDIA

Argonne National Lab
Intel Xeon / Xe

Oak Ridge National Lab
AMD Zen / Radeon

Lawrence Livermore National Lab
AMD Zen / Radeon

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

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Spack enables software distribution for HPC

- Spack automates the build and installation of scientific software
- Packages are *parameterized,* so that users can easily tweak and tune configuration

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 %clang@6.0
$ spack install hdf5@1.10.5 +threadssafe
$ spack install hdf5@1.10.5 cppflags="-O3 -g3"
$ spack install hdf5@1.10.5 target=haswell
$ 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
- In addition to CLI, Spack also:
  - Generates (but does **not** require) *modules*
  - Allows conda/virtualenv-like *environments*
  - Provides many devops features (CI, container generation, more)

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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

Package Manager

- Manages package installation
- Manages dependency relationships
- May drive package-level build systems

High Level Build System

- Cmake, Autotools
- Handle library abstractions
- Generate Makefiles, etc.

Low Level Build System

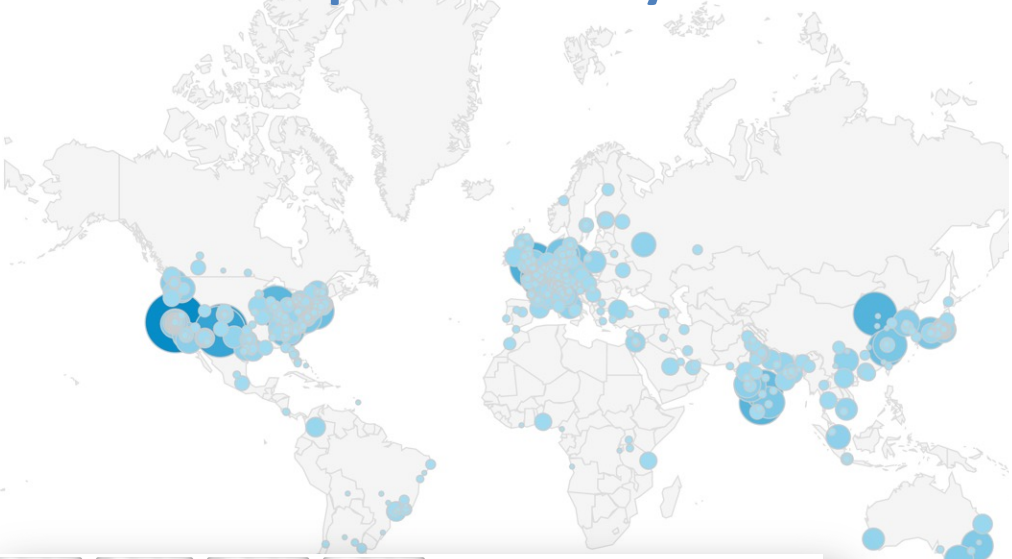
- Make, Ninja
- Handles dependencies among *commands* in a single build

Who can use Spack?

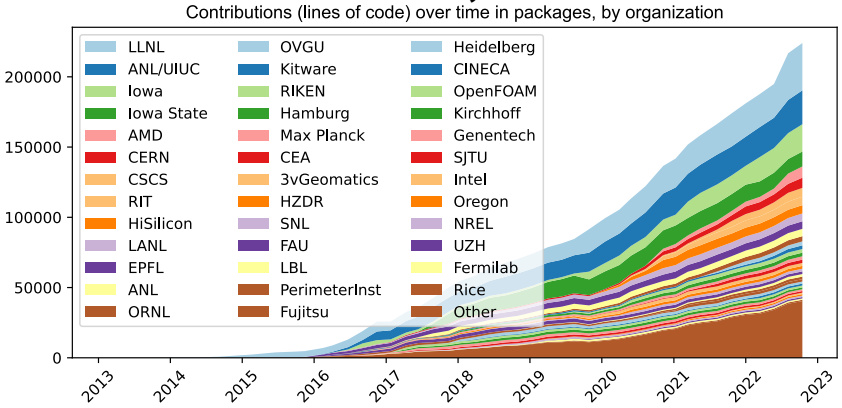
People who want to use or distribute software for HPC!

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

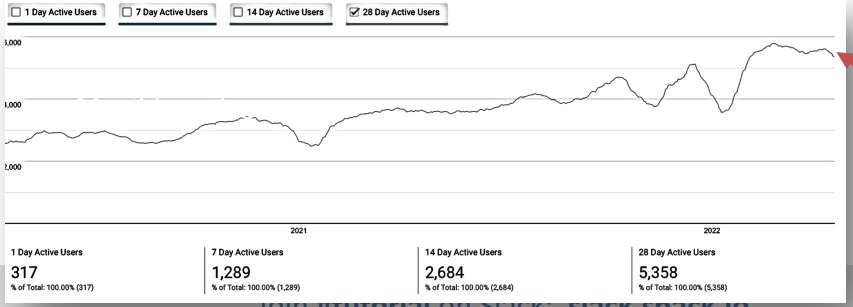
Spack sustains the HPC software ecosystem with the help of its many contributors



Over 6,700 software packages
Over 1,100 contributors

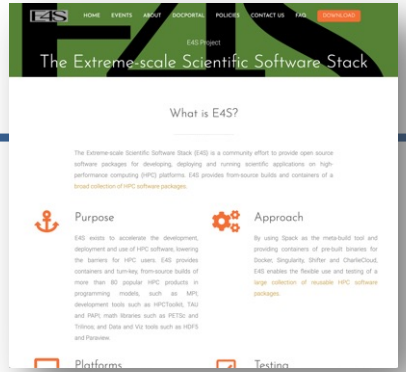


Most package contributions are ***not*** from DOE
But they help sustain the DOE ecosystem!



Nearly 6,000 monthly active users
(per documentation site)

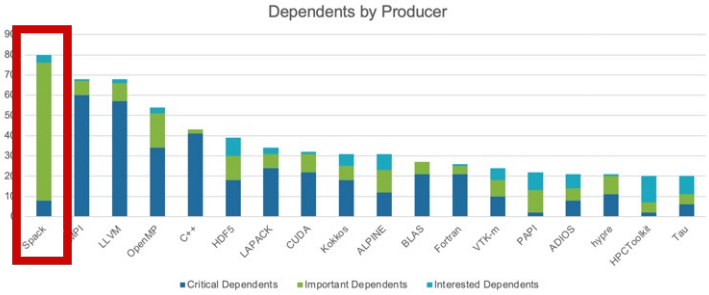
Spack is critical for ECP's mission to create a robust, capable exascale software ecosystem.



https://e4s.io

EXASCALE COMPUTING PROJECT

- Spack will be used to build software for the three upcoming U.S. exascale systems
- ECP has built the Extreme Scale Scientific Software Stack (E4S) with Spack – more at https://e4s.io
- Spack will be integral to upcoming ECP testing efforts.



Spack is the most depended-upon project in ECP

One month of Spack development is pretty busy!

October 12, 2021 – November 12, 2021

Period: 1 month

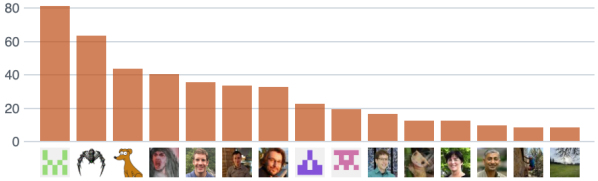
Overview

671 Active Pull Requests

145 Active Issues

536 Merged Pull Requests	**135** Open Pull Requests	**75** Closed Issues	**70** New Issues

Excluding merges, **173 authors** have pushed **571 commits** to develop and **634 commits** to all branches. On develop, **703 files** have changed and there have been **20,730 additions** and **3,807 deletions**.



1 Release published by **1** person

v0.17.0
published 7 days ago

536 Pull requests merged by **151** people

Spack's widespread adoption has drawn contributions and collaborations with many vendors

- **AWS** invests significantly in cloud credits for Spack build farm
  - Joint Spack tutorial with AWS had 125+ participants
  - Joint AWS/AHUG Spack Hackathon drew 60+ participants
- **AMD** has contributed ROCm packages and compiler support
  - 55+ PRs mostly from AMD, also others
  - ROCm, HIP, aocc packages are all in Spack now
- **HPE/Cray** is doing internal CI for Spack packages, in the Cray environment
- **Intel** contributing OneApi support and licenses for our build farm
- **NVIDIA** contributing NVHPC compiler support and other features
- **Fujitsu and RIKEN** have contributed a **huge** number of packages for ARM/a64fx support on Fugaku
- **ARM** and **Linaro** members contributing ARM support
  - 400+ pull requests for ARM support from various companies

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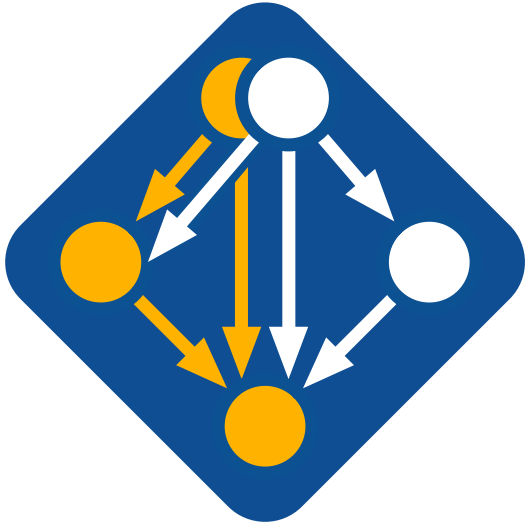
Spack v0.19.0 was released last week!

- Major new features:
  1. **Package requirements**
  2. **Environment UI improvements**
  3. **Packages with multiple build systems**
  4. Compiler/variant propagation
  5. Enhanced git versions
  6. Better Cray EX Support
  7. Testing and CI improvements
  8. Experimental binding link model

***Bold items covered in today's tutorial**



github.com/spack/spack

Full release notes:
https://github.com/spack/spack/releases/tag/v0.19.0

Spack is not the only tool that automates builds


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

2. **Build-from-source Package Managers**
   - Homebrew, LinuxBrew — http://brew.sh
   - MacPorts — https://www.macports.org
   - Gentoo — https://gentoo.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 has unoptimized binaries

Hands-on Time: Spack Basics

Follow script at **spack-tutorial.readthedocs.io**

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 provides a *spec* syntax to describe customized package 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=cascadelake         set target microarchitecture
$ spack install mpileaks@3.3 ^mpich@3.2 %gcc@4.9.3      ^ dependency constraints
```

- 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 packages are *parameterized* using the spec syntax

Python DSL defines many ways to build

```
from spack import *

class Kripke(CMakePackage):
    """Kripke is a simple, scalable, 3D Sn deterministic particle transport 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):
        mkdirp(prefix.bin)
        install('../spack-build/kripke', prefix.bin)
```

Base package (CMake support)

Metadata at the class level

Versions

Variants (build options)

Dependencies (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.

***One* package.py file per software project!**

Conditional variants simplify packages

CudaPackage: a mix-in for packages that use CUDA

```
class CudaPackage(PackageBase):
    variant('cuda', default=False,
            description='Build with CUDA')

    variant('cuda_arch',
            description='CUDA architecture',
            values=any_combination_of(cuda_arch_values),
            when='+cuda')

    depends_on('cuda', when='+cuda')

    depends_on('cuda@9.0:',     when='cuda_arch=70')
    depends_on('cuda@9.0:',     when='cuda_arch=72')
    depends_on('cuda@10.0:',    when='cuda_arch=75')

    conflicts('%gcc@9:', when='+cuda ^cuda@:10.2.89 target=x86_64:')
    conflicts('%gcc@9:', when='+cuda ^cuda@:10.1.243 target=ppc64le:')
```

cuda is a variant (build option)

cuda_arch is only present if cuda is enabled

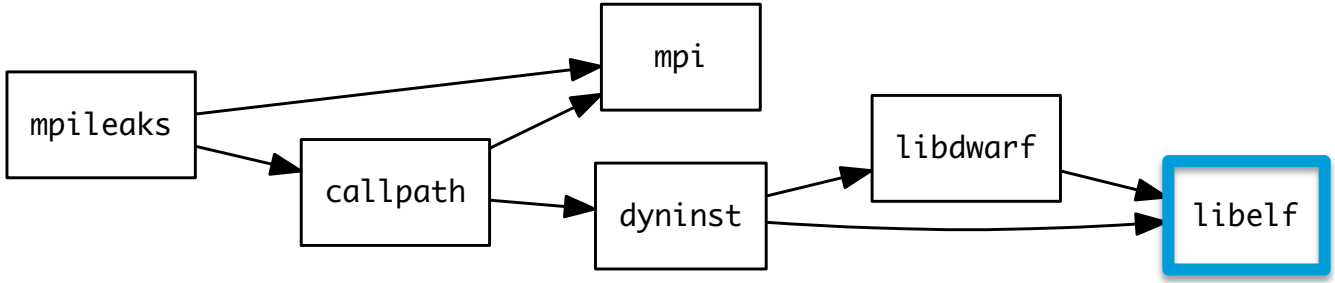
dependency on cuda, but only if cuda is enabled

constraints on cuda version

compiler support for x86_64 and ppc64le

There is a lot of expressive power in the Spack package DSL.

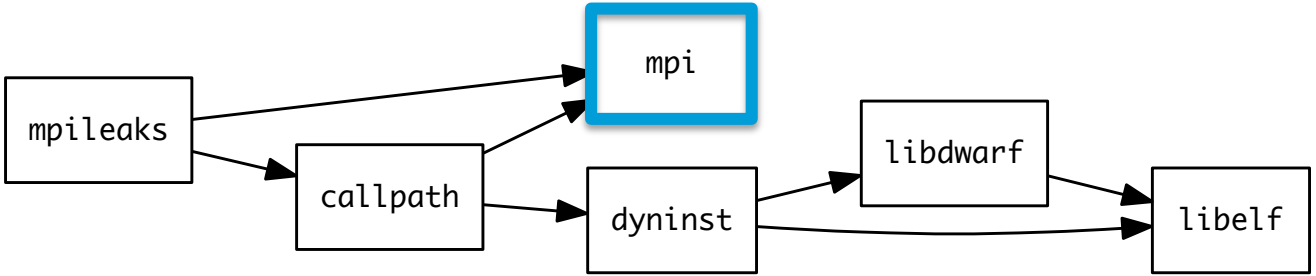
Spack Specs can constrain versions of dependencies




```
$ 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:
```

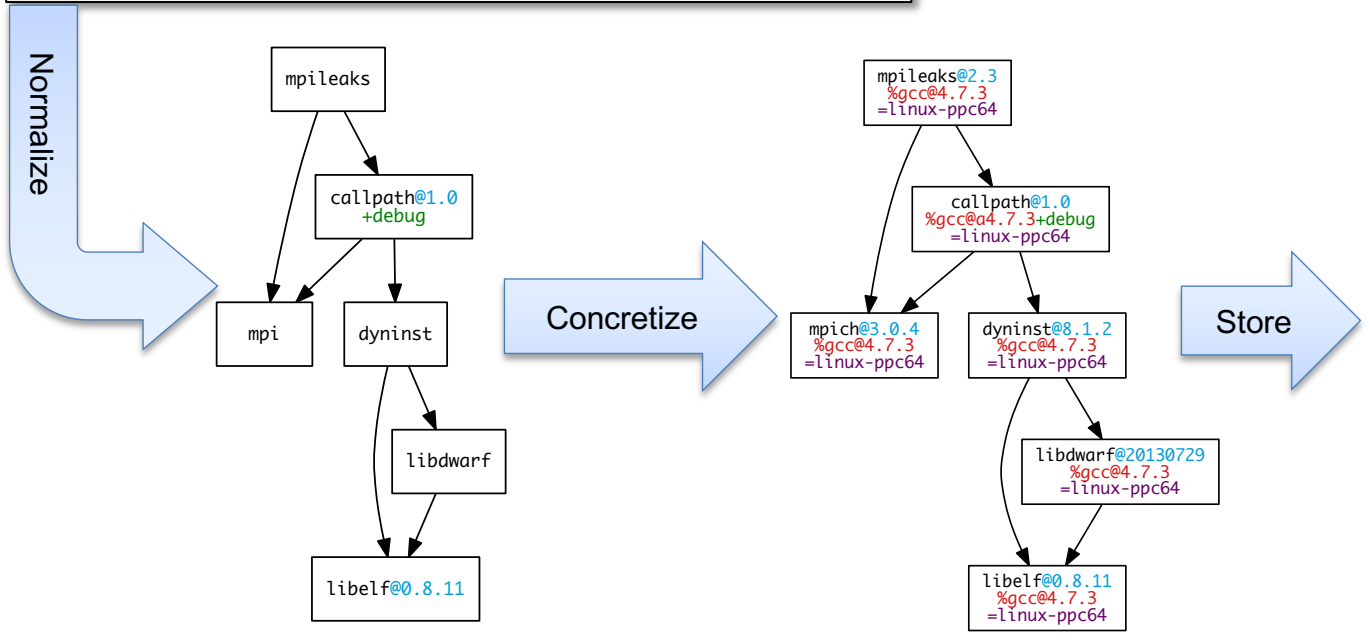
- Let Spack choose MPI implementation, as long as it provides MPI 2 interface:

```
$ 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



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
...
```

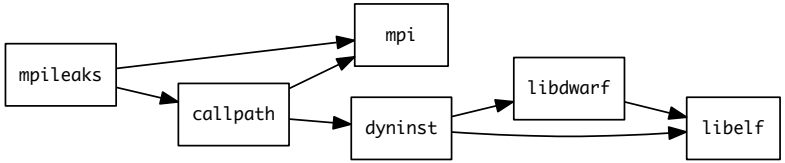

Abstract, normalized spec with some dependencies.

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

Detailed provenance is stored with the installed package

Hashing allows us to handle combinatorial complexity

Dependency DAG



Hash

Installation Layout

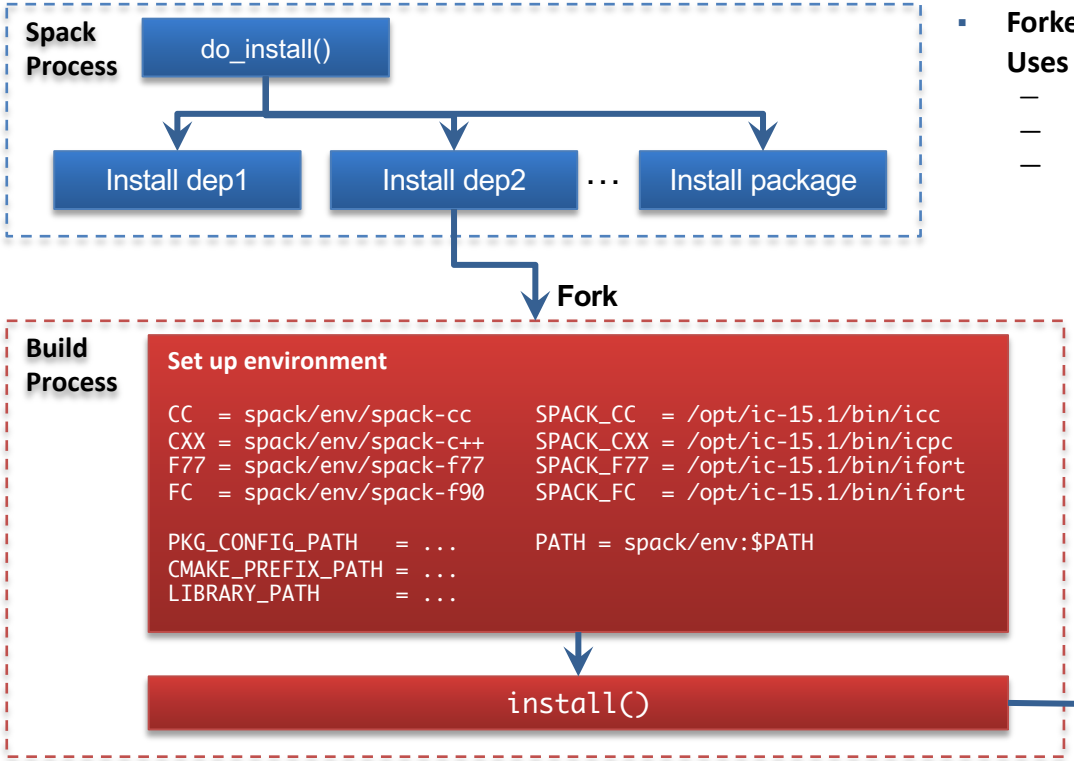
```
opt
└── spack
    ├── linux-rhel7-skylake
    |   └── gcc-8.3.0
    |       ├── mpileaks-1.0-hc4sm4vuzpm4znmvrfzri4ow2mkphe2e
    |       ├── callpath-1.0.4-daqqpssxb6qbfrztsezkmhus3xoflbsy
    |       ├── openmpi-4.1.4-u64v26igxvxyn23hysmklfums6tgjv5r
    |       ├── dyninst-12.1.0-u64v26igxvxyn23hysmklfums6tgjv5r
    |       ├── libdwarf-20180129-u5eawkvaoc7vonabe6nndkcfwuv233cj
    |       └── libelf-0.8.13-x46q4wm46ay4pltriijbgizxjrhbaka6
```

- Each unique dependency graph is a unique ***configuration***.
- Each configuration in a unique directory.
  - Multiple configurations of the same package can coexist.

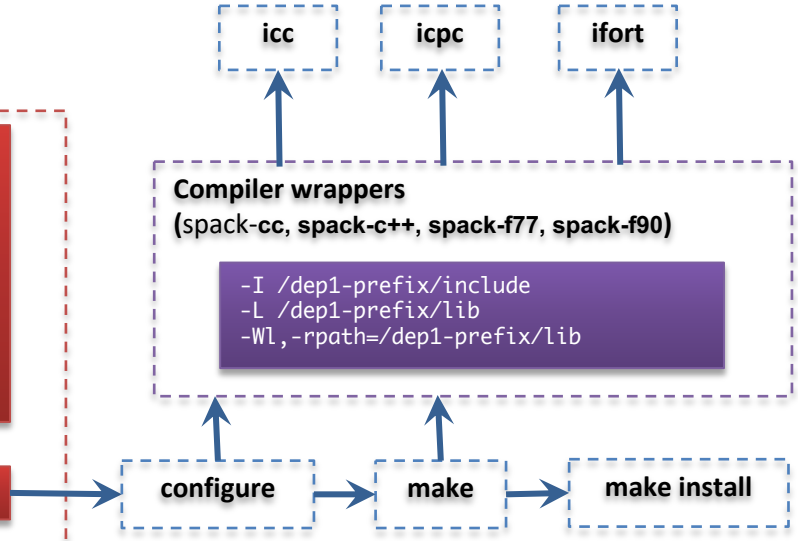
Hash of entire directed acyclic graph (DAG) is appended to each prefix.

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*

An isolated compilation environment allows Spack to easily swap compilers



- **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)



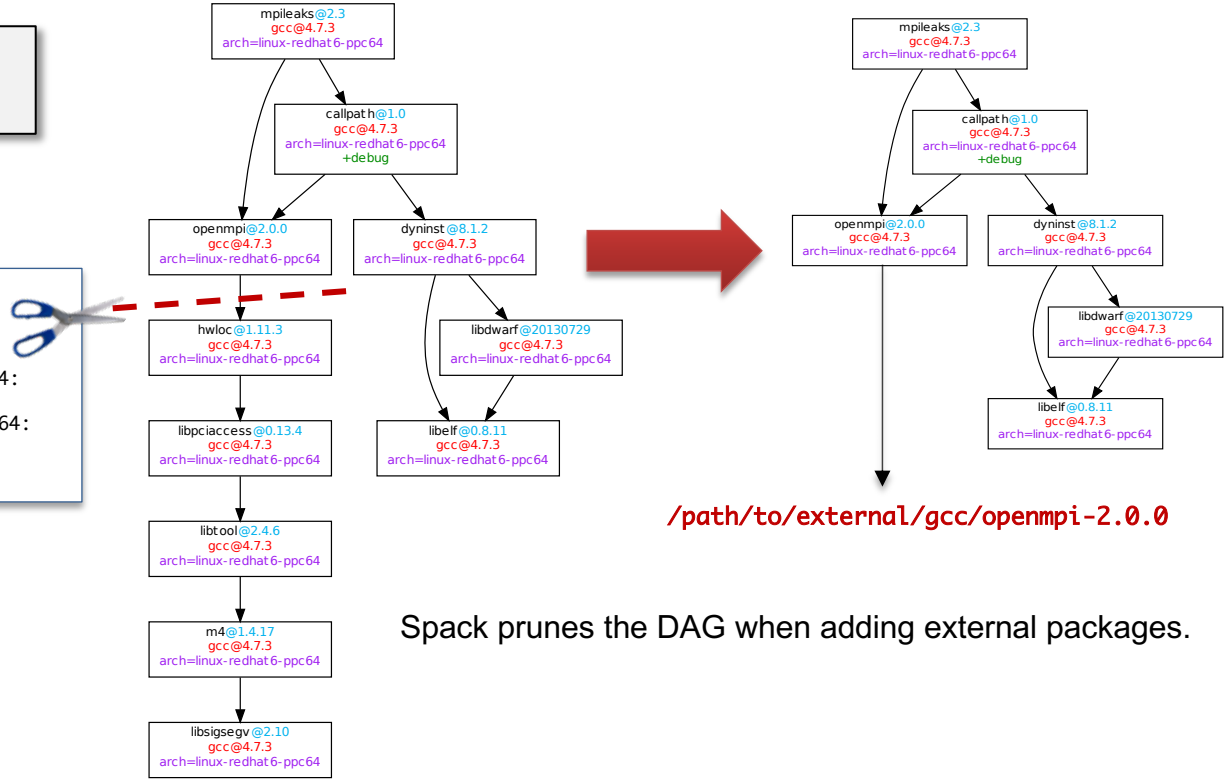
We can configure Spack to build with external software

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

packages.yaml

```yaml
packages:
  mpi:
    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
      ...
```

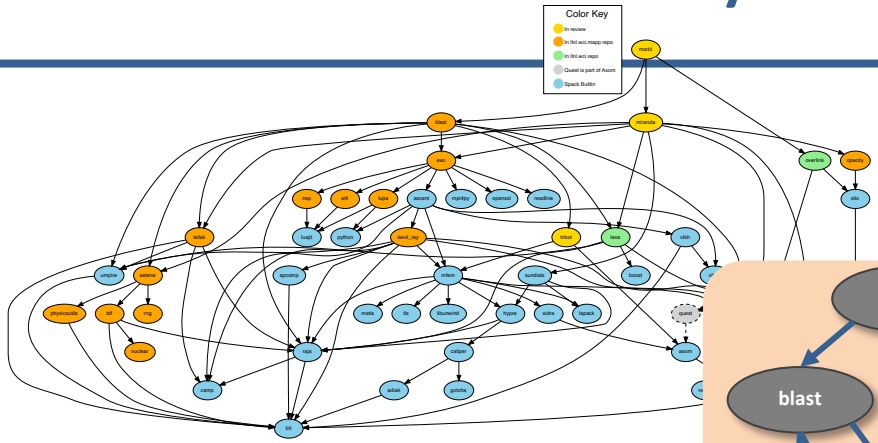
Users register external packages in a configuration file (more on these later).



Spack prunes the DAG when adding external packages.

Spack package repositories allow stacks to be layered

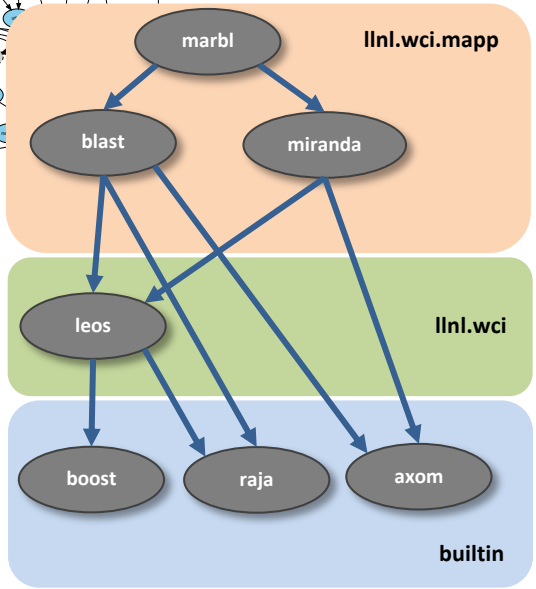
LLNL MARBL multi-physics application



MARBL Application Packages

Common internal packages

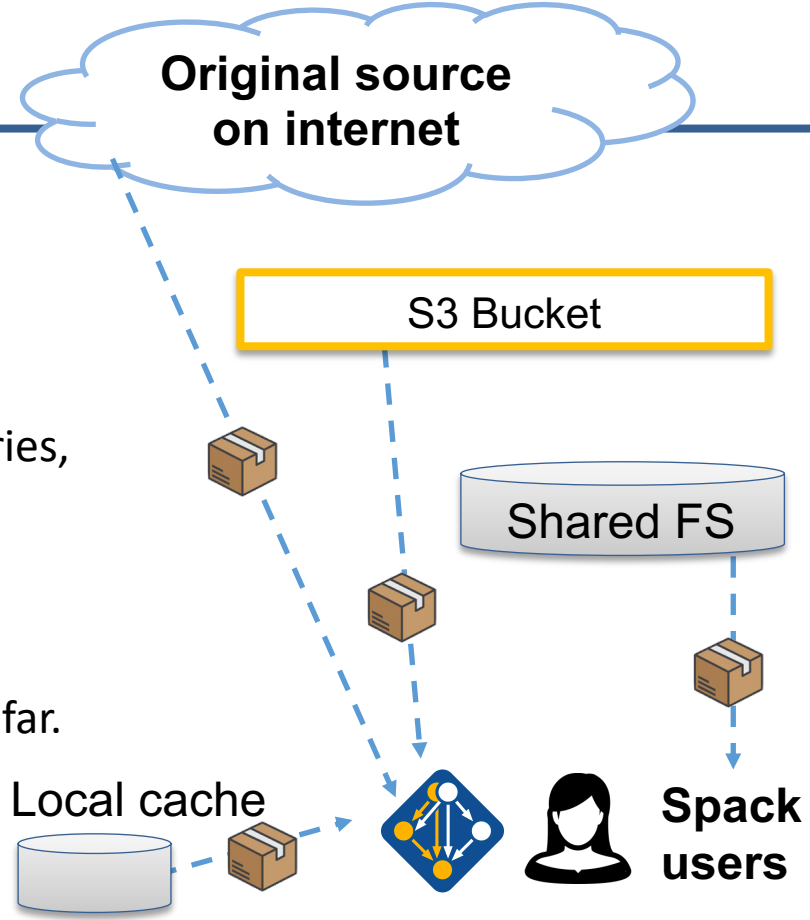
Open Source Spack packages




```
$ spack repo create /path/to/my_repo
$ spack repo add my_repo
$ spack repo list
==> 2 package repositories.
my_repo    /path/to/my_repo
builtin    spack/var/spack/repos/builtin
```

Spack mirrors

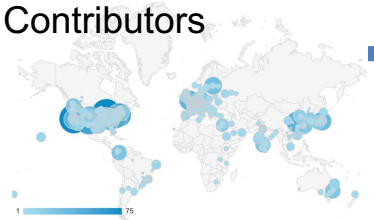
- Spack allows you to define *mirrors:*
  - Directories in the filesystem
  - On a web server
  - In an S3 bucket
- Mirrors are archives of fetched tarballs, repositories, and other resources needed to build
  - Can also contain binary packages
- By default, Spack maintains a mirror in var/spack/cache of everything you've fetched so far.
- You can host mirrors internal to your site
  - See the documentation for more details



The concretizer includes information from packages, configuration, and CLI

Dependency solving is NP-hard

Contributors



- new versions
- new dependencies
- new constraints

package.py repository

spack developers — default config `packages.yaml`

admins, users — local preferences config `packages.yaml`

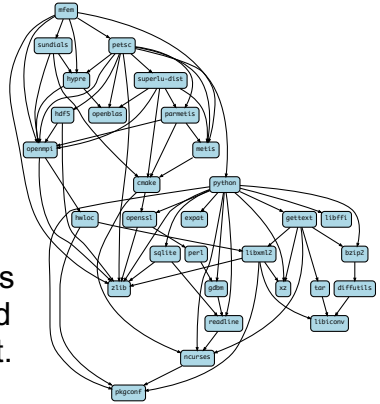
users — local environment config `spack.yaml`

users — Command line constraints

```
spack install hdf5@1.12.0 +debug
```

concretizer

Concrete spec is fully constrained and can be built.



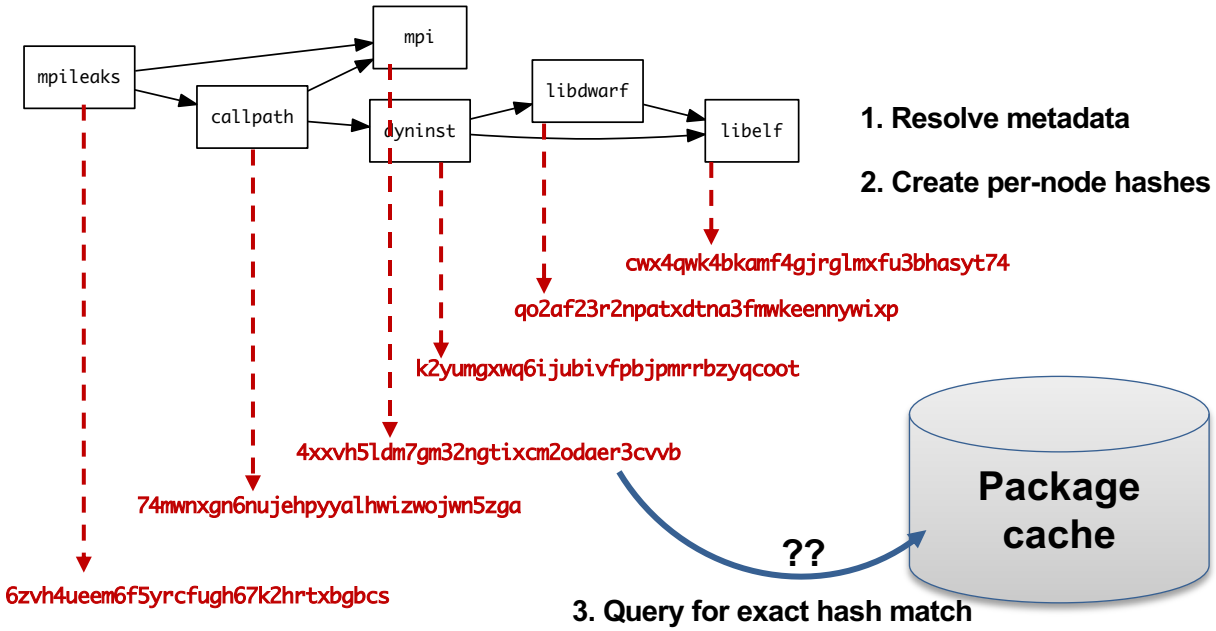
We use logic programming to simplify package solving

- New concretizer leverages Clingo (see potassco.org)
- Clingo is an Answer Set Programming (ASP) solver
  - ASP looks like Prolog; leverages SAT solvers for speed/correctness
  - ASP program has 2 parts:
    1. Large list of facts generated from our package repositories and config
    2. Small logic program (~800 lines)
       - includes constraints and optimization criteria
- New algorithm on the Spack side is conceptually simpler:
  - Generate facts for all possible dependencies, send to logic program
  - Optimization criteria express preferences more clearly
  - Build a DAG from the results
- New concretizer solves many specs that old concretizer can't
  - Backtracking is a huge win – many issues resolved
  - Conditional logic that was complicated before is now much easier

```
%-----------------------------------------------------------------------------
% Package: ucx
%-----------------------------------------------------------------------------
version_declared("ucx", "1.6.1", 0).
version_declared("ucx", "1.6.0", 1).
version_declared("ucx", "1.5.2", 2).
version_declared("ucx", "1.5.1", 3).
version_declared("ucx", "1.5.0", 4).
version_declared("ucx", "1.4.0", 5).
version_declared("ucx", "1.3.1", 6).
version_declared("ucx", "1.3.0", 7).
version_declared("ucx", "1.2.2", 8).
version_declared("ucx", "1.2.1", 9).
version_declared("ucx", "1.2.0", 10).

variant("ucx", "thread_multiple").
variant_single_value("ucx", "thread_multiple").
variant_default_value("ucx", "thread_multiple", "False").
variant_possible_value("ucx", "thread_multiple", "False").
variant_possible_value("ucx", "thread_multiple", "True").

declared_dependency("ucx", "numactl", "build").
declared_dependency("ucx", "numactl", "link").
node("numactl") :- depends_on("ucx", "numactl"), node("ucx").

declared_dependency("ucx", "rdma-core", "build").
declared_dependency("ucx", "rdma-core", "link").
node("rdma-core") :- depends_on("ucx", "rdma-core"), node("ucx").


%-----------------------------------------------------------------------------
% Package: util-linux
%-----------------------------------------------------------------------------
version_declared("util-linux", "2.29.2", 0).
version_declared("util-linux", "2.29.1", 1).
version_declared("util-linux", "2.25", 2).

variant("util-linux", "libuuid").
variant_single_value("util-linux", "libuuid").
variant_default_value("util-linux", "libuuid", "True").
variant_possible_value("util-linux", "libuuid", "False").
variant_possible_value("util-linux", "libuuid", "True").

declared_dependency("util-linux", "pkgconfig", "build").
declared_dependency("util-linux", "pkgconfig", "link").
node("pkgconfig") :- depends_on("util-linux", "pkgconfig"), node("util-linux").

declared_dependency("util-linux", "python", "build").
declared_dependency("util-linux", "python", "link").
node("python") :- depends_on("util-linux", "python"), node("util-linux").
```

Some facts for the HDF5 package

`--fresh` only reuses builds if hashes match



- Hash matches are very sensitive to small changes
- In many cases, a satisfying cached or already installed spec can be missed
- Nix, Spack, Guix, Conan, and others reuse this way

`--reuse` (now the default) is more aggressive

- --reuse tells the solver about all the installed packages!
- Add constraints for all installed packages, with their hash as the associated ID:

```
installed_hash("openssl","lwatuuysmwkhuahrncywvn77icdhs6mn").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node","openssl").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","version","openssl","1.1.1g").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_platform_set","openssl","darwin").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_os_set","openssl","catalina").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_target_set","openssl","x86_64").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","variant_set","openssl","systemcerts","True").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_compiler_set","openssl","apple-clang").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_compiler_version_set","openssl","apple-clang","12.0.0").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","concrete","openssl").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","depends_on","openssl","zlib","build").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","depends_on","openssl","zlib","link").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","hash","zlib","x2anksgssxsxa7pcnhzg5k3dhgacglze").
```

Telling the solver to minimize builds is surprisingly simple in ASP

1. Allow the solver to *choose* a hash for any package:

```
{ hash(Package, Hash) : installed_hash(Package, Hash) } 1 :- node(Package).
```

2. Choosing a hash means we impose its constraints:

```
impose(Hash) :- hash(Package, Hash).
```

3. Define a build as something *without* a hash:

```
build(Package) :- not hash(Package, _), node(Package).
```

4. Minimize builds!

```
#minimize { 1@100,Package : build(Package) }.
```

With and without --reuse optimization

```
(spackle):solver> spack solve -Il hdf5
==> Best of 9 considered solutions.
==> Optimization Criteria:
  Priority  Criterion                                          Installed  ToBuild
  1         number of packages to build (vs. reuse)                    -       20
  2         deprecated versions used                                   0        0
  3         version weight                                             0        0
  4         number of non-default variants (roots)                     0        0
  5         preferred providers for roots                              0        0
  6         default values of variants not being used (roots)          0        0
  7         number of non-default variants (non-roots)                 0        0
  8         preferred providers (non-roots)                            0        0
  9         compiler mismatches                                        0        0
  10        OS mismatches                                              0        0
  11        non-preferred OS's                                         0        0
  12        version badness                                            0        2
  13        default values of variants not being used (non-roots)      0        0
  14        non-preferred compilers                                    0        0
  15        target mismatches                                          0        0
  16        non-preferred targets                                      0        0

  -  zzngfs3  hdf5@1.10.7%apple-clang@13.0.0~cxx~fortran~hl~ipo~java+mpi+shared~szip~threadsafe+tools api=default b
  -  nsylovq      ^cmake@3.21.4%apple-clang@13.0.0~doc+ncurses+openssl+ownlibs~qt build_type=Release arch=darwin-bi
  -  xdbaqeo          ^ncurses@6.2%apple-clang@13.0.0~symlinks+termlib abi=none arch=darwin-bigsur-skylake
  -  kfureok              ^pkgconf@1.8.0%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -  5ekd4ap          ^openssl@1.1.1l%apple-clang@13.0.0~docs certs=system arch=darwin-bigsur-skylake
  -  xz6a265              ^perl@5.34.0%apple-clang@13.0.0+cpanm+shared+threads arch=darwin-bigsur-skylake
  -  xgt3tls                  ^berkeley-db@18.1.40%apple-clang@13.0.0+cxx~docs+stl patches=b231fcc4d5cff05e5c3a4814
  -  65edjf6                  ^bzip2@1.0.8%apple-clang@13.0.0~debug~pic+shared arch=darwin-bigsur-skylake
  -  662adoo                      ^diffutils@3.8%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -  fu7tfsr                          ^libiconv@1.16%apple-clang@13.0.0 libs=shared,static arch=darwin-bigsur-skyla
  -  vjg67nd                  ^gdbm@1.19%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -  tjceldr                      ^readline@8.1%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -  xevvljj                  ^zlib@1.2.11%apple-clang@13.0.0+optimize+pic+shared arch=darwin-bigsur-skylake
  -  xelfobh      ^openmpi@4.1.1%apple-clang@13.0.0~atomics~cuda~cxx~cxx_exceptions+gpfs~internal-hwloc~java~legacy
  -  zruns75          ^hwloc@2.6.0%apple-clang@13.0.0~cairo~cuda~gl~libudev+libxml2~netloc~nvml~opencl~pci~rocm+sha
  -  ib4fnkf              ^libxml2@2.9.12%apple-clang@13.0.0~python arch=darwin-bigsur-skylake
  -  dwiv2ys                  ^xz@5.2.5%apple-clang@13.0.0~pic libs=shared,static arch=darwin-bigsur-skylake
  -  blitnbl          ^libevent@2.1.12%apple-clang@13.0.0+openssl arch=darwin-bigsur-skylake
  -  h7jalyu          ^openssh@8.7p1%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -  7v7bqx2              ^libedit@3.1-20210216%apple-clang@13.0.0 arch=darwin-bigsur-skylake
```

Pure hash-based reuse: all misses

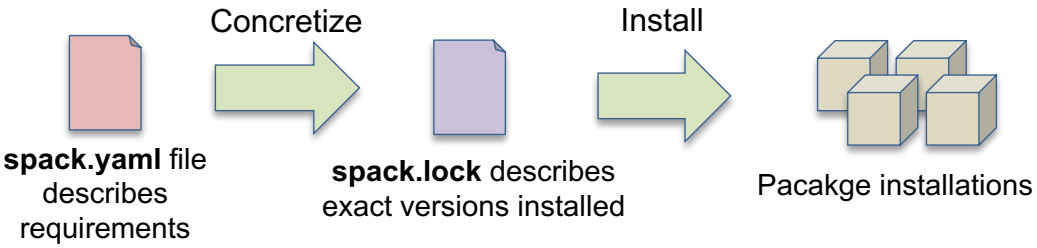
```
(spackle):spack> spack solve --reuse -Il hdf5
==> Best of 10 considered solutions.
==> Optimization Criteria:
  Priority  Criterion                                          Installed  ToBuild
  1         number of packages to build (vs. reuse)                    -        4
  2         deprecated versions used                                   0        0
  3         version weight                                             0        0
  4         number of non-default variants (roots)                     0        0
  5         preferred providers for roots                              0        0
  6         default values of variants not being used (roots)          0        0
  7         number of non-default variants (non-roots)                 2        0
  8         preferred providers (non-roots)                            0        0
  9         compiler mismatches                                        0        0
  10        OS mismatches                                              0        0
  11        non-preferred OS's                                         0        0
  12        version badness                                            6        0
  13        default values of variants not being used (non-roots)      1        0
  14        non-preferred compilers                                   15        4
  15        target mismatches                                          0        0
  16        non-preferred targets                                      0        0

  -  yfkfnsp  hdf5@1.10.7%apple-clang@12.0.5~cxx~fortran~hl~ipo~java+mpi+shared~szip~threadsafe+tools api=default
  [+] zd4m26e     ^cmake@3.21.1%apple-clang@12.0.5~doc+ncurses+openssl+ownlibs~qt build_type=Release arch=darwin-
  [+] 63i52xr         ^ncurses@6.2%apple-clang@12.0.5~symlinks+termlib abi=none arch=darwin-bigsur-skylake
  [+] us36bwr         ^openssl@1.1.1l%apple-clang@12.0.5~docs+systemcerts arch=darwin-bigsur-skylake
  [+] 74mwnxg             ^zlib@1.2.11%apple-clang@12.0.5+optimize+pic+shared arch=darwin-bigsur-skylake
  -  3ijfnel      ^openmpi@4.1.1%apple-clang@12.0.5~atomics~cuda~cxx~cxx_exceptions+gpfs~internal-hwloc~java~leg
  -  jxexyb7          ^hwloc@2.6.0%apple-clang@12.0.5~cairo~cuda~gl~libudev+libxml2~netloc~nvml~opencl~pci~rocm+
  [+] ckdn5zf             ^libxml2@2.9.12%apple-clang@12.0.5~python arch=darwin-bigsur-skylake
  [+] k7auat3                 ^libiconv@1.16%apple-clang@12.0.5 libs=shared,static arch=darwin-bigsur-skylake
  [+] kzyumgx                 ^xz@5.2.5%apple-clang@12.0.5~pic libs=shared,static arch=darwin-bigsur-skylake
  [+] grgtlcd         ^pkgconf@1.8.0%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  -  nnc66ug          ^libevent@2.1.12%apple-clang@12.0.5+openssl arch=darwin-bigsur-skylake
  [+] 63xbksk         ^openssh@8.6p1%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  [+] snhgldt             ^libedit@3.1-20210216%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  [+] gbkmtdd         ^perl@5.34.0%apple-clang@12.0.5+cpanm+shared+threads arch=darwin-bigsur-skylake
  [+] cnvkifs             ^berkeley-db@18.1.40%apple-clang@12.0.5+cxx~docs+stl patches=b231fcc4d5cff05e5c3a4814f
  [+] 7d5woqt             ^bzip2@1.0.8%apple-clang@12.0.5~debug~pic+shared arch=darwin-bigsur-skylake
  [+] vh6di3i             ^gdbm@1.19%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  [+] ggy3v4l                 ^readline@8.1%apple-clang@12.0.5 arch=darwin-bigsur-skylake
```

With reuse: 16 packages were reusable

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
```

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



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
```

- spack.yaml describes project requirements
- spack.lock describes exactly what versions/configurations were installed, allows them to be reproduced.
- Can be used to maintain configuration of a software stack.
  - Can easily version an environment in a repository

Concrete spack.lock file (generated)


```
{
 "concrete_specs": {
   "6s63so2kstp3zyvjezglndmavy6l3nul": {
     "hdf5": {
         "version": "1.10.5",
         "arch": {
             "platform": "darwin",
             "platform_os": "mojave",
             "target": "x86_64"
         },
         "compiler": {
             "name": "clang",
             "version": "10.0.0-apple"
         },
         "namespace": "builti
         "parameters":
```

We'll resume at: 10:30am

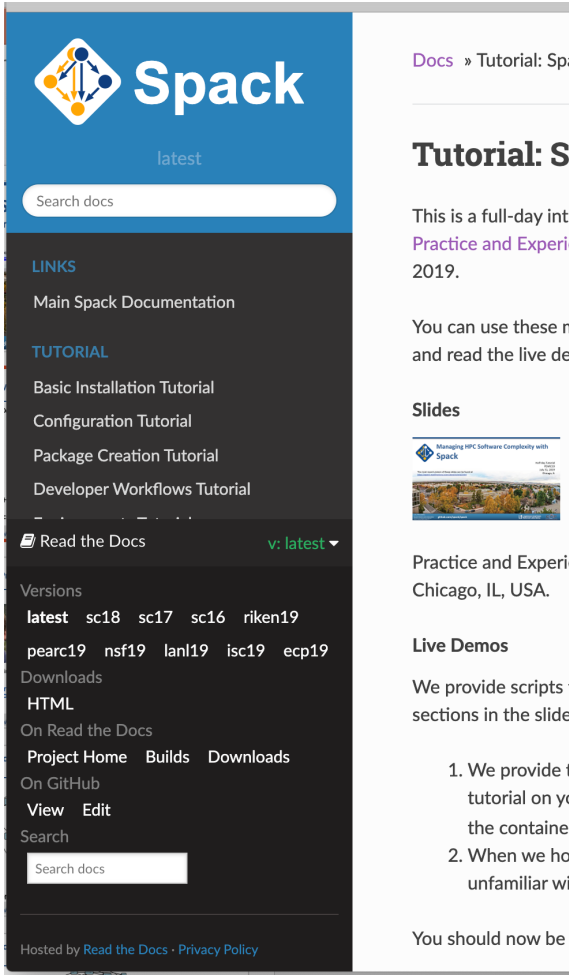
Find the slides and associated scripts here:

spack-tutorial.readthedocs.io

Remember to join Spack slack so you can get help after ISC!

slack.spack.io

Join the **#tutorial** channel!



Environments, `spack.yaml` and `spack.lock`

Follow script at **spack-tutorial.readthedocs.io**

Hands-on Time: Configuration

Follow script at **spack-tutorial.readthedocs.io**

We'll resume at:
1:30pm

Find the slides and associated scripts here:

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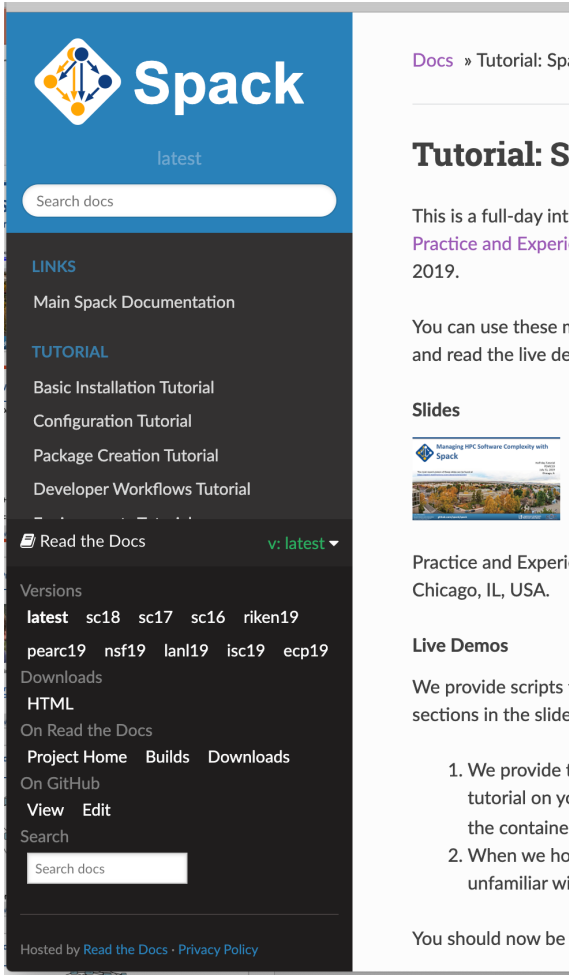

Hands-on Time:
Stacks

Follow script at **spack-tutorial.readthedocs.io**

Hands-on Time:
Creating Packages

Follow script at **spack-tutorial.readthedocs.io**

We'll resume at: 3:30pm

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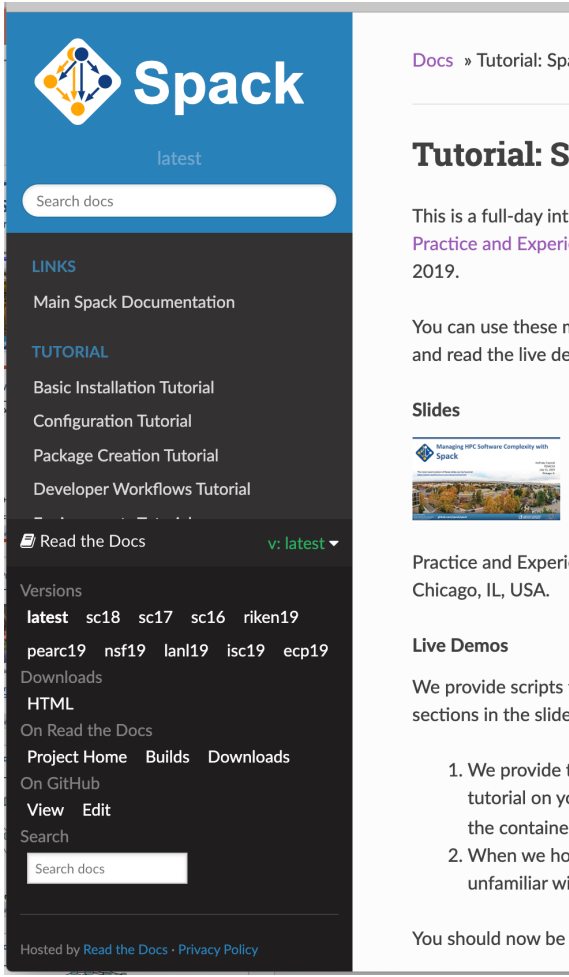


Hands-on Time:
Developer Workflows

Follow script at **spack-tutorial.readthedocs.io**

Hands-on Time: Scripting

Follow script at **spack-tutorial.readthedocs.io**

Hands-on Time:
Mirrors and Build Caches

Follow script at **spack-tutorial.readthedocs.io**

More Features and the Road Ahead

Environments have enabled us to add build many features to support developer workflows

```
class Cmake(Package):
    executables = ['cmake']

    @classmethod
    def determine_spec_details(cls, prefix, exes_in_prefix):
        exe_to_path = dict(
            (os.path.basename(p), p) for p in exes_in_prefix
        )
        if 'cmake' not in exe_to_path:
            return None

        cmake = spack.util.executable.Executable(exe_to_path['cmake'])
        output = cmake('--version', output=str)
        if output:
            match = re.search(r'cmake.*version\s+(\S+)', output)
            if match:
                version_str = match.group(1)
                return Spec('cmake@{0}'.format(version_str))
```

package.py

```
packages:
  cmake:
    externals:
      - spec: cmake@3.15.1
        prefix: /usr/local
```

spack.yaml configuration

spack external find

Automatically find and configure external packages on the system

```
class Libsigsegv(AutotoolsPackage, GNUMirrorPackage):
    """GNU libsigsegv is a library for handling page faults in user mode."""

    # ... spack package contents ...

    extra_install_tests = 'tests/.libs'

    def test(self):
        data_dir = self.test_suite.current_test_data_dir
        smoke_test_c = data_dir.join('smoke_test.c')

        self.run_test(
            'cc', [
                '-I%s' % self.prefix.include,
                '-L%s' % self.prefix.lib, '-lsigsegv',
                smoke_test_c,
                '-o', 'smoke_test'
            ]
            purpose='check linking')

        self.run_test(
            'smoke_test', [], data_dir.join('smoke_test.out'),
            purpose='run built smoke test')

        self.run_test('sigsegv1': ['Test passed'], purpose='check sigsegv1 output')
        self.run_test('sigsegv2': ['Test passed'], purpose='check sigsegv2 output')
```

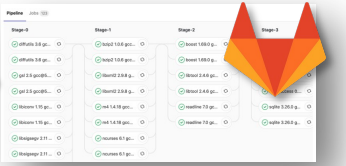
package.py

spack test

Packages know how to run their own test suites

```
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
```

spack.yaml



.gitlab-ci.yml CI pipeline

spack ci

Automatically generate parallel build pipelines
(more on this later)

```
spack:
  specs:
  - gromacs+mpi
  - mpich

  container:
    # Select the format of the recipe e.g. docker,
    # singularity or anything else that is currently sup
    format: docker

    # Select from a valid list of images
    base:
      image: "centos:7"
      spack: develop

    # Whether or not to strip binaries
    strip: true

    # Additional system packages that are needed at runt
    os_packages:
    - libgomp

    # Extra instructions
    extra_instructions:
      final: |
RUN echo 'export PS1="\[$(tput bold)\]\[$(tput setaf 1)"

    # Labels for the image
    labels:
      app: "gromacs"
      mpi: "mpich"
```

```
# Build stage with Spack pre-installed and ready to be used
FROM spack/centos7:latest as builder

# What we want to install and how we want to install it
# is specified in a manifest file (spack.yaml)
RUN mkdir /opt/spack-environment \
&&  echo "spacks= " \
&&  echo "  specs2= " \
&&  echo "  - gromacs+mpi" \
&&  echo "  - mpich" \
&&  echo "  concretization: together" \
&&  echo "  unify: true" \
&&  echo "  install_tree: /opt/software" \
&&  echo ". view: /opt/view" > /opt/spack-environment/spack.yaml

# Install the software, remove unnecessary deps
RUN cd /opt/spack-environment && spack install && spack gc -y

# Strip all the binaries
RUN find -L /opt/view/* -type f -exec readlink -f '{}' \; | \
    xargs file -i | \
    grep 'charset=binary' | \
    grep 'x-executable\|x-archive\|x-sharedlib' | \
    awk -F: '{print $1}' | xargs strip -s

# Modifications to the environment that are necessary to run
RUN cd /opt/spack-environment && \
    spack env activate --sh -d . >> /etc/profile.d/z10_spack_environment.sh


# Bare OS image to run the installed executables
FROM centos:7

COPY --from=builder /opt/spack-environment /opt/spack-environment
COPY --from=builder /opt/software /opt/software
COPY --from=builder /opt/view /opt/view
COPY --from=builder /etc/profile.d/z10_spack_environment.sh /etc/profile.d/z10_spack_envi

RUN yum update -y && yum install -y epel-release && yum update -y
&& yum install -y libgomp \
&& rm -rf /var/cache/yum  && yum clean all

RUN echo 'export PS1="\[$(tput bold)\]\[$(tput setaf 1)\][gromacs]\[$(tput setaf 2)\]\u\[$(tput
```

spack containerize

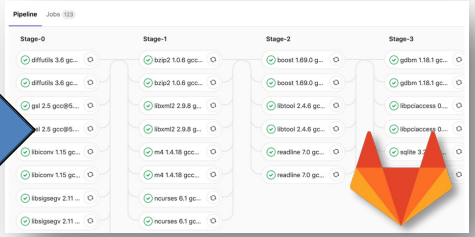
Turn environments into container build recipes

Spack environments are the foundation of Spack CI

- `spack ci` enables any environment to be turned into a build pipeline
- Pipeline generates a `.gitlab-ci.yml` file from spack.lock
- Pipelines can be used just to build, or to generate relocatable binary packages
  - Binary packages can be used to keep the same build from running twice
- Same repository used for spack.yaml can generate pipelines for project

```yaml
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_18.0
      - 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
```

spack.yaml



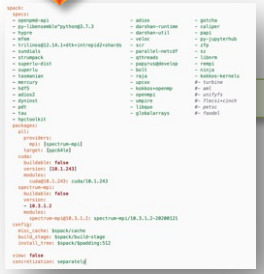
Parallel GitLab build pipeline

We are building a supply chain for HPC

Spack Contributions on GitHub

ci/gitlab/gitlab.spack.io — Pipeline passed on GitLab

gitlab.spack.io



spack.yaml configurations (E4S, SDKs, others)

spack ci

x86_64 and **aarch64** pipelines in **AWS**

ppc64le, GPU pipelines at **U. Oregon**

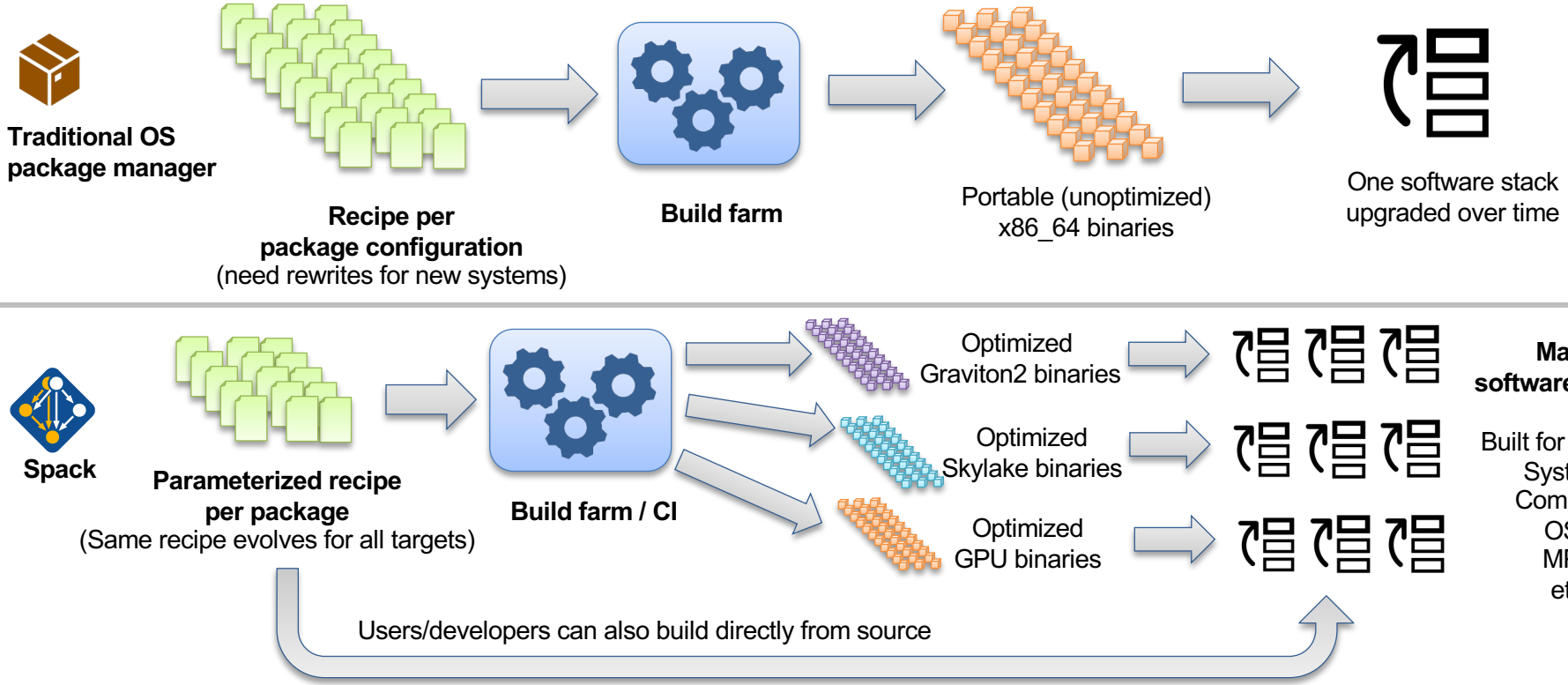
Pipelines at **LLNL** **(Cray PE soon, hopefully)**

GitLab CI builds (changed) packages
- On every pull request
- On every release branch

- **New security model supports untrusted contributions from forks**
  - Sandboxed build caches for test builds; Authoritative builds on mainline only after approved merge

This CI has *greatly* increased reliability of builds for users

Spack's model lowers the maintenance burden of optimized software stacks



We started providing public binaries in June 2022

```
# latest v0.18.x release binaries
spack mirror add https://binaries.spack.io/releases/v0.18

# rolling release: bleeding edge binaries
spack mirror add https://binaries.spack.io/develop
```

- Over 3,000 builds in the cache so far:
  - Amazon Linux 2 x86_64_v4
  - Amazon Linux 2 aarch64
  - Amazon Linux 2 graviton2
  - Ubuntu 18.04 x86_64
- Expect this list to expand!

Our infrastructure enables us to sustainably manage a binary distro

Separate, untrusted S3 buckets

Per-PR build caches

github/pr-28468 | github/pr-28469 | ...

Public, signed binaries in CloudFront distribution

https://binaries.spack.io

develop | releases/v0.18 | ...

Contributors submit package changes

- Iterate on builds in PR
- Caches prevent unnecessary rebuilds

Maintainers review PRs

- Verify PR build succeeded
- Review package code
- Merge to develop

Rebuild and Sign

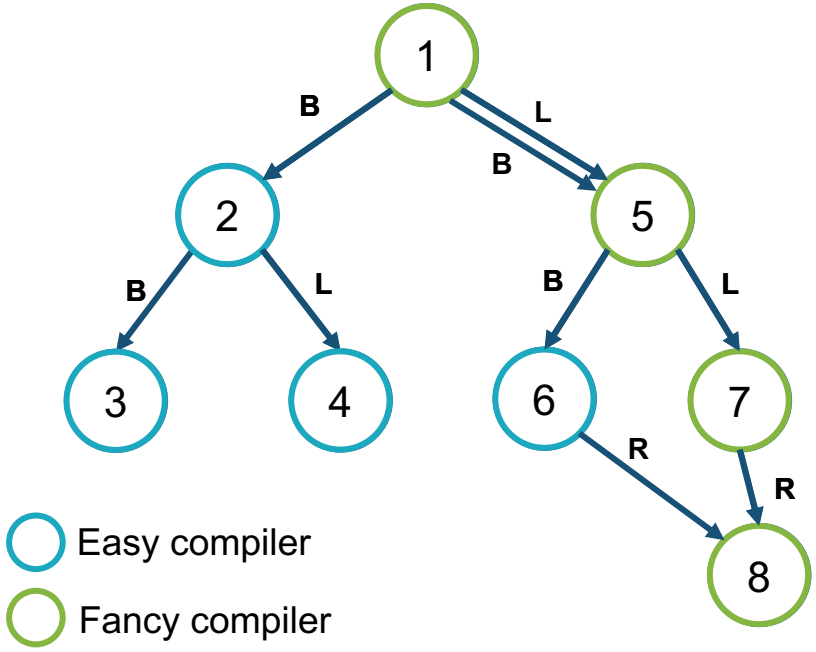
- Published binaries built ONLY from approved code
- Protected signing runners
- Ephemeral keys

- Moves bulk of binary maintenance upstream, onto PRs
  - Production binaries never reuse binaries from untrusted environment

Spack v0.20 roadmap: Separate concretization of build dependencies

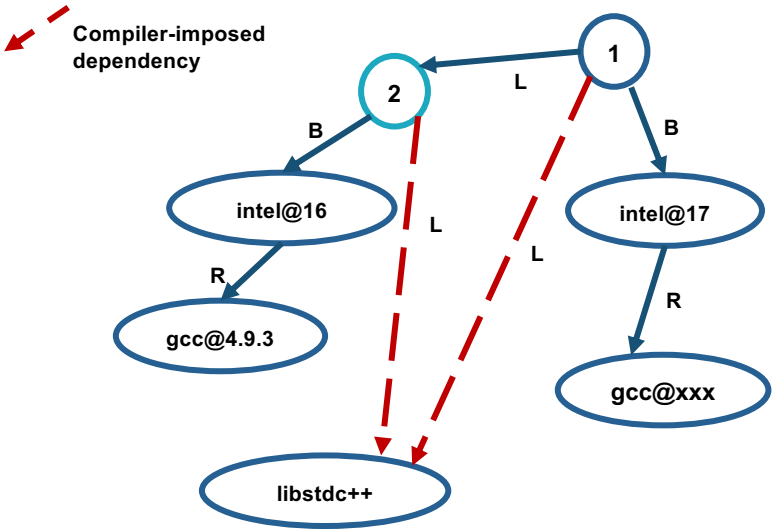
- We want to:
  - Build build dependencies with the "easy" compilers
  - Build rest of DAG (the link/run dependencies) with the fancy compiler
- 2 approaches to modify concretization:
  1. **Separate solves**
     - Solve run and link dependencies first
     - Solve for build dependencies separately
     - May restrict possible solutions (build ←→ run env constraints)
  2. **Separate models**
     - *Allow* a bigger space of packages in the solve
     - Solve *all* runtime environments together
     - May explode (even more) combinatorially

```
spack install pkg1 %intel
```



Spack 0.20 Roadmap: compilers as dependencies

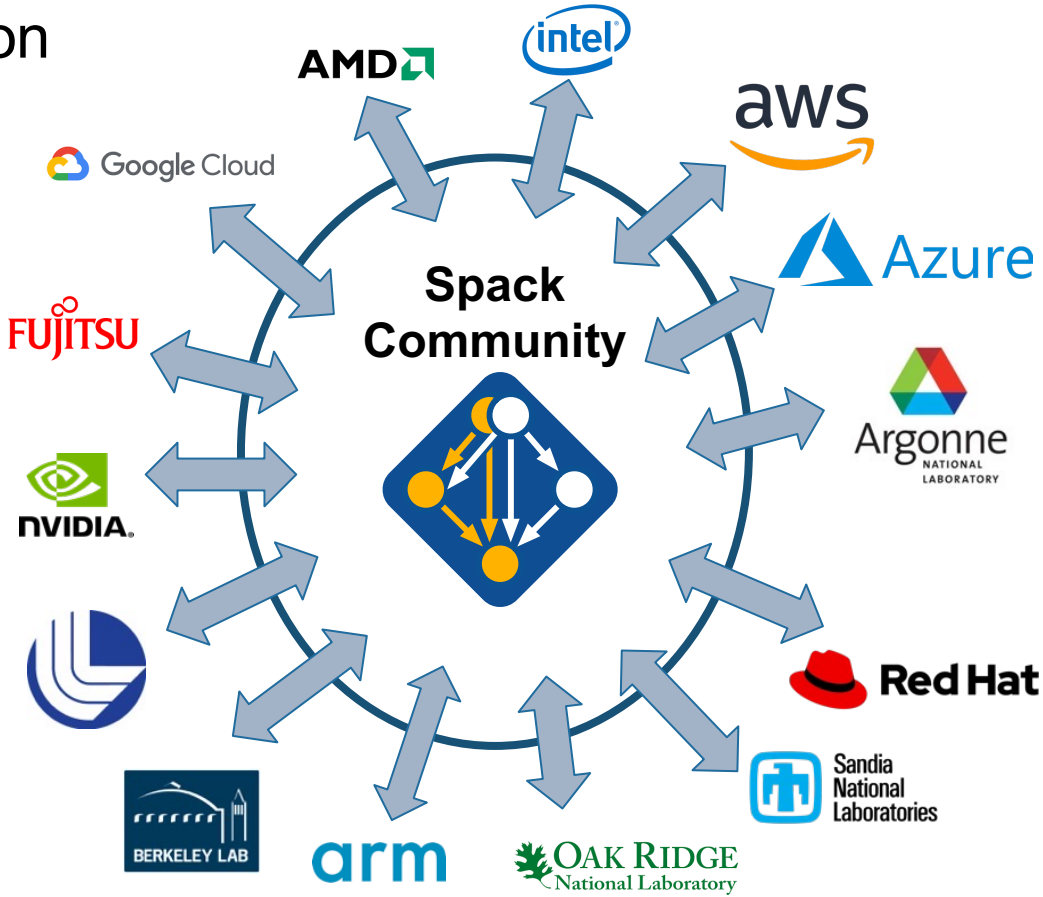
- **We need deeper modeling of compilers to handle compiler interoperability**
  - libstdc++, libc++ compatibility
  - Compilers that depend on compilers
  - Linking executables with multiple compilers
- **First prototype is complete!**
  - We've done successful builds of some packages using compilers as dependencies
  - We need the new concretizer to move forward!
- **Packages that depend on languages**
  - Depend on **cxx@2011**, **cxx@2017**, **fortran@1995**, etc
  - Depend on **openmp@4.5**, other compiler features
  - Model languages, openmp, cuda, etc. as virtuals



Compilers and runtime libs fully modeled as dependencies

Spack's long-term strategy is based around broad adoption and collaboration

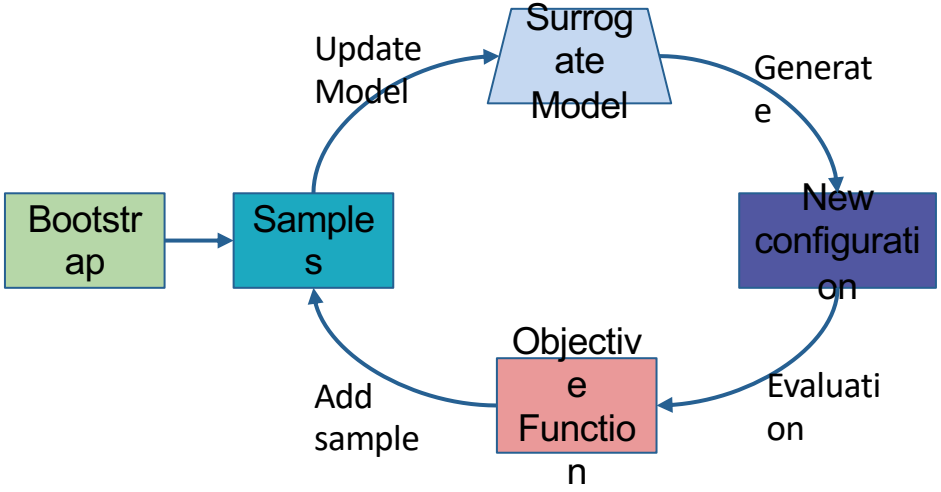
- **Not sustainable without a community**
  - Broad adoption incentivizes contributors
  - Cloud resources and automation absolutely necessary
- **Spack preserves build knowledge in a cross-platform, reusable way**
  - Minimize rewriting recipes when porting
- **CI ensures builds continue to work as packages evolve**
  - Keep packages flexible but verify key configurations
- **Growing contributor base and continuing to automate are the most important priorities**
  - **377 contributors to 0.18 release!**



When would we go 1.0?

- Big things we've wanted for 1.0 are:
  - New concretizer
  - production CI
  - production public build cache
  - Compilers as dependencies
  - Stable package API
    - Enables separate package repository
- After 0.19 we will hopefully have all of these
  - Maybe there won't be a 0.20!

Reliabuild: An Active Learning based Configuration Selection Framework*

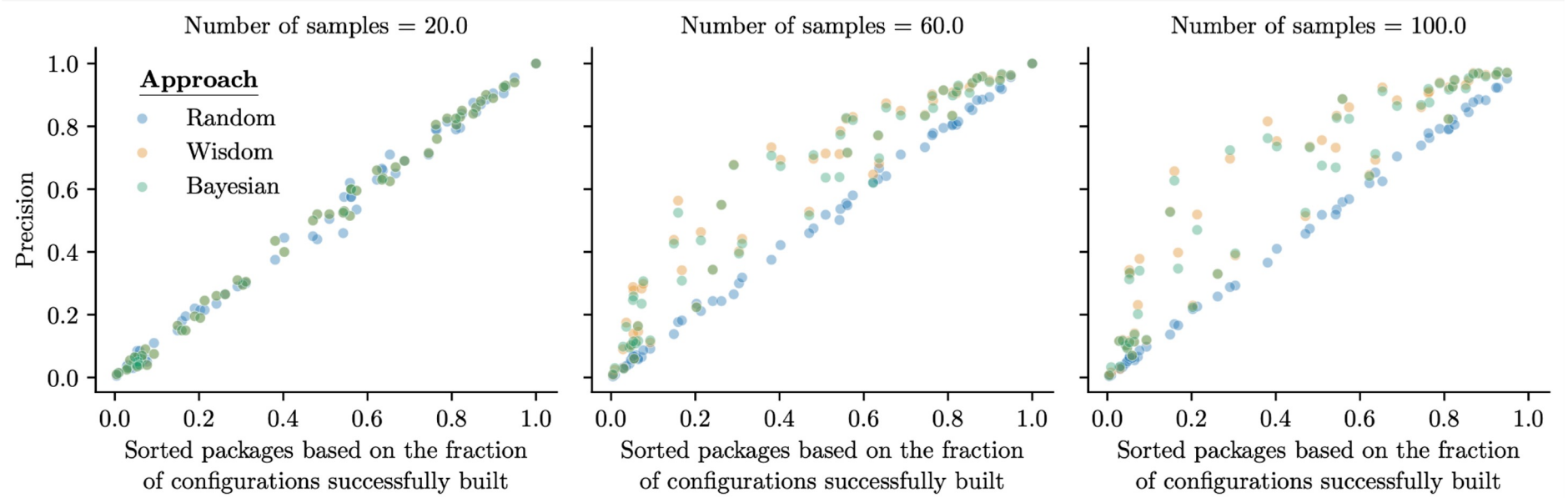


Reliabuild iterates between fitting model and using it to select samples

- An active-learning-based approach for identifying high-fidelity package build configurations
- Iterative sampling method using only a limited set of samples.
  - —Suitable when the true objective function evaluations are expensive
- Surrogate model is used to compute the value of the objective for a configuration

*Reliabuild: Searching for High-Fidelity Builds Using Active Learning; H.Menon, K. Parasyris, T. Scogland, T. Gamblin; MSR'2022

Reliabuild has significantly higher precision than *Random* selection



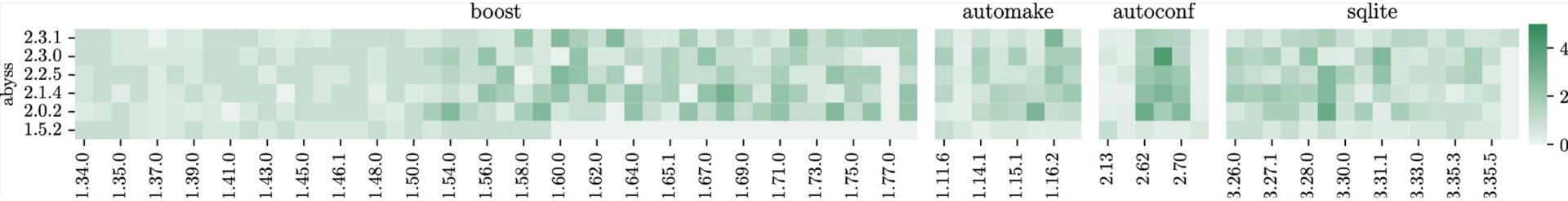
Package Importance Analysis

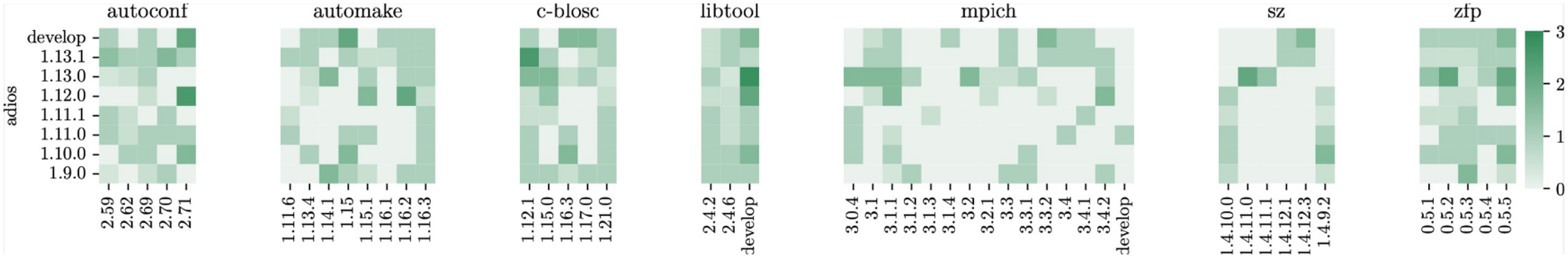
Root package	Dependency ranking				
abyss	autoconf: 0.37	autoconf+m4: 0.37	autoconf+perl: 0.37	libtool+autoconf: 0.29	abyss+autoconf: 0.27
adios	autoconf+perl: 0.27	autoconf+m4: 0.27	autoconf: 0.27	libtool: 0.22	libtool+m4: 0.22
ascent	vtk-h+openmpi: 0.14	vtk-h: 0.14	vtk-h+vtk-m: 0.14	conduit+zlib: 0.12	conduit+hdf5: 0.12
axom	lua: 0.08	lua+ncurses: 0.08	lua+readline: 0.08	lua+unzip: 0.08	axom+openmpi: 0.07
bolt	autoconf+perl: 0.37	autoconf+m4: 0.37	autoconf: 0.37	automake+autoconf: 0.32	automake+perl: 0.30
hypre	openblas+perl: 0.07	openblas: 0.07	hypre+openblas: 0.03	hypre+mpich: 0.02	mpich+findutils: 0.01
hpx	hpx+boost: 0.24	hpx+hwloc: 0.24	hpx+pkgconf: 0.24	hpx+python: 0.24	hpx: 0.24
heffte	heffte: 0.35	heffte+openmpi: 0.30	heffte+fftw: 0.24	cuda+libxml2: 0.19	mpich+findutils: 0.19
hdf5	mpich+findutils: 0.03	mpich+pkgconf: 0.03	mpich+libxml2: 0.03	mpich: 0.03	mpich+libpciaccess: 0.03
ninja	ninja+python: 0.03	python+ncurses: 0.01	python+readline: 0.01	python+pkgconf: 0.01	python+libffi: 0.01
omega-h	omega-h+zlib: 0.24	trilinos: 0.24	trilinos+openblas: 0.24	omega-h: 0.24	omega-h+trilinos: 0.18
openmpi	json-c: 0.30	mariadb+lz4: 0.30	meson: 0.30	gmp: 0.30	python+libffi: 0.30
openpmd-api	hdf5: 0.19	hdf5+zlib: 0.19	hdf5+openmpi: 0.19	hdf5+pkgconf: 0.19	hdf5+cmake: 0.19
papyrus	papyrus+mpich: 0.11	cmake+ncurses: 0.08	cmake: 0.08	papyrus+cmake: 0.08	mpich+findutils: 0.04
plasma	plasma: 0.52	plasma+openblas: 0.26	openblas+perl: 0.13	openblas: 0.13	plasma+cmake: 0.12

- A particular choice of version for packages can significantly affect the build outcome
- Importance metric: We use Jensen-Shannon (JS) divergence to compute the difference between the good and bad distribution.
- Some packages impact the build outcome more than others

Relative ranking of dependencies based on importance can guide the exploration process

Pairwise Version Constraints Analysis





Join us for more SC22 events!

- **Wed Nov 16:**
  - **2 Spack-related papers:**
    - Mapping out the HPC Dependency Chaos 1:30pm
    - Using Answer Set Programming for HPC Dependency Solving 2:00pm
  - **Spack Community BOF** 5:15pm

We'll be giving away more T-shirts at the BOF! Tell your friends!

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!
  - You're already on our **Slack channel** (spackpm.herokuapp.com)
  - Join our **Google Group** (see GitHub repo for info)
  - Submit **GitHub issues** and **pull requests**!

★ Star us on GitHub!

github.com/spack/spack

Follow us on Twitter!

@spackpm

We hope to make distributing & using HPC software easy!

Lawrence Livermore National Laboratory