



# Managing HPC Software Complexity with Spack

**SC25** Tutorial

November 17, 2025

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**Gregory Becker, Todd Gamblin, Kathleen Shea, Caetano Melone,  
Alec Scott, and Phil Sakievich**

The most recent version of these slides can be found at:  
<https://spack-tutorial.readthedocs.io>



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# Tutorial Materials

Find these slides and associated scripts here:

<https://spack-tutorial.readthedocs.io>

Join us on Slack

- <https://slack.spack.io>
- Join the #tutorial channel!
- You can ask questions here after the conference is over.
- **Over 3,800** people can help you on Slack!

latest

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LINKS

Main Spack Documentation

TUTORIAL

Basic Installation Tutorial

Environments Tutorial

Configuration Tutorial

Package Creation Tutorial

Stacks Tutorial

Developer Workflows Tutorial

Binary Caches Tutorial

Scripting with Spack

ADDITIONAL SECTIONS

Module Files Tutorial

Spack Package Build Systems

Advanced Topics in Packaging

## Tutorial: Spack 101

This is an introduction to Spack with lectures and live demos. It was last presented at the [Managing HPC Software Complexity with Spack](#) session at the [PEARC25 Conference](#). The presentation was a full-day tutorial.

You can use these materials to teach a course on Spack at your own site or online. You can also read the live demo scripts to see how Spack is used in practice.

### Slides



[Download Slides](#).

**Full citation:** Todd Gamblin, Alec Scott, Kathleen Meehan, and Michael L. Johnson. Managing HPC Software Complexity with Spack. In [Advanced Research Computing 2025 \(PEARC25\)](#), 2025.

### Video

For the last recorded video of this tutorial, see the [HPCIC Tutorial 2024](#).

### Live Demos

We provide scripts that take you step-by-step through basic Spack tasks. You can run these scripts by following the steps in the sections in the slides above.

To run through the scripts, we provide the [spack/tutorial](#) container image.

```
$ docker pull ghcr.io/spack/tutorial:pearc25
$ docker run -it ghcr.io/spack/tutorial:pearc25
```

to start using the container. You should now be ready to run through our live demos.

# Claim a VM Instance

**bit.ly/spack-vms**



	A	B	C	D	E
1	<b>Spack Tutorial VM Instances</b>				
2	Instructions:	1. Put your name in a box below to claim an account on a VM instance			
3		2. Log in to your VM:			
4		ssh <IP address>			
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6					
7		<b>Login / Password</b>			
8	<b>IP Address</b>	spack1	spack2	spack3	spack4
9	35.90.43.21				
10	35.91.36.120		Your Name		
11	34.217.149.171				
12	35.90.450.155				

If you're in the **spack2** column,  
your login and password are  
*both spack2*

**ssh spack2@35.91.36.120**

## Claim a login by putting your name in the Google Sheet



# Agenda (Approximate)

## Morning

Intro	8:30 am
Basics	
Concepts	
Break	10:00 am
Environments	10:30 am
Configuration	
Lunch	12:00 pm

## Afternoon

Software Stacks	1:30 pm
Packaging	
Break	3:00 pm
Developer Workflows	3:30 pm
Mirrors & Binary Caches	
End	5:00 pm

# Modern scientific codes are built from hundreds of small, complex pieces

*“Just when we’re starting to solve the problem of how to create software using reusable parts, it founders on the nuts-and-bolts problems outside the software itself.”*

P. DuBois & T. Epperly. *Why Johnny Can’t Build*. Scientific Programming. Sep/Oct 2003.

- Component-based software development dates back to the 60’s
  - M.D. McIlroy, *Mass Produced Software Components*. NATO SE Conf., 1968
- **Pros are well known:**
  - Teams can and must reuse each others’ work
  - Teams write less code, meet deliverables faster
- **Cons:**
  - Teams must ensure that components work together
  - Integration burden increases with each additional library
  - Integration must be repeated with each update to components
  - **Components must be vetted!**
- **Managing changes over time is becoming intractable**

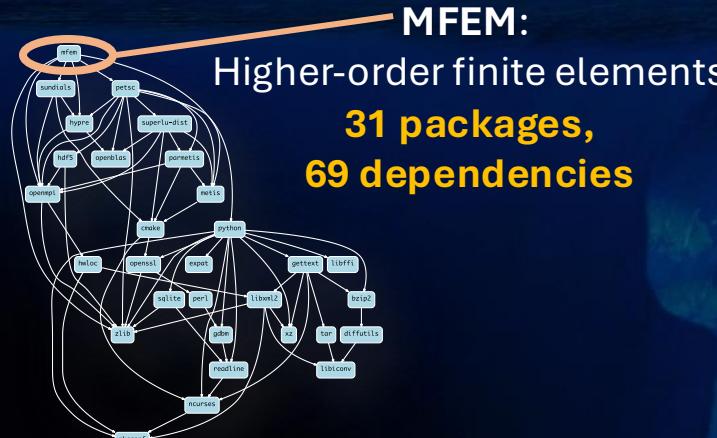


Build-time incompatibility; fail fast



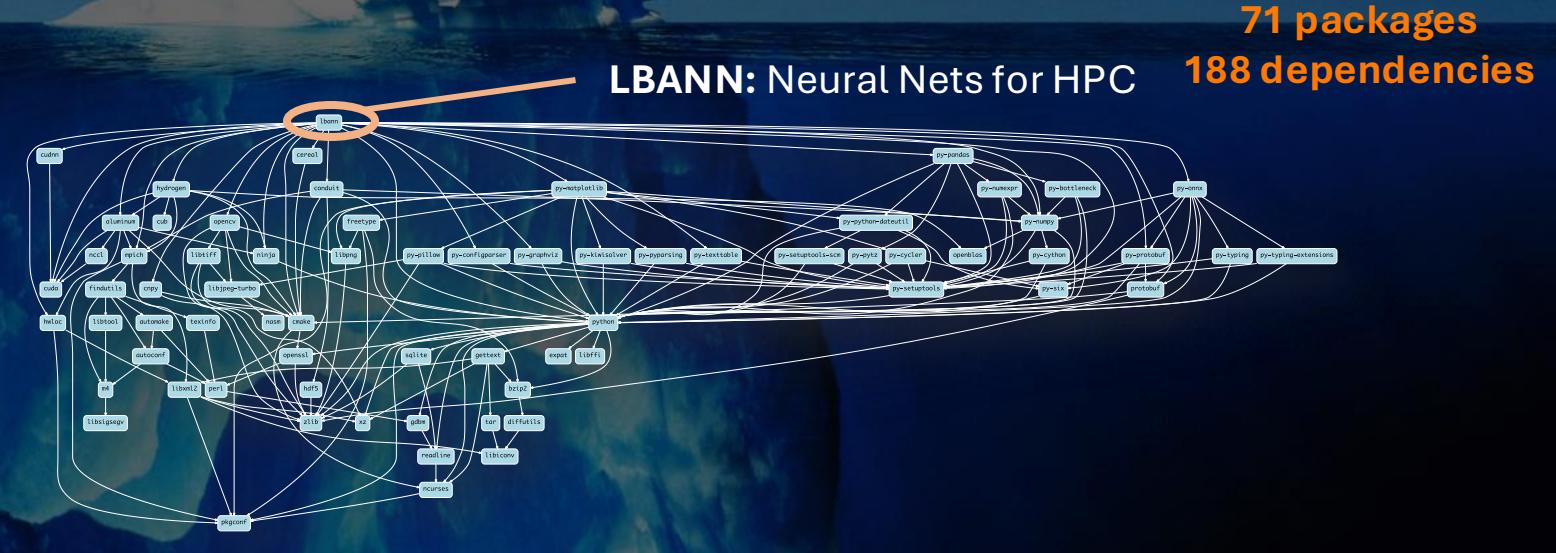
Appears to work; subtle errors later

# Modern scientific codes rely on icebergs of dependency libraries

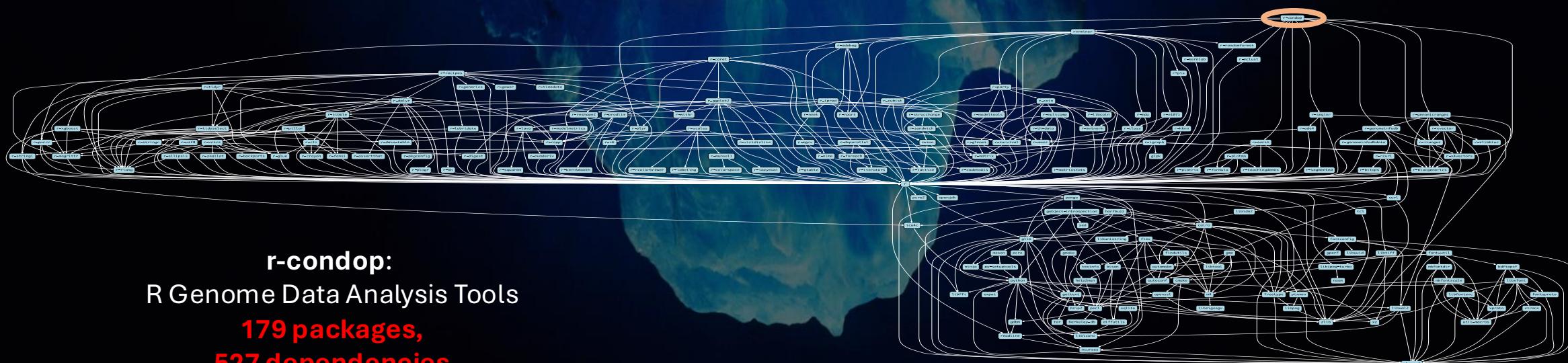


# Higher-order finite elements

## 31 packages, 69 dependencies



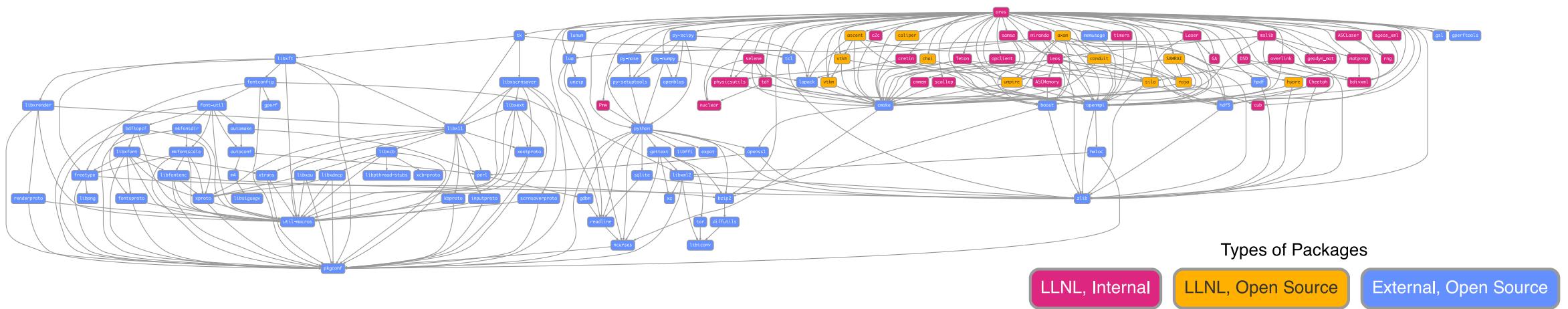
**LBANN: Neural Nets for HPC** **188 dependencies**



# r-condop: R Genome Data Analysis Tools

**179 packages,  
527 dependencies**

# **Modern software integrates open source and internal packages**



- Most modern software uses **tons** of open source
  - We *cannot* replace all these OSS components with our own
    - How do we put them all together effectively?
    - Do you *have* to integrate this stuff by hand?



# Some fairly common (but questionable) assumptions made by package managers

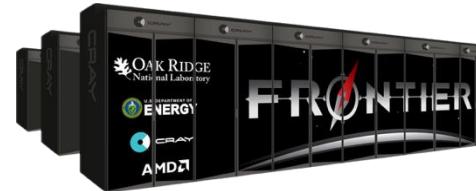
- **1:1 relationship between source code and binary (per platform)**
  - Good for reproducibility (e.g., Debian)
  - Bad for performance optimization
- **Binaries should be as portable as possible**
  - What most distributions do
  - Again, bad for performance
- **Toolchain is the same across the ecosystem**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

# High Performance Computing (HPC) violates many of these assumptions

- 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
- Code is typically distributed as source
  - With exception of vendor libraries, compilers
- 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



Lawrence Livermore  
National Lab  
AMD Zen / MI300A



Oak Ridge National Lab  
AMD Zen / MI250X



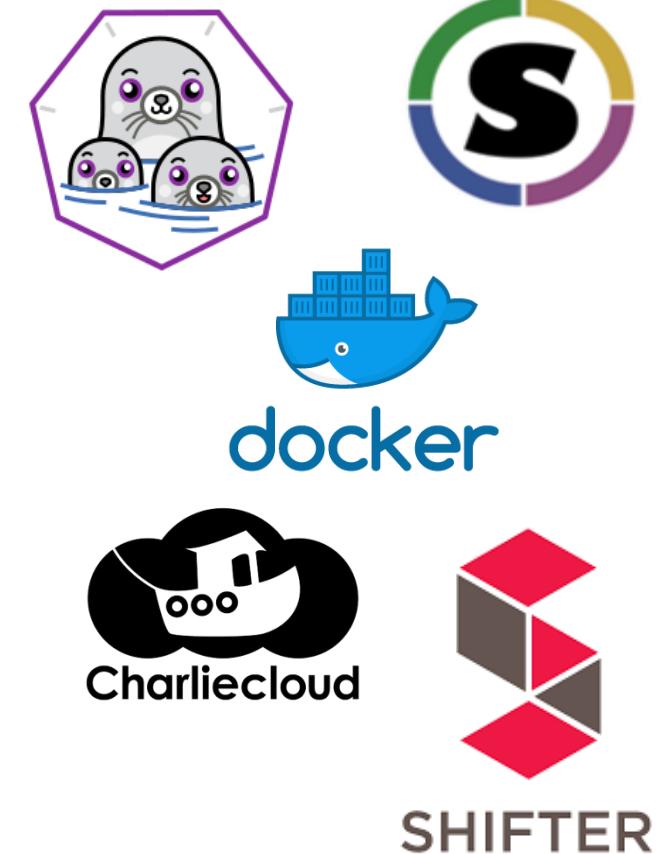
RIKEN  
Fujitsu ARM a64fx



Argonne National Lab  
Intel Xeon / Xe

# 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





# Spack enables Software distribution for HPC



## No installation required: clone and go

```
$ git clone --depth=2 https://github.com/spack/spack  
$ spack install hdf5
```

## Simple syntax enables complex installs

```
$ spack install hdf5@1.10.5           $ 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 +threadsafe    $ spack install hdf5@1.10.5 +mpi ^mpich@3.2
```

- Packages are **parameterized**, so that users can easily tweak and tune configuration
- Ease of use of mainstream tools, with flexibility needed for HPC



# 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

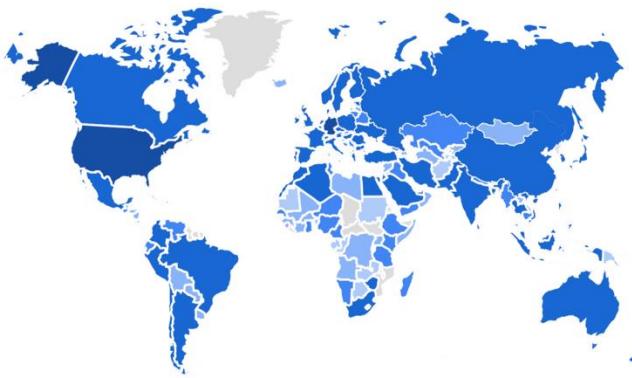
## 3. Package Developers

- 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

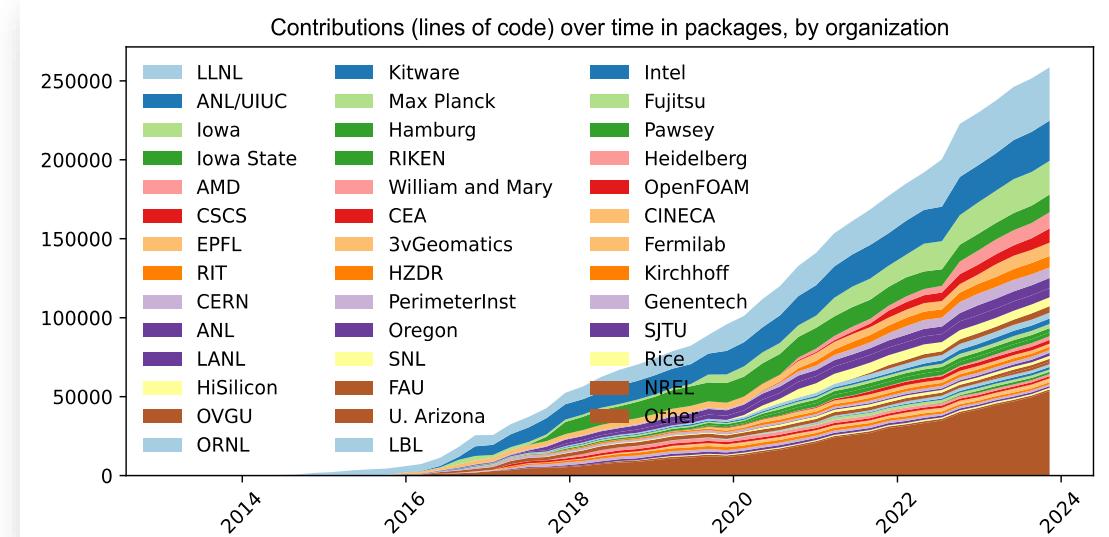
# Spack sustains the HPC software ecosystem with the help of many contributors



COUNTRY	USERS
United States	23K
Germany	5.3K
China	4.6K
India	4.5K
United Kingdom	3.3K
France	3K
Japan	2.4K

2023 aggregate documentation user counts from GA4  
(note: yearly user counts are almost certainly too large)

**Over 8,600 software packages**  
**Over 1,500 contributors**



**Contributors continue to grow worldwide!**

# One month of Spack development is pretty busy!

October 16, 2025 – November 16, 2025

Period: 1 month ▾

## Overview

504 Active pull requests

23 Active issues

361  
Merged pull requests

143  
Open pull requests

8  
Closed issues

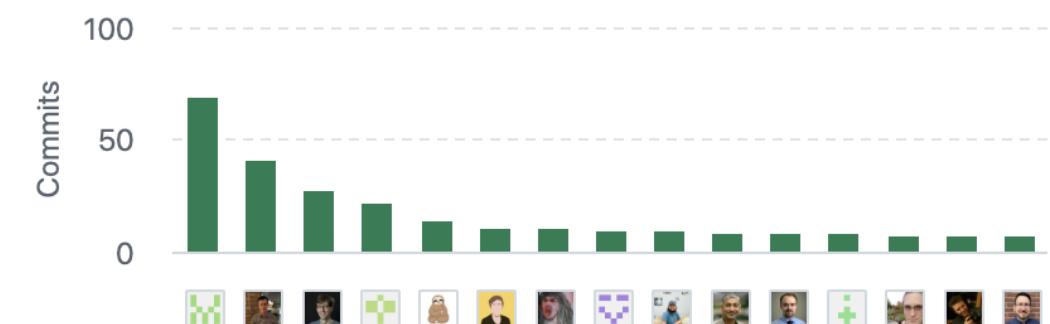
15  
New issues

## Summary

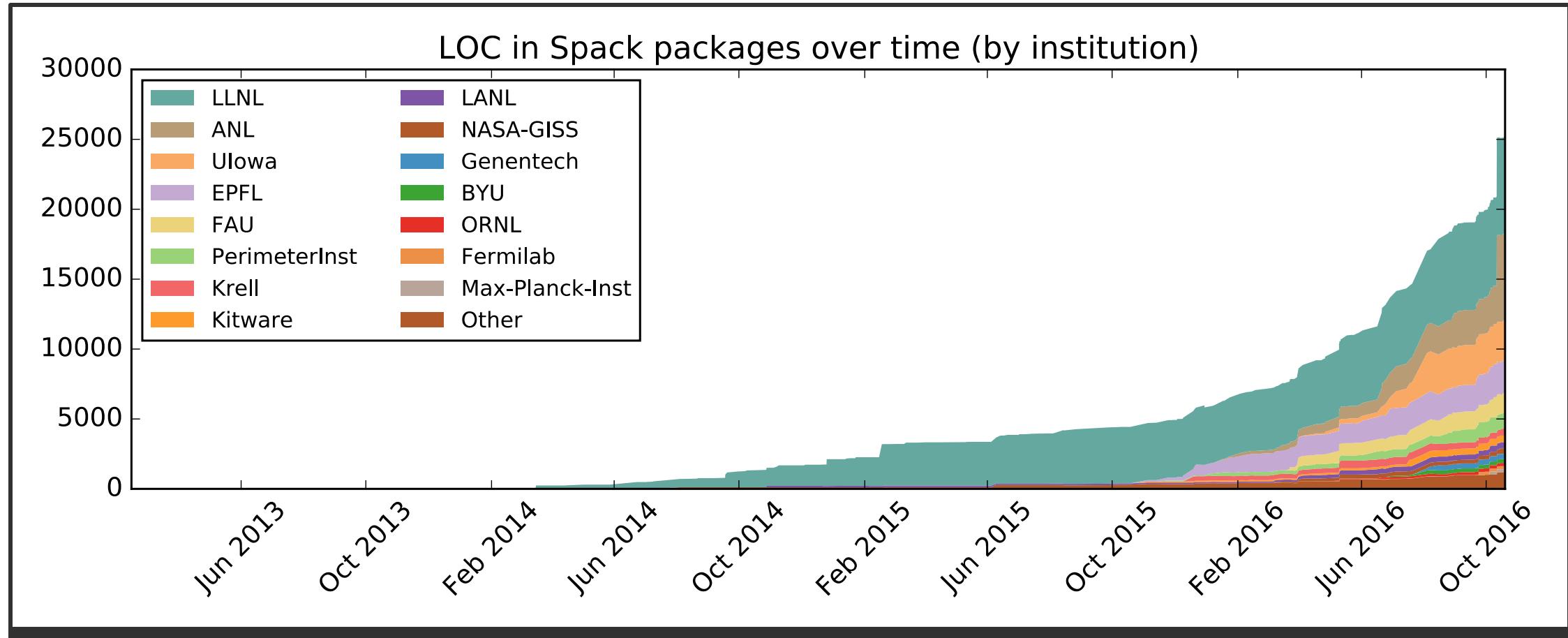
Excluding merges, **116 authors** have pushed **361 commits** to develop and **402 commits** to all branches.

On develop, **848 files** have changed and there have been **7,676 additions** and **1,868 deletions**

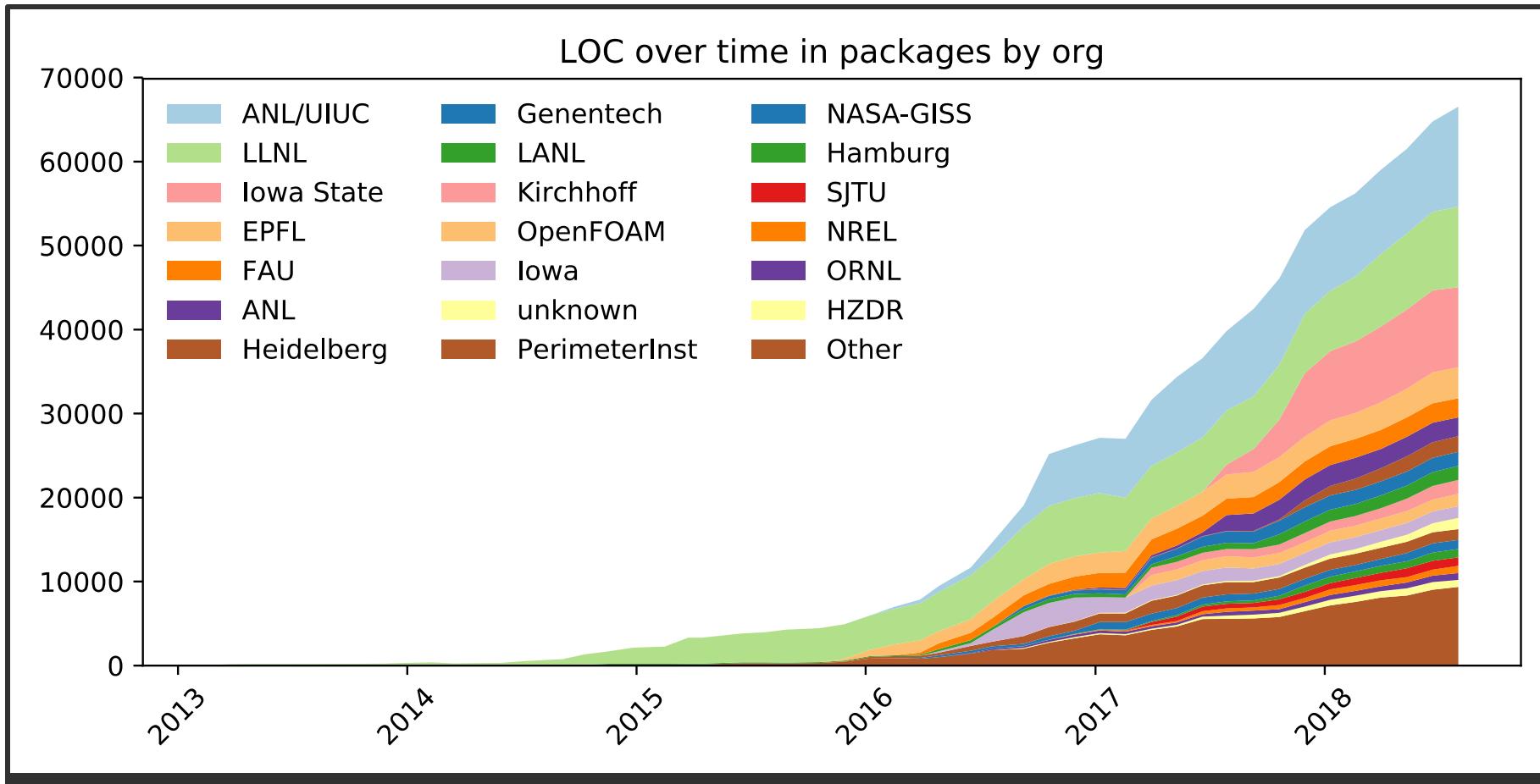
## Top Committers



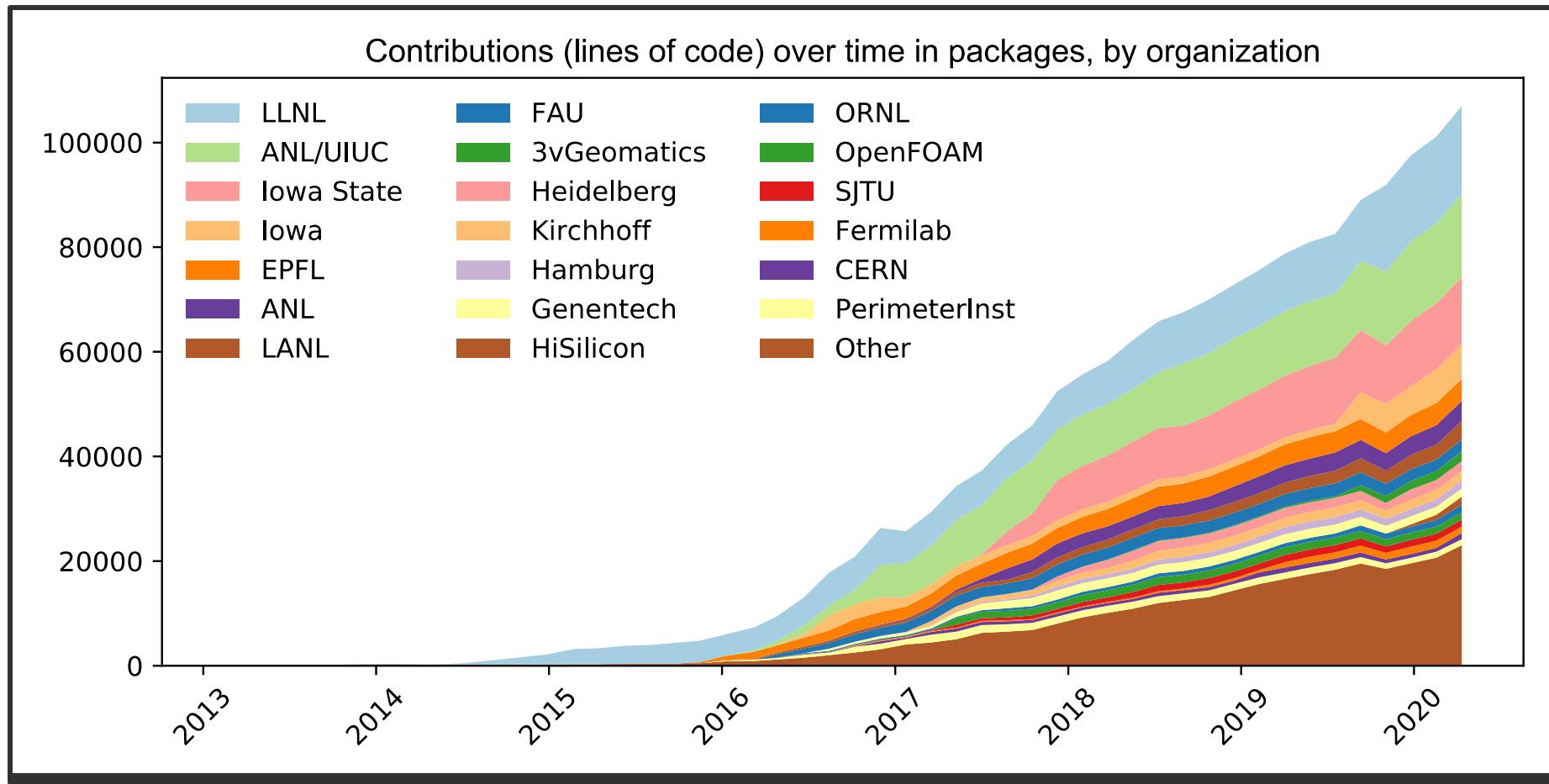
# 2016



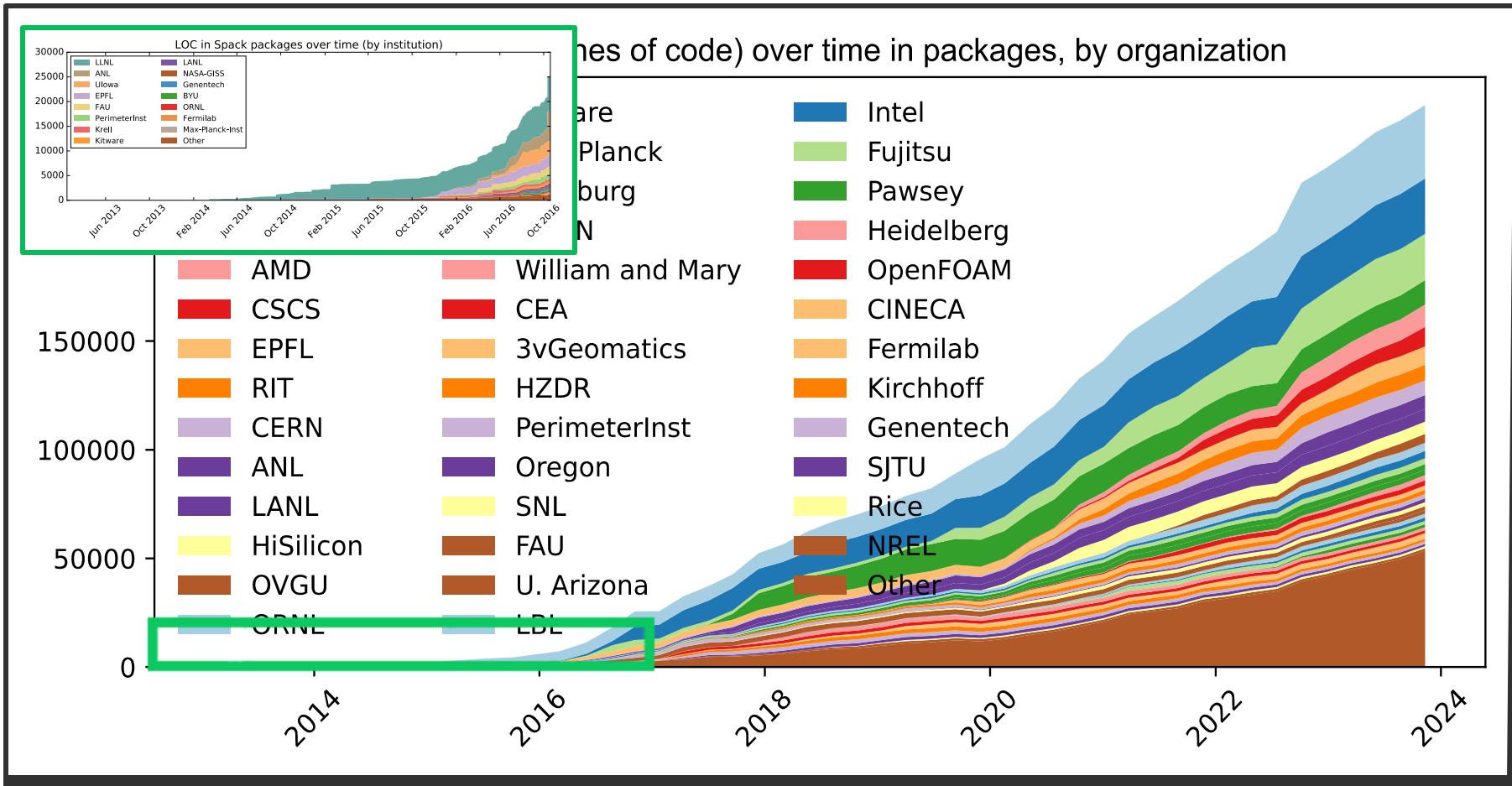
# 2018



# 2020



# 2024



# Spack's widespread adoption has made it a de facto standard, drawing contribution and collaboration from vendors

- **AWS** is investing significantly in cloud credits for Spack
  - Supporting highly scalable cloud CI system with ~250k+/year in credits
  - Integrating Spack with ParallelCluster product
  - Joint Spack tutorial with AWS drew 125+ participants
- **Google** is using Spack in their HPC Toolkit cloud cluster product
  - List packages to deploy; automatically built and cached in cluster deployment
- **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 allowing us to do CI in the cloud for the Cray PE environment
  - Looking at tighter Spack integration with Cray PE
- **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





# Spack is a part of the High Performance Software Foundation (HPSF)

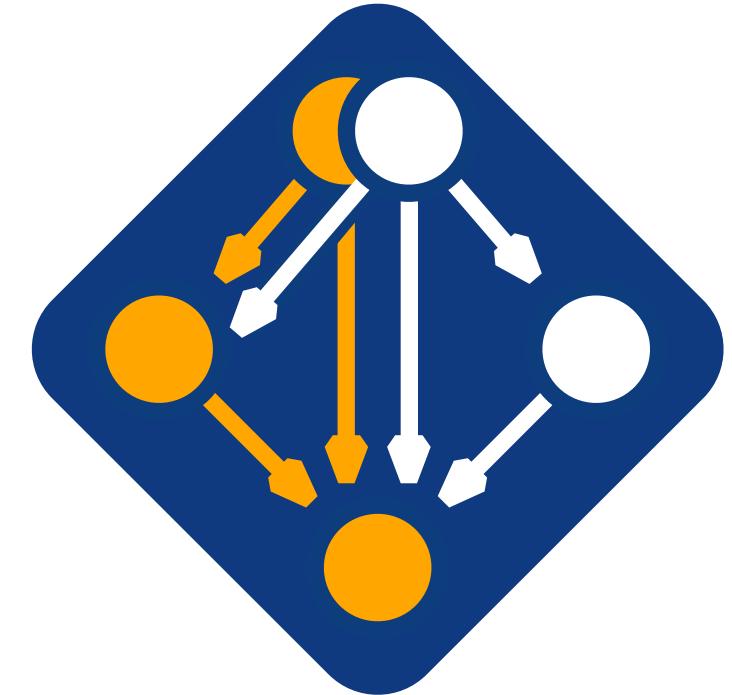
- Project has a neutral legal entity
  - 501(c)(6) non-profit company
- Project has a Technical Steering Committee (TSC)
  - Charter mandates TSC to make decisions
  - Governance defined at [github.com/spack/governance](https://github.com/spack/governance)
- Trademark (Spack name, logo) assigned to Linux Foundation
- Project resources owned by Linux Foundation
  - [spack.io](https://spack.io) website
  - GitHub Organization



# Spack v1.1.0 was released on November 14!

## New Features:

1. More compiler control
  - Propagated compiler preferences with %%
  - Unmixing preferences
2. Customizable/overridable configuration scopes
3. Git fetching
4. External packages can have dependencies



## Experimental Features:

5. New installer UI for parallel builds
6. Concretizer caching



[github.com/spack/spack](https://github.com/spack/spack)

**Full release notes:** <https://github.com/spack/spack/releases/tag/v1.1.0>

# Spack is not the only HPC/AI/data science package manager out there



## 1. Nix, Guix: “Functional” Package Managers

- Pioneered using hashes to identify installations/configurations
- No concretizer/solver; handling multiple versions requires coding packages

<https://hpc.guix.info>



## 2. Build-from-source Package Managers

- Homebrew, LinuxBrew
- MacPorts
- Gentoo

<https://brew.sh>

<https://www.macports.org>

<https://hpc.guix.info>



## 3. Pip, UV

- Package managers for PyPI, Python ecosystem
- **Very** widely used, increasingly for (unoptimized) software binaries beyond Python <https://docs.astral.sh/uv/>

<https://pypi.org/project/pip/>

<https://docs.astral.sh/uv/>



## 4. Easybuild

- Installation tool Focused on HPC system administrators
- Different model w/fixed software stack – harder to tweak recipes for experimentation

<https://easybuild.io>



## 5. Conda / Mamba / Pixi

- Very popular binary package ecosystem for data science
- Not targeted at HPC; generally, has unoptimized binaries

<https://conda.io>

<https://mamba.readthedocs.io>

<https://prefix.dev>



# Claim a VM Instance

**bit.ly/spack-vms**



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your login and password are  
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**ssh spack2@35.91.36.120**

## Claim a login by putting your name in the Google Sheet



# Hands on Section

## Basics



# Presentation

# Core Spack Concepts

# Spack supports 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"

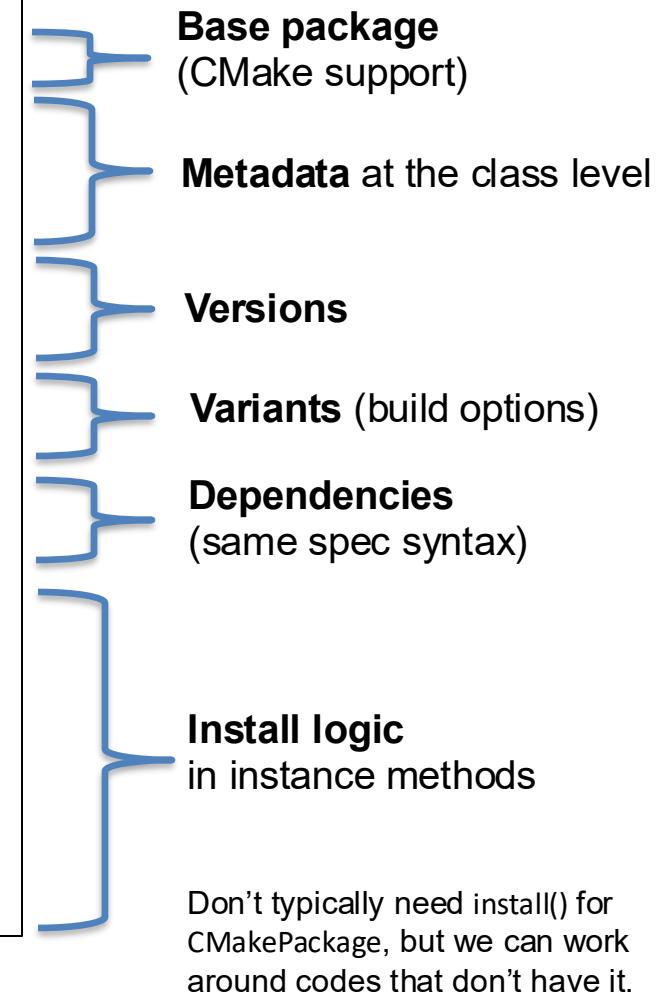
    version('1.2.3', sha256='3f7f2eef0d1ba5825780d626741eb0b3f026a096048d7ec4794d2a7dfbe2b8a6')
    version('1.2.2', sha256='eaf9ddf562416974157b34d00c3a1c880fc5296fce2aa2efa039a86e0976f3a3')
    version('1.1', sha256='232d74072fc7b848fa2adc8a1bc839ae8fb5f96d50224186601f55554a25f64a')

    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)
```



**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

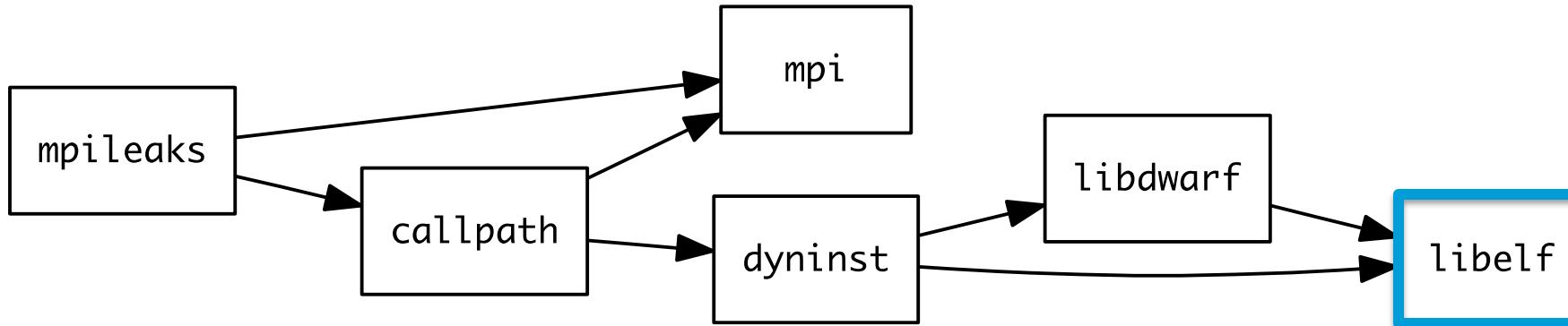
constraints on cuda version

compiler support for x86\_64  
and ppc64le

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



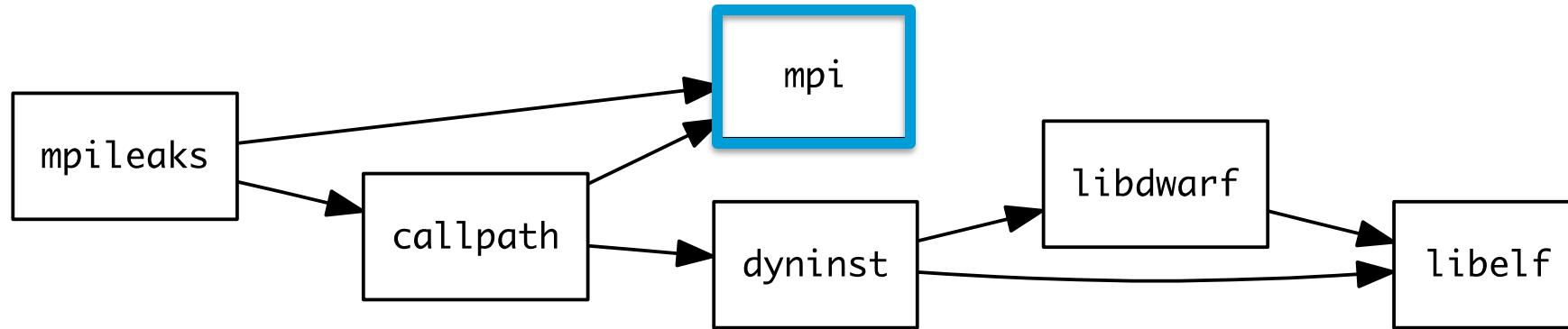
# Spack Specs can constrain versions of dependencies



```
$ 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:

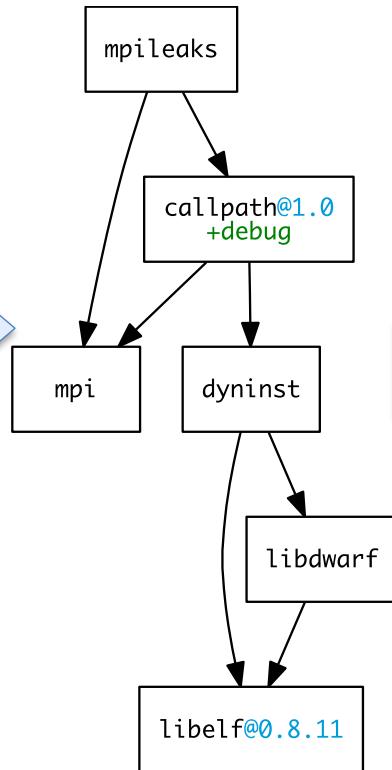
```
$ spack install mpileaks ^mpi@2
```

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

mpileaks ^callpath@1.0+debug ^libelf@0.8.11

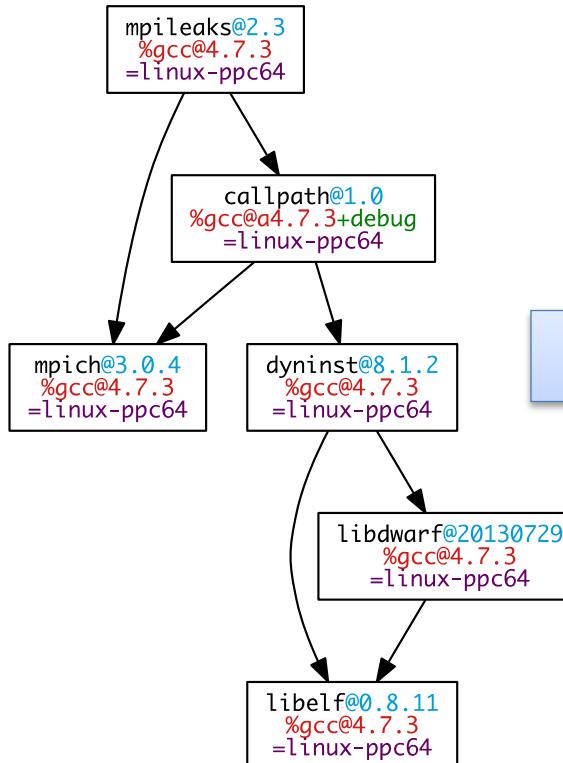
User input: abstract spec with some constraints

Normalize



Abstract, normalized spec with some dependencies.

Concretize



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

spec.yaml

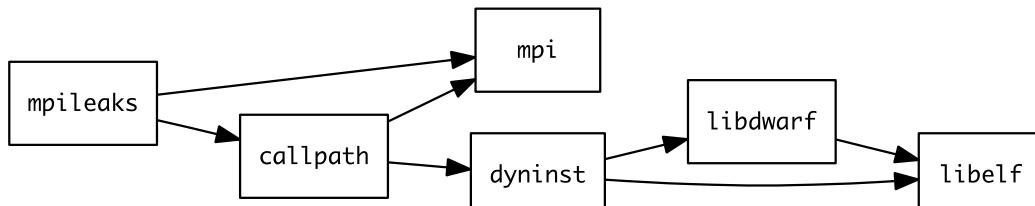
```
spec:  
- mpileaks:  
  arch: linux-x86_64  
  compiler:  
    name: gcc  
    version: 4.9.2  
  dependencies:  
    adept-utils: ksrtkpzbac3ss2ixjkorlaybnptp4  
    callpath: bah5f4h4d2n47mgycce2mtrnrvvxy77  
    mpich: aa4ar6ifj23yijqmdabeakpejcli72t3  
    hash: 33hjhxi7p6gyzn5ptgyes7sghypujh  
  variants: {}  
  version: '1.0'  
- adept-utils:  
  arch: linux-x86_64  
  compiler:  
    name: gcc  
    version: 4.9.2  
  dependencies:  
    boost: teesvj7ehpe5ksspjm5dk43a7qnowlq  
    mpich: aa4ar6ifj23yijqmdabeakpejcli72t3  
    hash: ksrtkpzbac3ss2ixjkorlaybnptp4  
  variants: {}  
  version: 1.0.1  
- boost:  
  arch: linux-x86_64  
  compiler:  
    name: gcc  
    version: 4.9.2  
  dependencies: {}  
  hash: teesvj7ehpe5ksspjm5dk43a7qnowlq  
  variants: {}  
  version: 1.59.0  
...
```

Detailed provenance is stored with the installed package



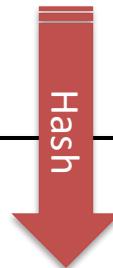
# Hashing allows us to handle combinatorial complexity

## Dependency DAG



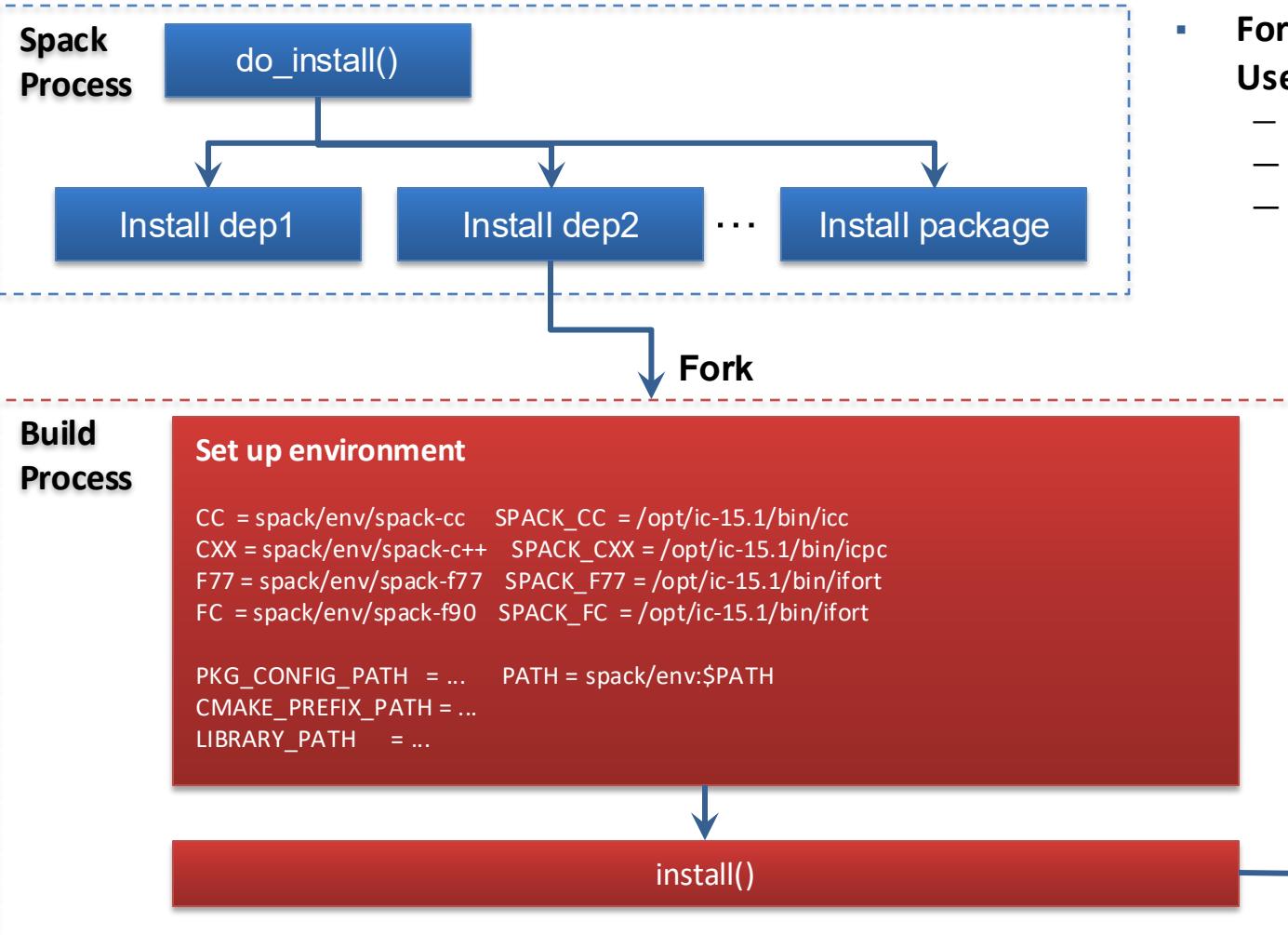
## Installation Layout

```
opt
└── spack
    ├── darwin-mojave-skylake
    │   └── clang-10.0.0-apple
    │       ├── bzip2-1.0.8-hc4sm4vuzpm4znmvrfzri4ow2mkphe2e
    │       ├── python-3.7.6-daqqpssxb6qbfrztsezkmhus3xoflbsy
    │       ├── sqlite-3.30.1-u64v26igvxyn23hysmklfums6tgjv5r
    │       ├── xz-5.2.4-u5eawkvaoc7vonabe6nnndkcfwuv233cj
    │       └── zlib-1.2.11-x46q4wm46ay4pltrijbgizxjrhbaka6
    ├── darwin-mojave-x86_64
    │   └── clang-10.0.0-apple
    └── coreutils-8.29-p12kcytejqcys5dzecfrtjqxfdssvnob
```



- 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*

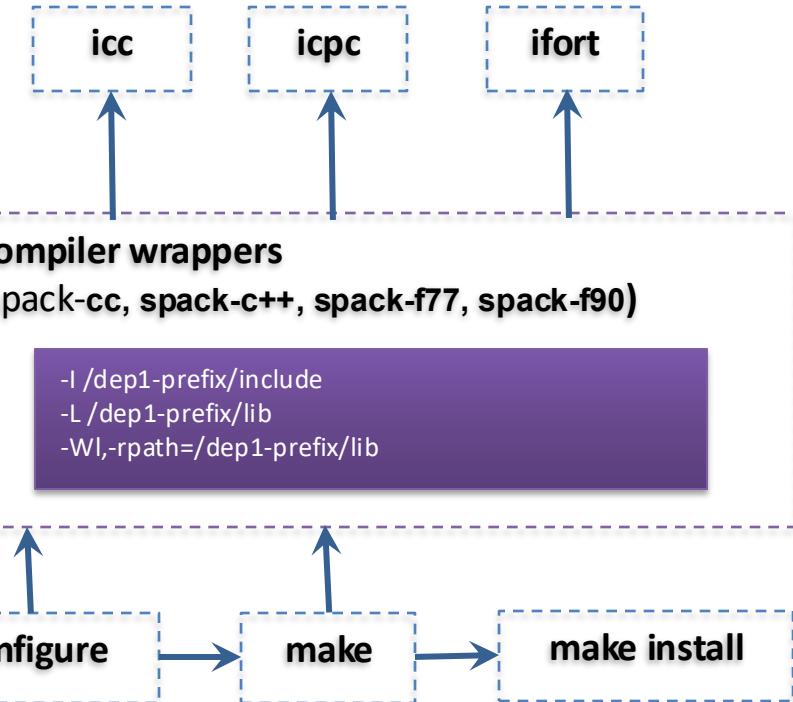
# An isolated compilation environment allows Spack to easily swap compilers



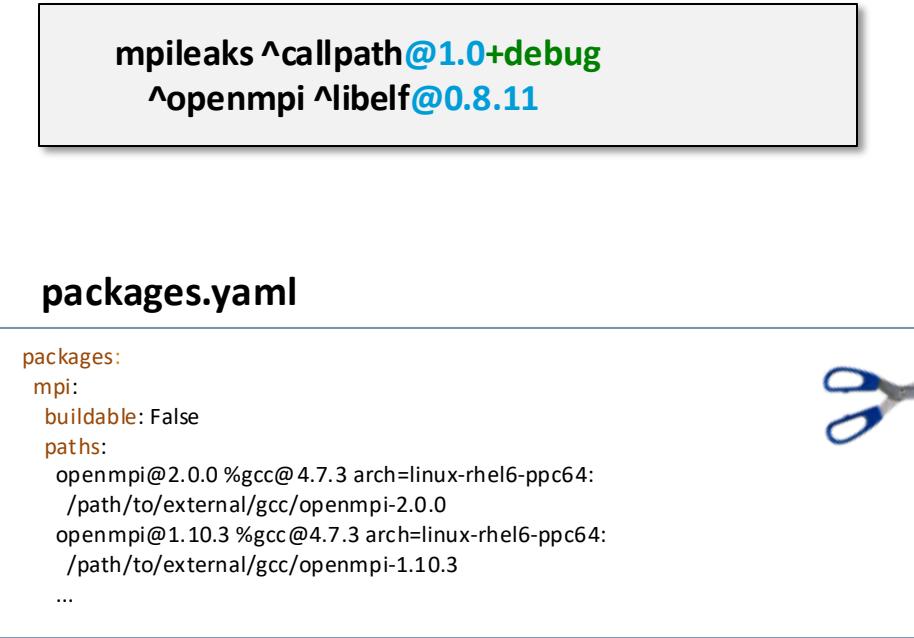
- Forked build process isolates environment for each build.

## Uses compiler wrappers to:

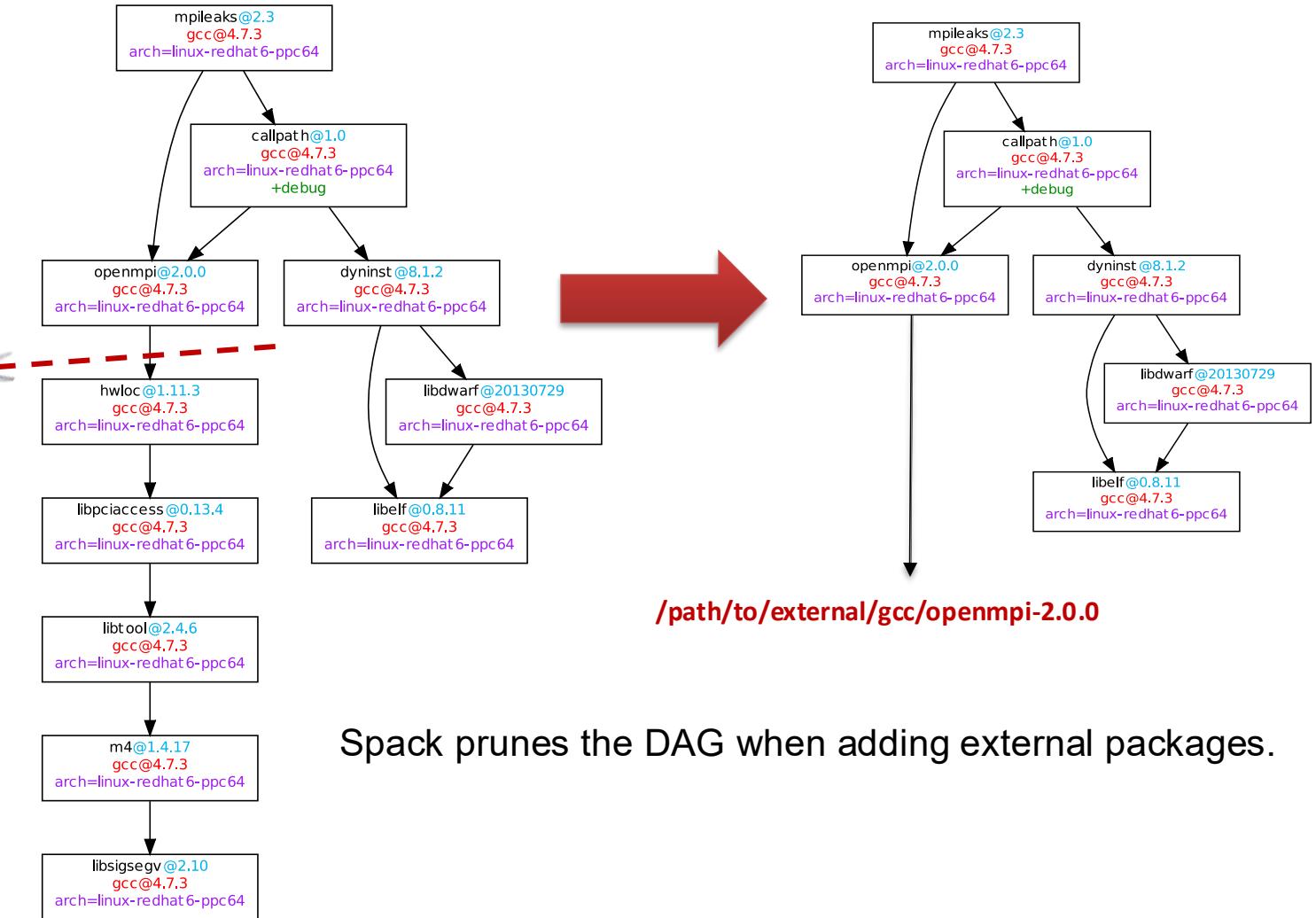
- Add include, lib, and RPATH flags
- Ensure that dependencies are found automatically
- Load Cray modules (use right compiler/system deps)



# We can configure Spack to build with external software



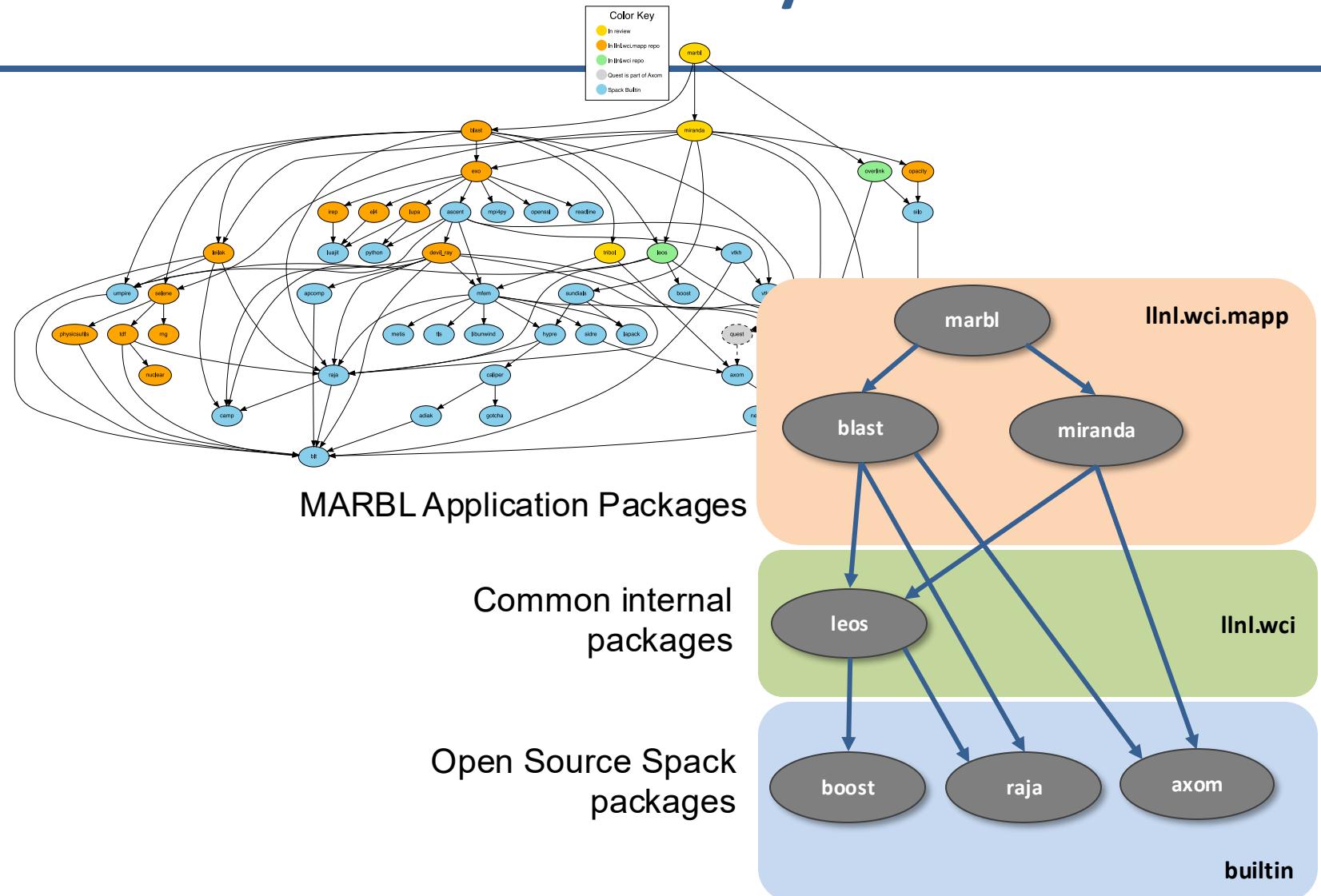
Users register external packages in a configuration file (more on these later).



Spack prunes the DAG when adding external packages.

# Spack package repositories allow stacks to be layered

LLNL MARBL multi-physics application

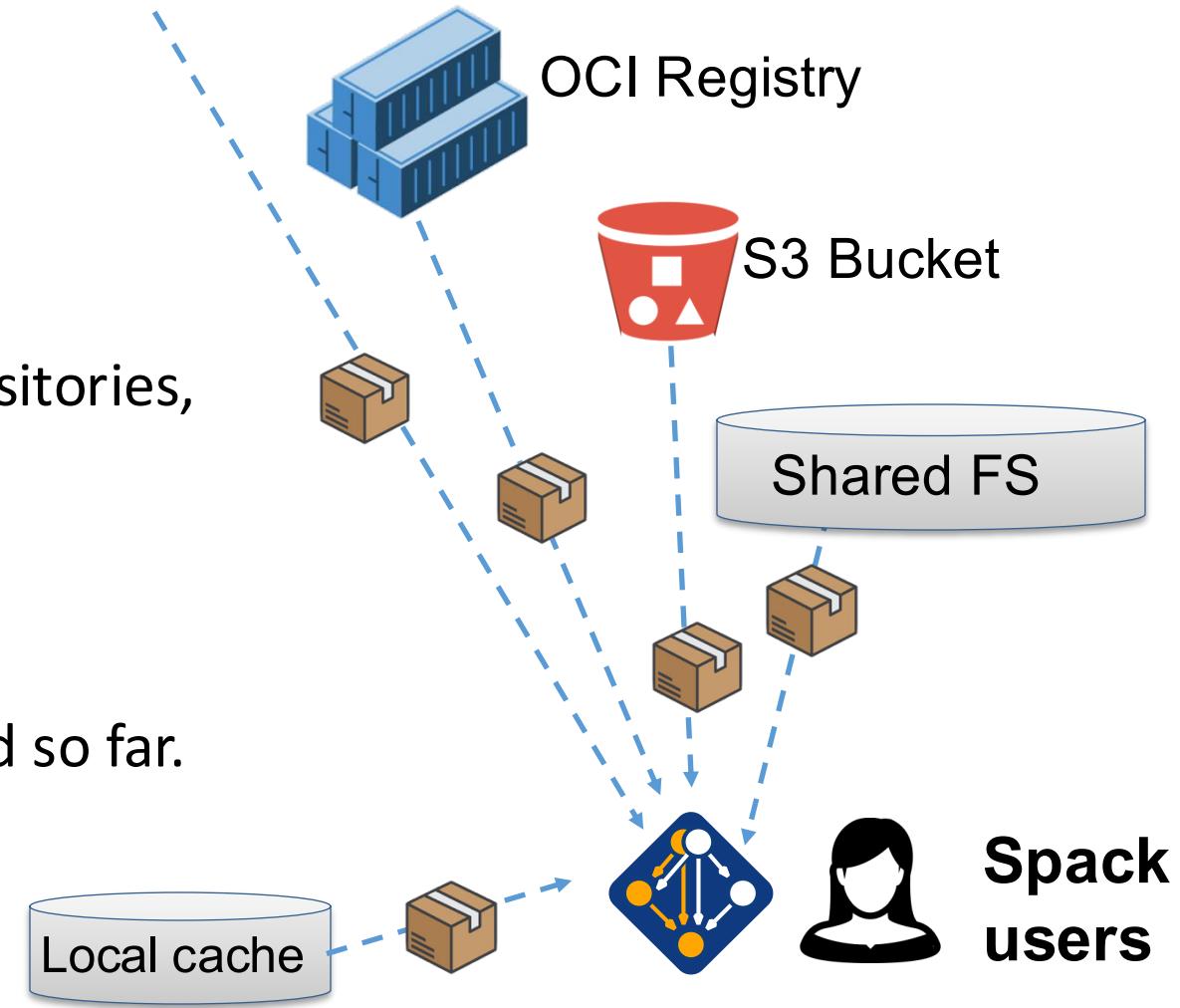


```
$ spack repo create /path/to/my_repo  
$ spack repo add my_repo  
$ spack repo list  
==> 2 package repositories.  
my_repo  /path/to/my_repo  
builtin  spack/var/spack/repos/builtin
```

# Spack mirrors



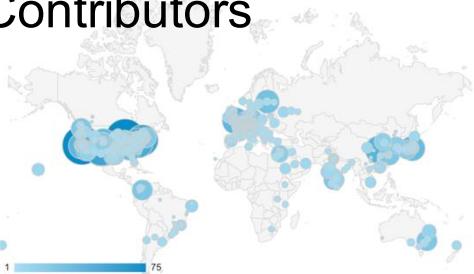
- Spack allows you to define *mirrors*:
  - Directories in the filesystem
  - On a web server
  - In an S3 bucket
- Mirrors are archives of fetched tarballs, repositories, and other resources needed to build
  - Can also contain binary packages
- By default, Spack maintains a mirror in `var/spack/cache` 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

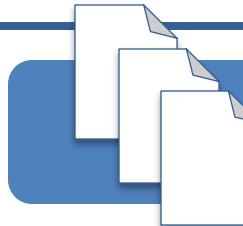
users

local environment config  
spack.yaml

users

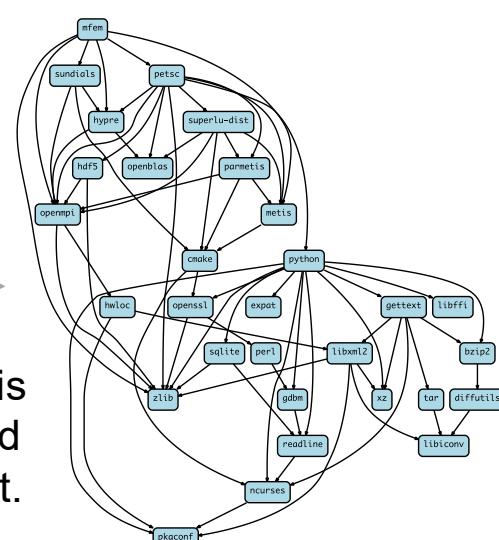
Command line constraints

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

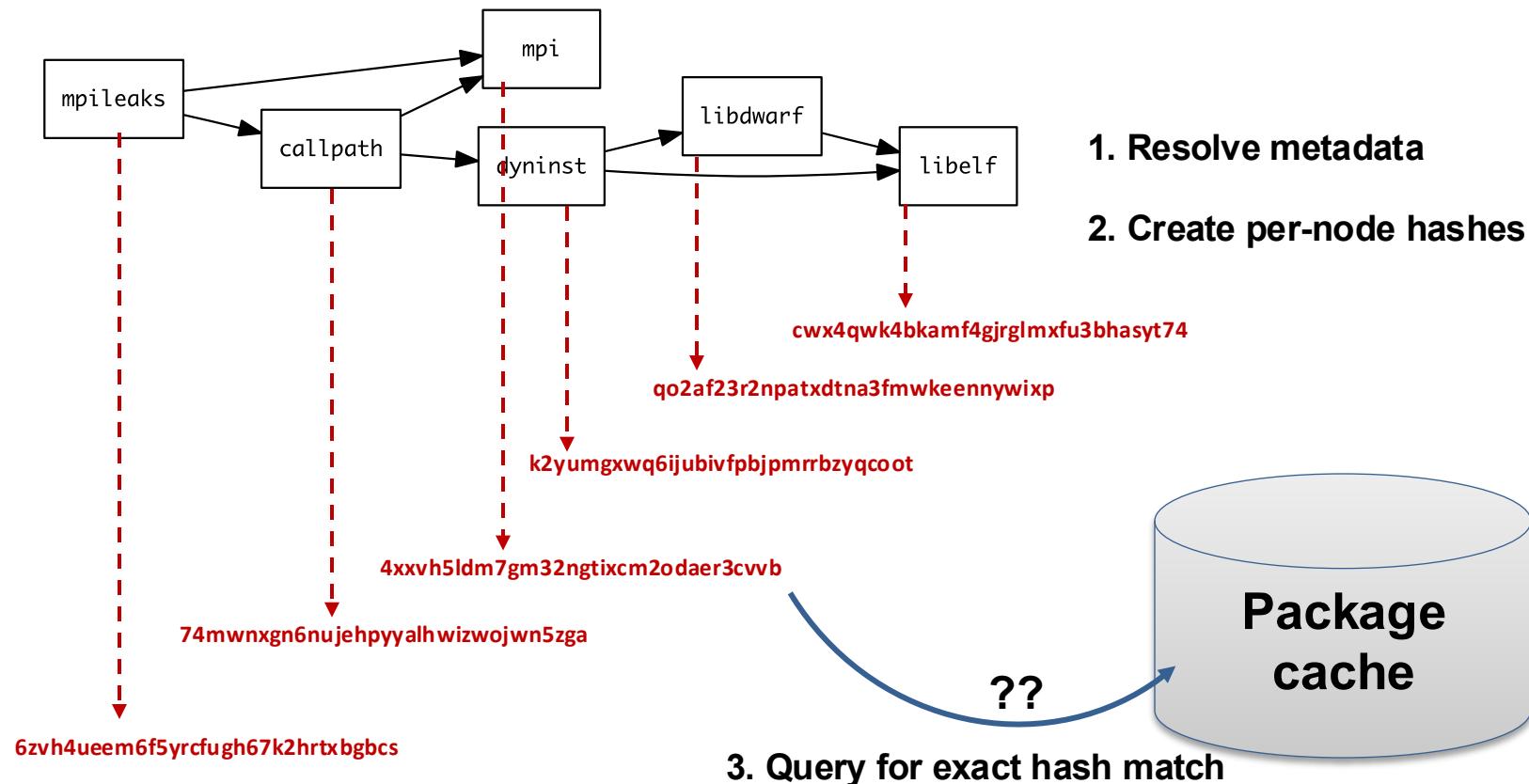
- New concretizer leverages Clingo (see [potassco.org](http://potassco.org))
- Clingo is an Answer Set Programming (ASP) solver
  - ASP looks like Prolog; leverages SAT solvers for speed/correctness
  - ASP program has 2 parts:
    1. Large list of facts generated from our package repositories and config
    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", "1.4.8", 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

```
(spack):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+nurses+openssl+ownlibs+qt build_type=Release arch=darwin-bi
- xdbaquo  ^ncurses@6.2%apple-clang@13.0.0~symlinks+termibl 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+cpam+shared+threads arch=darwin-bigsur-skylake
- xgt3tls   ^berkeley-db@18.1.40%apple-clang@13.0.0~cxx~docs+stl patches=b231fcc4d5cff05e5c3a4814f
- 65edjf6   ^bzip2@1.0.8%apple-clang@13.0.0~debug~pic+shared arch=darwin-bigsur-skylake
- 662ad0o   ^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-skylake
- 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
- xevlijj   ^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+sh
- 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   ^openssl@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

```
(spack):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 b
- zd4m26e   ^cmake@3.21.1%apple-clang@12.0.5~doc+nurses+openssl+ownlibs+qt build_type=Release arch=darwin-bi
- 53i52xr   ^ncurses@6.2%apple-clang@12.0.5~symlinks+termibl abi=none arch=darwin-bigsur-skylake
- us36bwr   ^openssl@1.1.1l%apple-clang@12.0.5~docs+systemcerts arch=darwin-bigsur-skylake
- 74mwmxg   ^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~lega
- jxexyb7   ^hwloc@2.6.0%apple-clang@12.0.5~cairo~cuda~gl~libudev+libxml2~netloc~nvml~opencl~pci~rocm+
- ckdnn5zf  ^libxml2@2.9.12%apple-clang@12.0.5~python arch=darwin-bigsur-skylake
- k7uat43   ^libiconv@1.16%apple-clang@12.0.5 libs=shared,static arch=darwin-bigsur-skylake
- k2zymgx   ^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   ^openssl@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
- qbkmttd   ^perl@5.34.0%apple-clang@12.0.5~cpam+shared+threads arch=darwin-bigsur-skylake
- tnvkif5   ^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
- qgy3v4l   ^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
    ^bzzip2@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": "builtin",  
        "parameters": {  
          "cxx": false,  
          "debug": false,  
          "fortran": false,  
          "hl": false,  
          "mpi": true,  
          "shared": false  
        }  
      }  
    }  
  }  
}
```





## Hands on Section

# Environments



## Hands on Section

# Configuration



## Hands on Section

# Software Stacks



## Hands on Section

# Creating Packages



## Hands on Section

# Binary Caches & Mirrors



## Hands on Section

# Developer Workflows



## Hands on Section

# Scripting



# Join us at other Spack-related events at SC25!

- HPSF BOF                    Tuesday            12:15pm, 230
- Spack BOF                    Wednesday        12:15pm, 275



## And after the conference!



 @spack@hpc.social

 ★ Star us on GitHub!  
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 @spackpm.bsky.social

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