

Managing HPC Software Complexity with Spack

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

PEARC21 Full-day Tutorial
July 19, 2021



Tutorial Materials

Find these slides and associated scripts here:

spack-tutorial.readthedocs.io

We will also have a chat room on Spack slack.
Get an invite here:

slack.spack.io

Join the “tutorial” channel!

We will give you login credentials for the hands-on exercises once you join Slack.

Join #tutorial on Slack: slack.spack.io

Materials: spack-tutorial.readthedocs.io

The screenshot shows the homepage of the spack-tutorial.readthedocs.io website. The header features the Spack logo and the word "Spack". Below the header is a search bar labeled "Search docs". A sidebar on the left contains links for "LINKS" (Main Spack Documentation), "TUTORIAL" (Basic Installation Tutorial, Configuration Tutorial, Package Creation Tutorial, Developer Workflows Tutorial), and "Read the Docs" with a dropdown menu for "v: latest". The main content area includes sections for "Versions" (latest, sc18, sc17, sc16, riken19, pearc19, nsf19, lanl19, isc19, ecp19), "Downloads", "HTML", "On Read the Docs" (Project Home, Builds, Downloads), "On GitHub", "View", "Edit", and "Search". At the bottom, it says "Hosted by [Read the Docs](#) · [Privacy Policy](#)".

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Practice and Experi
2019.

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Slides



Practice and Experi
Chicago, IL, USA.

Live Demos

We provide scripts
sections in the slide

1. We provide a
tutorial on yo
the containe
2. When we ha
unfamiliar wi

You should now be



Tutorial Presenters



Greg Becker
LLNL



Robert Blake
LLNL



Massimiliano
Culpo
np-complete, S.r.l.



Tamara
Dahlgren
LLNL



Adam Stewart
UIUC



Todd Gamblin
LLNL

Agenda (times are approximate)

Morning:

- | | |
|-----------------|--------|
| — Intro | 10 min |
| — Basics | 45 min |
| — Concepts | 20 min |
| Break | 30 min |
| — Environments | 45 min |
| — Configuration | 45 min |
| Break | 30 min |

Afternoon:

- | | |
|-----------------------|--------|
| — Packaging | 60 min |
| — Developer Workflows | 30 min |
| Break | 30 min |
| — Mirrors | 20 min |
| — Stacks | 20 min |
| — Scripting | 15 min |
| — Roadmap | 10 min |

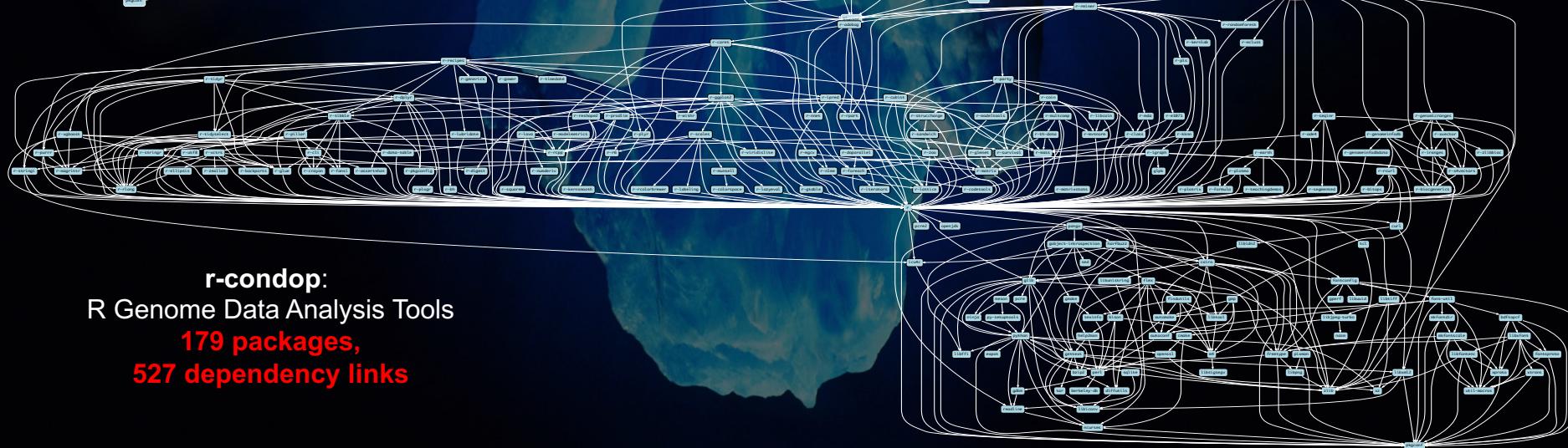
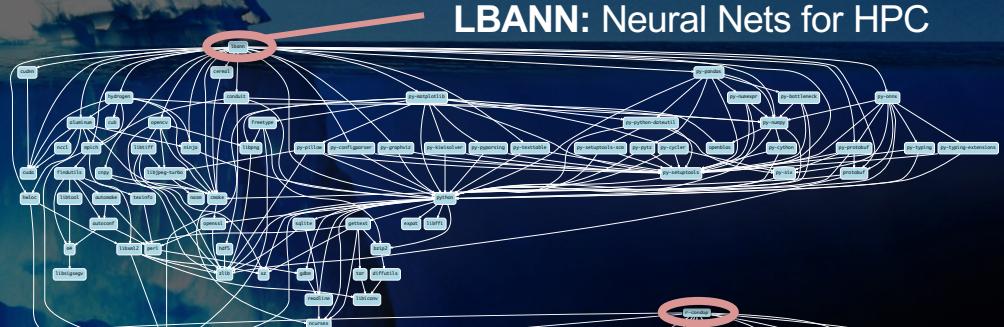


Modern scientific codes rely on icebergs of dependency libraries



A large iceberg is visible in the background of the slide, partially submerged in dark blue water.

71 packages
188 dependency links



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



Summit

Oak Ridge National Lab
Power9 / NVIDIA



Fugaku

RIKEN
Fujitsu/ARM a64fx

Upcoming



Perlmutter

Lawrence Berkeley
National Lab
AMD Zen / NVIDIA



Aurora

Argonne National Lab
Intel Xeon / Xe



FRONTIER
Oak Ridge National Lab
AMD Zen / Radeon



EL CAPITAN
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

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

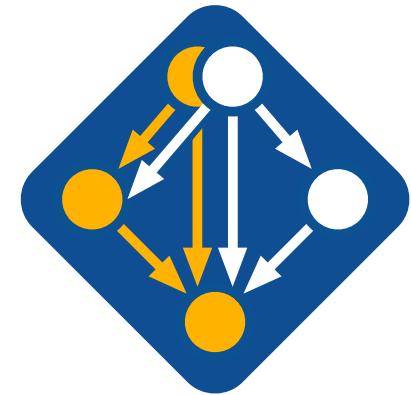
No installation required: clone and go

```
$ 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 +threadsafe
```

```
$ 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)

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

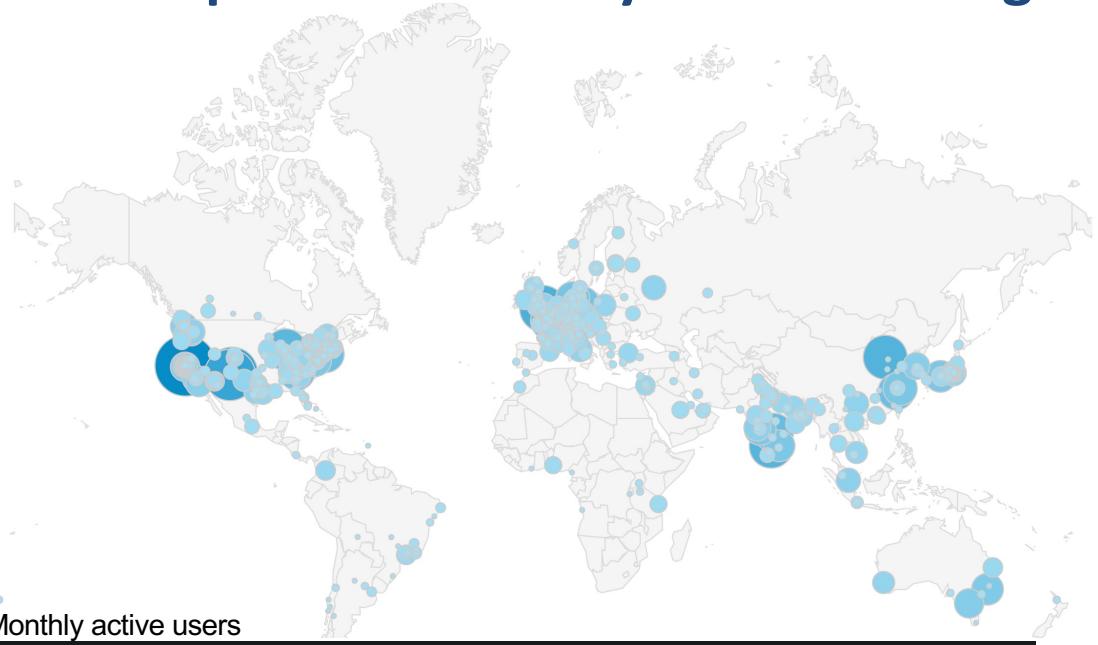
4. User support teams at HPC Centers

- People who deploy software for users at large HPC sites

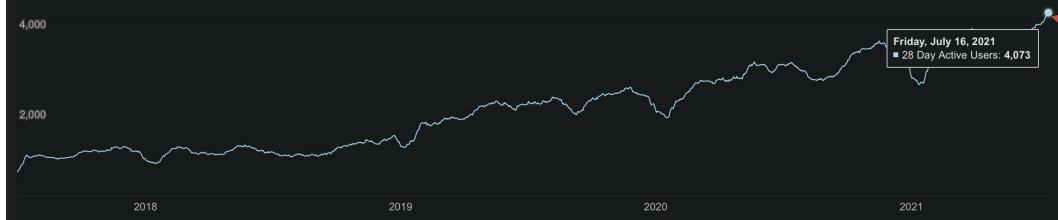


The Spack community continues to grow!

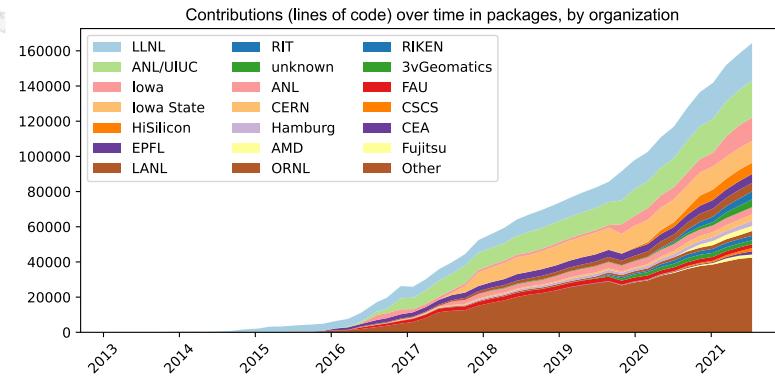
5,700+ software packages
840 contributors



Monthly active users



Package contribution rate increased in 2020



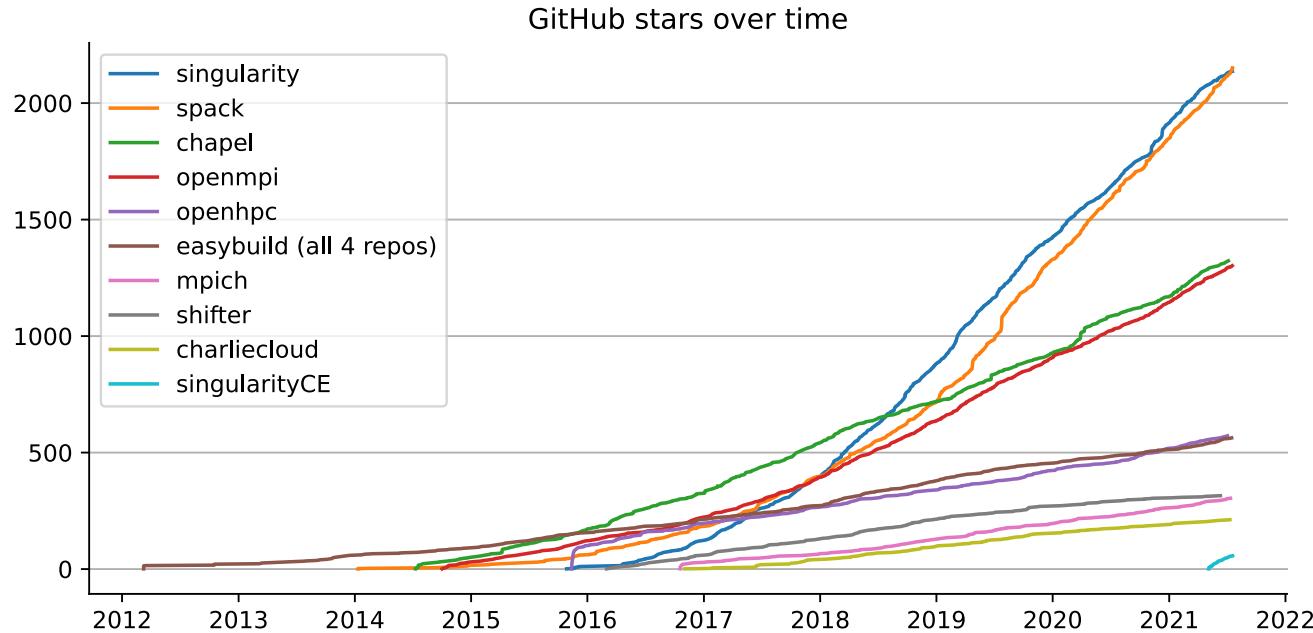
All time high of 4,073
monthly active users last week

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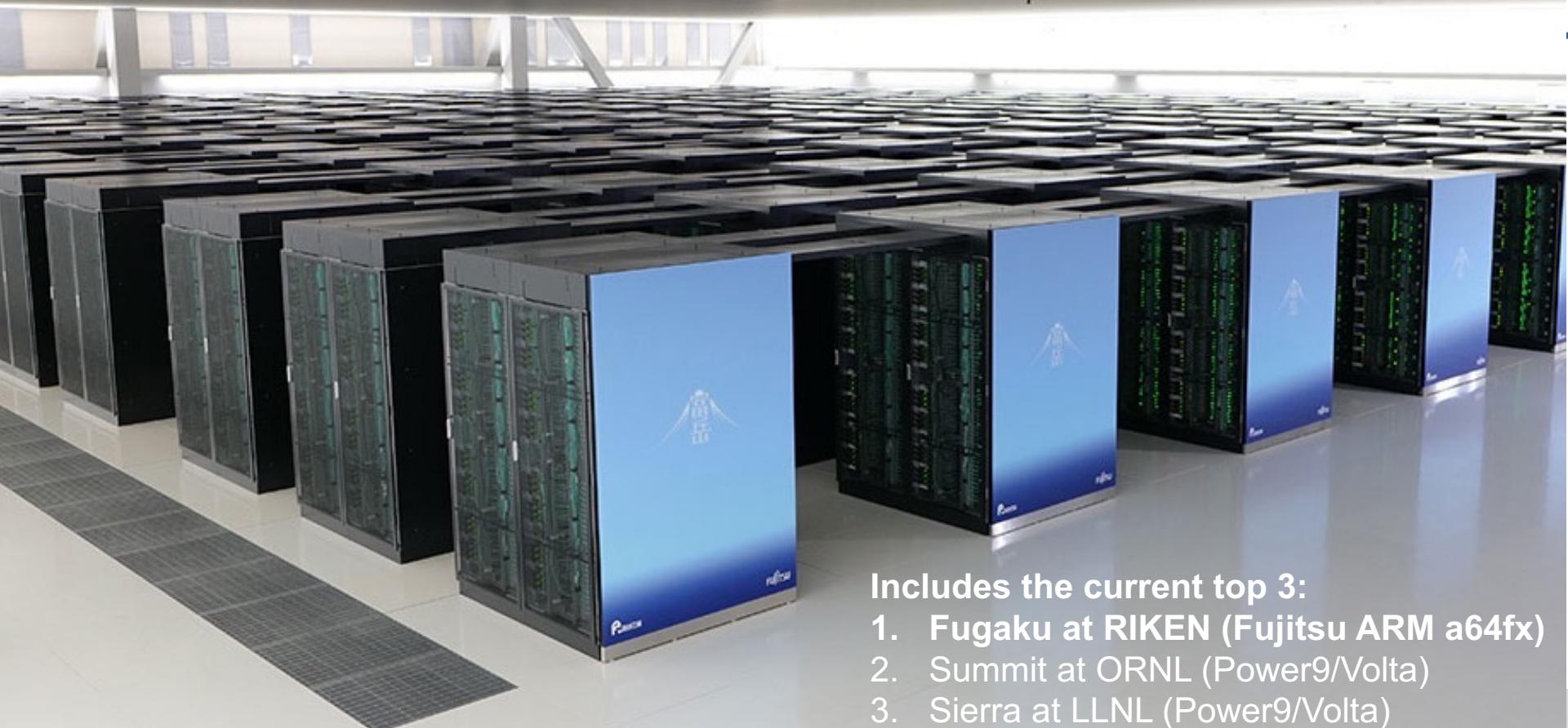


Spack has gained adoption rapidly (if stars are an indicator)



★ Star Spack at github.com/spack/spack if you like the tutorial!

Spack is used on the fastest supercomputers in the world



Includes the current top 3:

1. Fugaku at RIKEN (Fujitsu ARM a64fx)
2. Summit at ORNL (Power9/Volta)
3. Sierra at LLNL (Power9/Volta)

Spack is the deployment tool for the U.S. Exascale Computing Project



- Spack will be used to build software for the US's three upcoming exascale systems
- ECP has built the Extreme Scale Scientific Software Stack (E4S) with Spack – more at <https://e4s.io>
- We are helping ECP fulfill its mission – to create a robust and capable exascale software ecosystem

A screenshot of the E4S Project website. The header features the E4S logo and navigation links for Home, Events, About, DocPortal, Policies, Contact Us, FAQ, and Download. The main banner reads "The Extreme-scale Scientific Software Stack". Below the banner, a section titled "What is E4S?" contains a brief description of the project. Further down, there are four sections: "Purpose" (with an anchor icon), "Approach" (with a gear icon), "Platforms" (with a server icon), and "Testing" (with a test tube icon).

The Extreme-scale Scientific Software Stack (E4S) is a community effort to provide open source software packages for developing, deploying and running scientific applications on high-performance computing (HPC) platforms. E4S provides from-source builds and containers of a broad collection of HPC software packages.

Purpose
E4S exists to accelerate the development, deployment and use of HPC software, lowering the barriers for HPC users. E4S provides containers and turn-key, from-source builds of more than 80 popular HPC products in programming models such as MPI; development tools such as HPCToolkit, TAU and PAPI; math libraries such as PETSc and Trilinos; and Data and Viz tools such as HDF5 and Paraview.

Approach
By using Spack as the meta-build tool and providing containers of pre-built binaries for Docker, Singularity, Shifter and CharlieCloud, E4S enables the flexible use and testing of a large collection of reusable HPC software packages.

Platforms

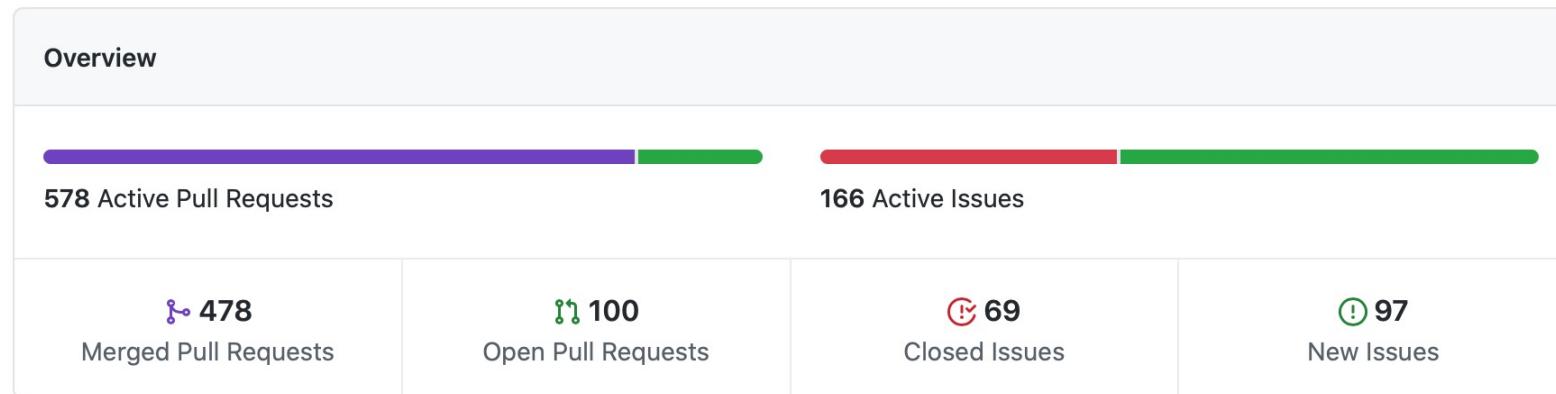
Testing

<https://e4s.io>

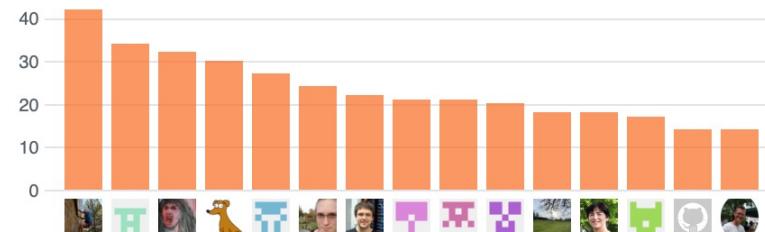
One month of Spack development is pretty busy!

April 20, 2021 – May 20, 2021

Period: 1 month ▾



Excluding merges, **147 authors** have pushed **467 commits** to develop and **566 commits** to all branches. On develop, **596 files** have changed and there have been **8,995 additions** and **3,311 deletions**.



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We have seen an increase in industry contributions to Spack

- **Fujitsu and RIKEN** have contributed a **huge** number of packages for ARM/a64fx support on Fugaku
- **AMD** has contributed ROCm packages and compiler support
 - 55+ PRs mostly from AMD, also others
 - ROCm, HIP, aocc packages are all in Spack now
- **Intel** contributing oneapi support and compiler licenses for our build farm
- **NVIDIA** contributing NVHPC compiler support and other features
- **ARM** and **Linaro** members contributing ARM support
 - 400+ pull requests for ARM support from various companies
- **AWS** is collaborating with us on our build farm, making optimized binaries for ParallelCluster
 - Joint Spack tutorial in July with AWS had 125+ participants

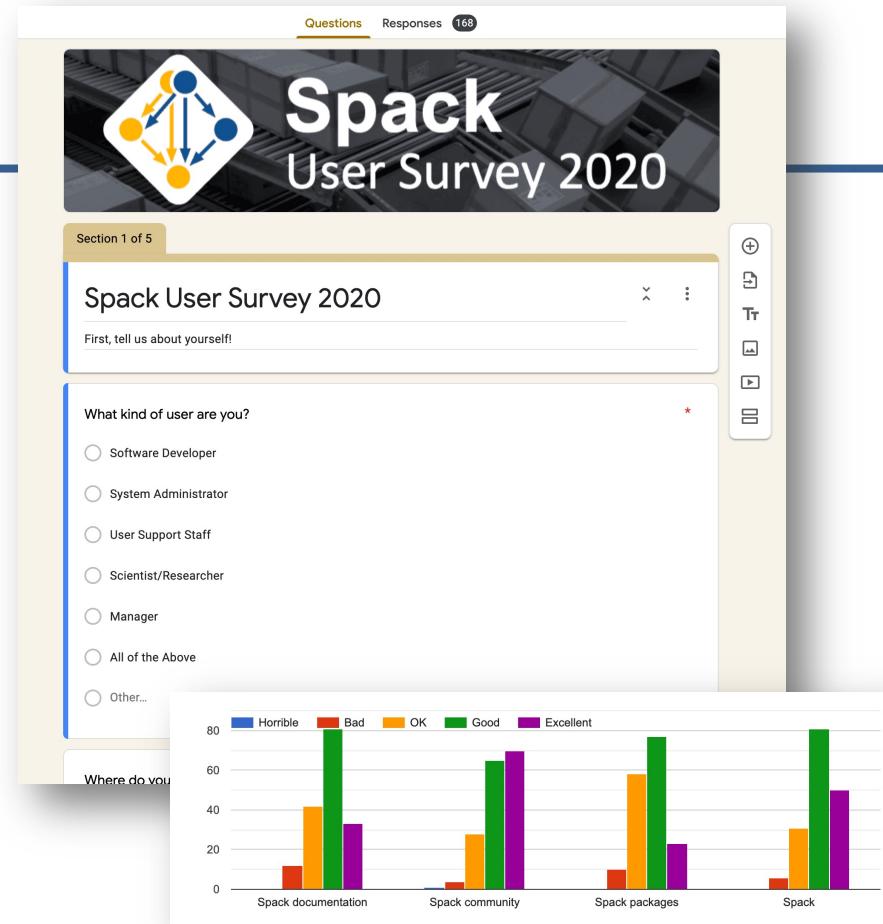


Spack User Survey 2020

- First widely distributed Spack Survey
 - Sent to all of Slack (900+ users)
 - All of Spack mailing list, ECP mailing list
- Got **169 responses!**
- **Takeaways:**
 - People like Spack and its community!
 - Docs and package stability need the most work
 - Concretizer features and dev features are the most wanted improvements

Results writeup and full survey data at:

<https://spack.io/spack-user-survey-2020>



Spack is not the only tool that automates builds



1.

"Functional" Package Managers

- Nix
- GNU Guix

<https://nixos.org/>
<https://www.gnu.org/s/guix/>

2.

Build-from-source Package Managers

- Homebrew, LinuxBrew
- MacPorts
- Gentoo

<http://brew.sh>
<https://www.macports.org>
<https://gentoo.org>

Other tools in the HPC Space:



- **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

<http://hpcugent.github.io/easybuild/>

- **Conda**

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

<https://conda.io>



Hands-on Time: Spack Basics

Follow script at spack-tutorial.readthedocs.io



Core Spack Concepts

If you have not yet joined us on slack,
get an invite here, join the tutorial channel,
and ask for a VM login!

Follow along with the tutorial here

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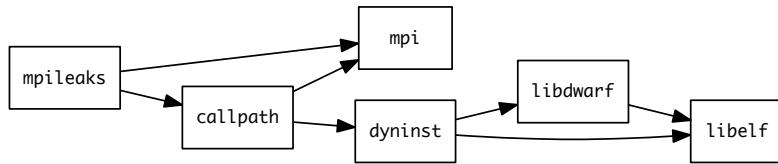
Most existing tools do not support combinatorial versioning

- Traditional binary package managers
 - RPM, yum, APT, yast, etc.
 - Designed to manage a single stack.
 - Install *one* version of each package in a single prefix (/usr).
 - Seamless upgrades to a *stable, well tested* stack
- Port systems
 - BSD Ports, portage, Macports, Homebrew, Gentoo, etc.
 - Minimal support for builds parameterized by compilers, dependency versions.
- Virtual Machines and Linux Containers (Docker)
 - Containers allow users to build environments for different applications.
 - Does not solve the build problem (someone has to build the image)
 - Performance, security, and upgrade issues prevent widespread HPC deployment.



Spack handles combinatorial software complexity

Dependency DAG

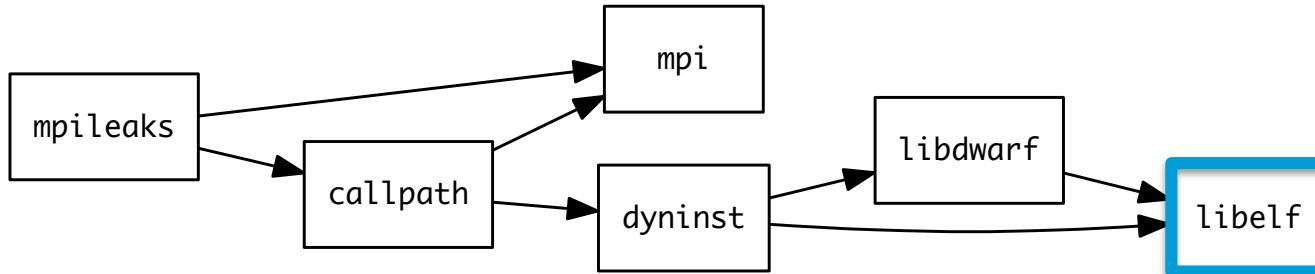


Installation Layout

```
opt
└── spack
    ├── darwin-mojave-skylake
    │   └── clang-10.0.0-apple
    │       ├── bzip2-1.0.8-hc4sm4vuzpm4znmvrfzri4ow2mkphe2e
    │       ├── python-3.7.6-daqqpsssxb6qbfrztsezkmhus3xoflbsy
    │       ├── sqlite-3.30.1-u64v26igvxyn23hysmk1fums6tgjv5r
    │       ├── xz-5.2.4-u5eawkvaoc7vonabe6nndkcfwuv233cj
    │       └── 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*

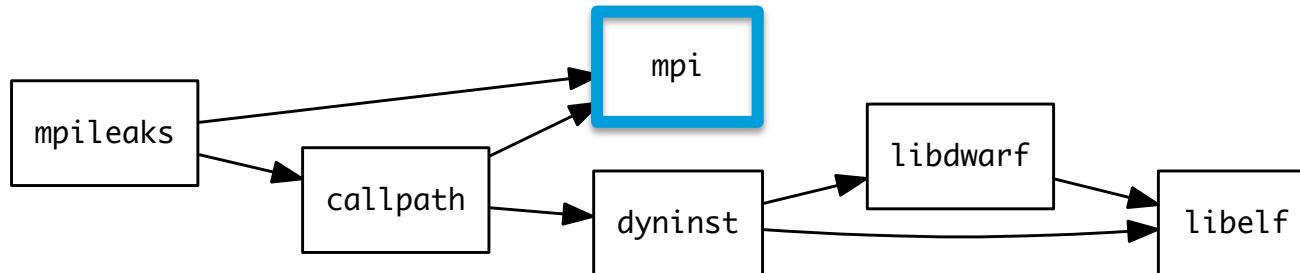
Spack Specs can constrain versions of dependencies



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

- Spack ensures *one* configuration of each library per DAG
 - Ensures ABI consistency.
 - User does not need to know DAG structure; only the dependency *names*.
- Spack can ensure that builds use the same compiler, or you can mix
 - Working on ensuring ABI compatibility when compilers are mixed.

Spack handles ABI-incompatible, versioned interfaces like MPI



- *mpi* is a *virtual dependency*
- Install the same package built with two different MPI implementations:

```
$ spack install mpileaks ^mvapich@1.9
```

```
$ spack install mpileaks ^openmpi@1.4:
```

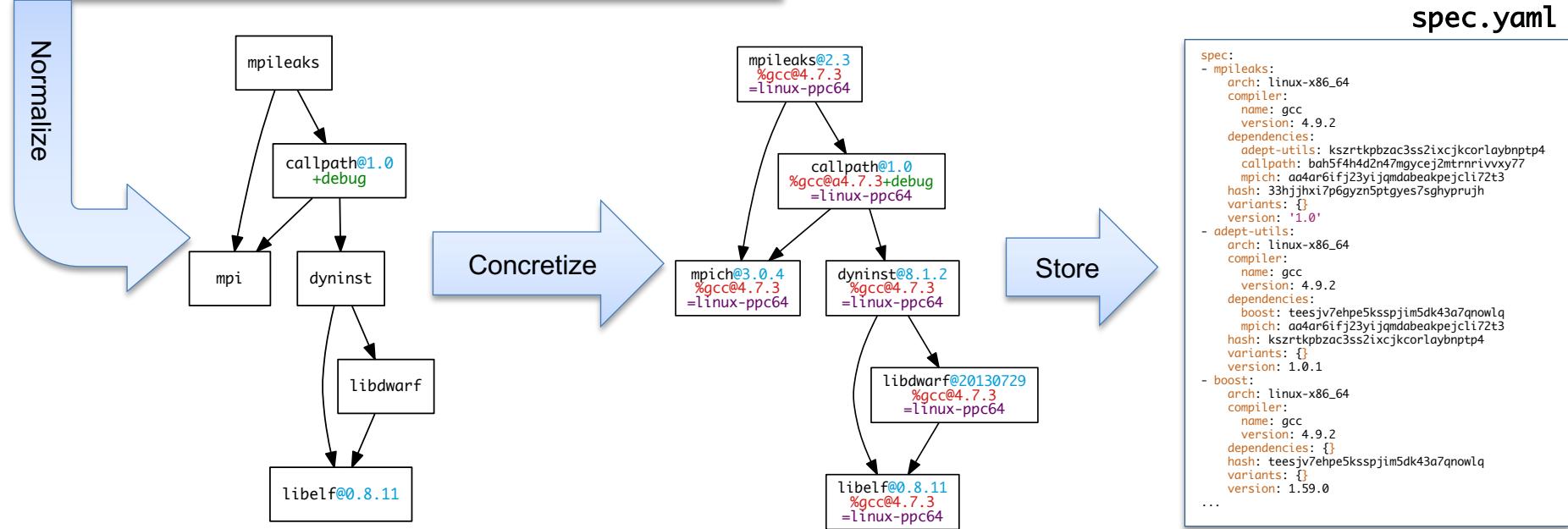
- Let Spack choose MPI implementation, as long as it provides MPI 2 interface:

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

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

mpileaks ^callpath@1.0+debug ^libelf@0.8.11

User input: *abstract spec with some constraints*



Abstract, normalized spec with some dependencies.

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

Detailed provenance is stored with the installed package

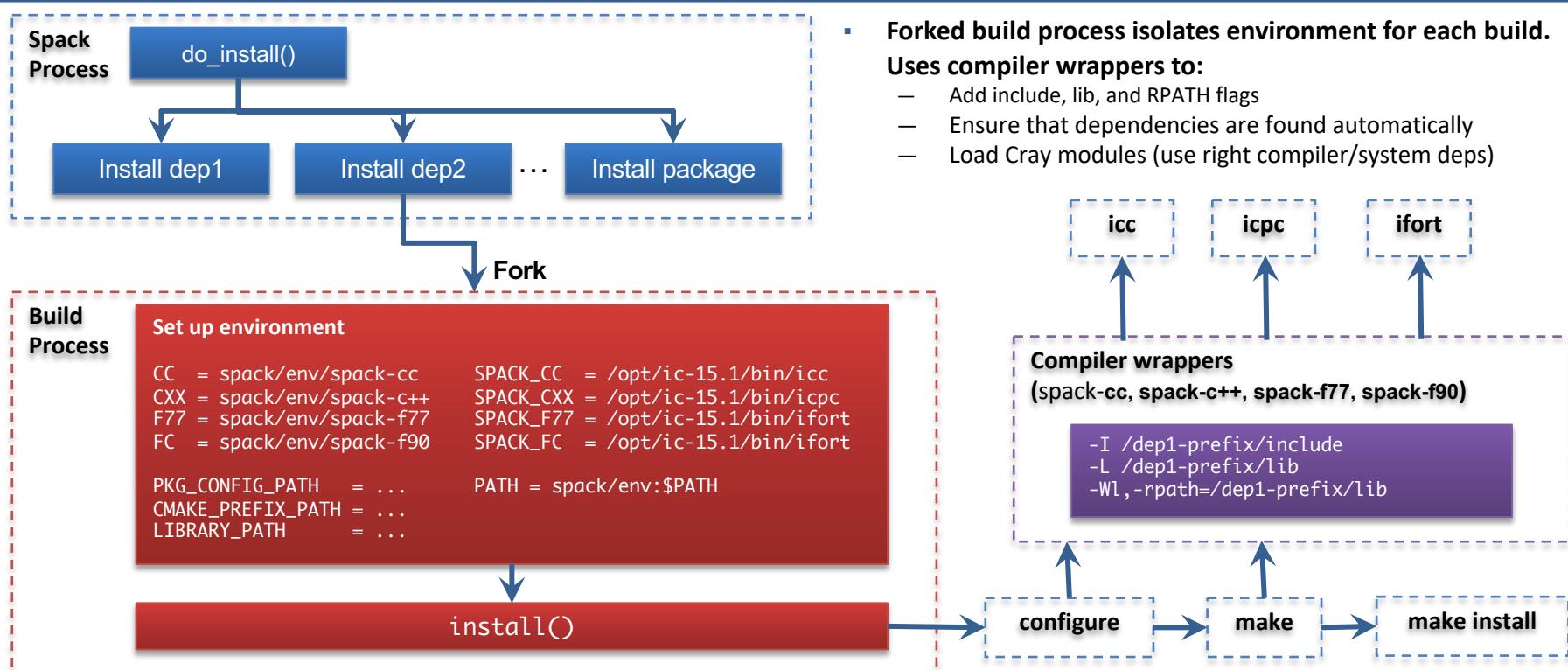
Use `spack spec` to see the results of concretization

```
$ spack spec mpileaks
Input spec
-----
mpileaks

Concretized
-----
mpileaks@1.0%gcc@5.3.0 arch=darwin-elcapitan-x86_64
  ^adept-utils@1.0.1%gcc@5.3.0 arch=darwin-elcapitan-x86_64
    ^boost@1.61.0%gcc@5.3.0+atomic+chrono+date_time~debug+filesystem~graph
      ~icu_support+iostreams+locale+log+math~mpi+multithreaded+program_options
      ~python+random +regex+serialization+shared+signals+singlethreaded+system
      +test+thread+timer+wave arch=darwin-elcapitan-x86_64
    ^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~cxxm~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 builds each package in its own compilation environment



Extensions and Python Support

- Spack installs each package in its own prefix
- Some packages need to be installed within directory structure of other packages
 - i.e., Python modules installed in \$prefix/lib/python-<version>/site-packages
 - Spack supports this via extensions

```
class PyNumpy(Package):
    """NumPy is the fundamental package for scientific computing with Python."""

    homepage = "https://numpy.org"
    url      = "https://pypi.python.org/packages/source/n/numpy/numpy-1.9.1.tar.gz"
    version('1.9.1', '78842b73560ec378142665e712ae4ad9')

    extends('python')

    def install(self, spec, prefix):
        setup_py("install", "--prefix={0}".format(prefix))
```



Spack extensions

- Some packages need to be installed within directory structure of other packages
- Examples of extension packages:
 - python libraries are a good example
 - R, Lua, perl
 - Need to maintain combinatorial versioning

```
$ spack activate py-numpy @1.10.4
```

- Symbolic link to Spack install location
- This is an older feature – we are encouraging users to use **spack environments** instead
 - More on this later!

```
spack/opt/
linux-rhel6-x86_64/
gcc-4.7.2/
python-2.7.12-6y6vvaw/
lib/python2.7/site-packages/
..
py-numpy-1.10.4-oaxix36/
lib/python2.7/site-packages/
numpy/
...
```

```
spack/opt/
linux-rhel6-x86_64/
gcc-4.7.2/
python-2.7.12-6y6vvaw/
lib/python2.7/site-packages/
numpy@
py-numpy-1.10.4-oaxix36/
lib/python2.7/site-packages/
numpy/
...
```

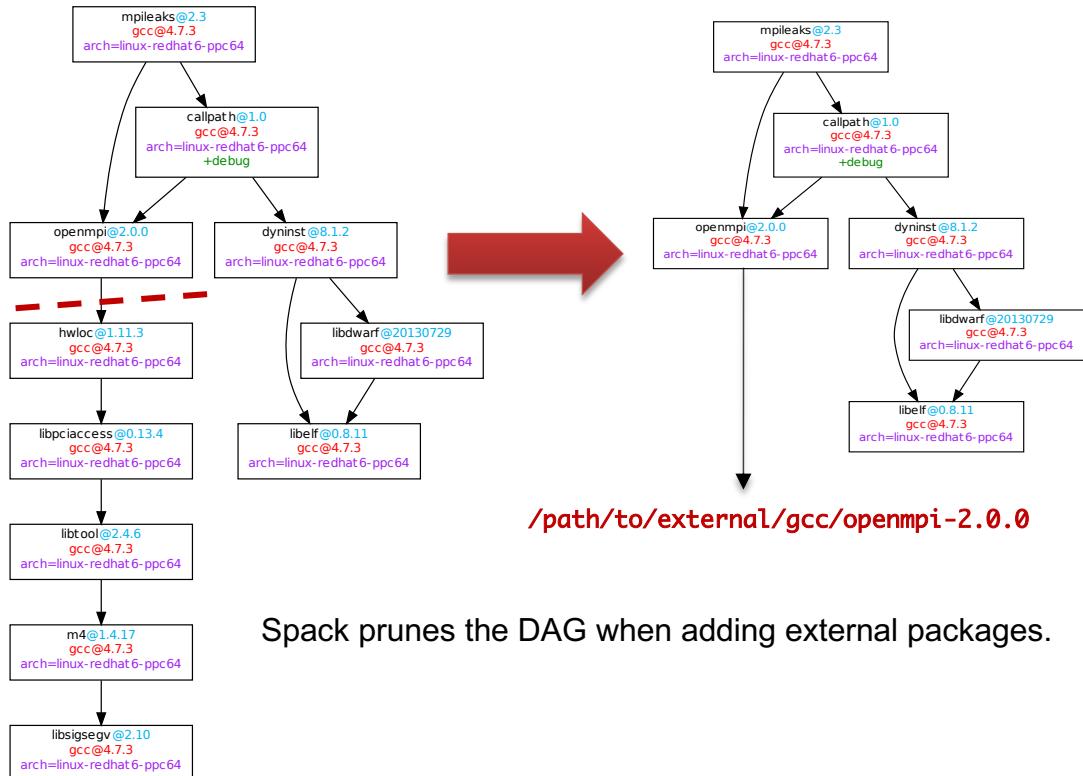


Building against externally installed software

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

packages.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

- Spack supports external package repositories
 - Separate directories of package recipes
- Many reasons to use this:
 - Some packages can't be released publicly
 - Some sites require ~~bizarre~~ custom builds
 - Override default packages with site-specific versions
- Packages are composable:
 - External repositories can be layered on top of the built-in packages
 - Custom packages can depend on built-in packages (or packages in other repos)

```
$ 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
```

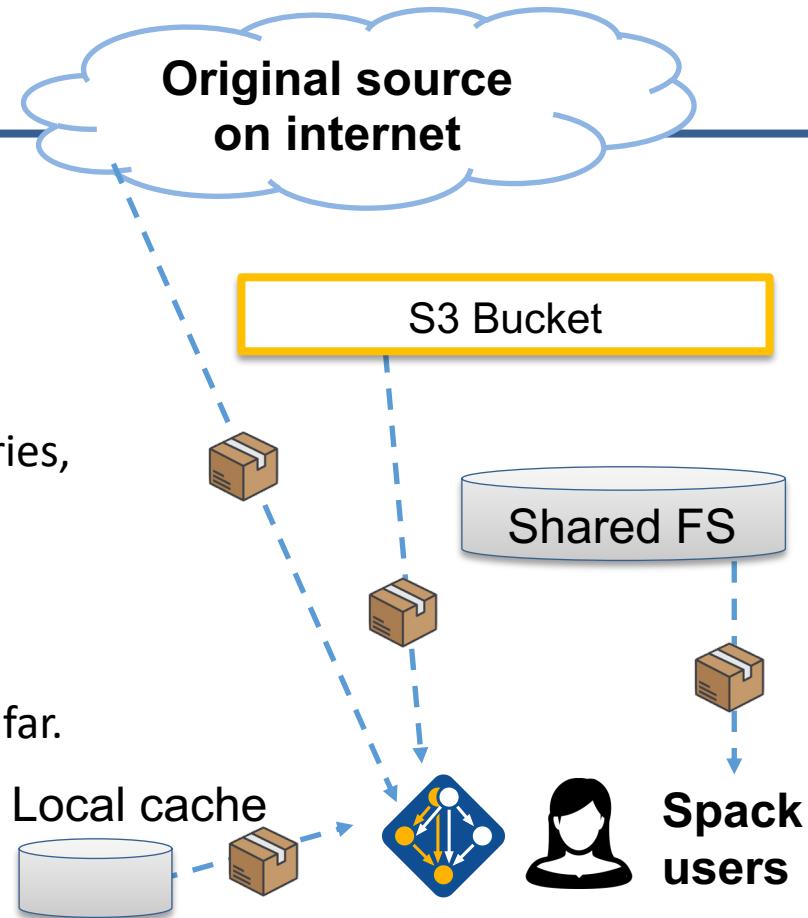
my_repo
proprietary packages, pathological builds

spack/var/spack/repos/builtin
“standard” packages in the spack mainline.



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



Environments, spack.yaml and spack.lock

Follow script at spack-tutorial.readthedocs.io



We'll resume at: 4:20pm CET (7:20am PDT)

Find the slides and associated scripts here:

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We also have a chat room on Spack slack. Get an invite here:

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Join the “tutorial” channel!

We will give you login credentials for the hands-on exercises once you join Slack.

The screenshot shows the "Spack" documentation page on Read the Docs. The top navigation bar includes links for "Docs" and "Tutorial". The main content area features a search bar and a sidebar with sections for "LINKS" (Main Spack Documentation), "TUTORIAL" (Basic Installation Tutorial, Configuration Tutorial, Package Creation Tutorial, Developer Workflows Tutorial), and "Read the Docs" (v: latest). Below the sidebar are sections for "Versions" (latest, sc18, sc17, sc16, riken19, pearc19, nsf19, lanl19, isc19, ecp19), "Downloads", "HTML", "On Read the Docs" (Project Home, Builds, Downloads), "On GitHub", "View", "Edit", and "Search". At the bottom, it says "Hosted by Read the Docs · Privacy Policy".

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This is a full-day int
Practice and Experi
2019.

You can use these n
and read the live de

Slides



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Chicago, IL, USA.

Live Demos

We provide scripts
sections in the slide

1. We provide a
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2. When we ha
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You should now be

Hands-on Time: Configuration

Follow script at spack-tutorial.readthedocs.io



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The screenshot shows a dark-themed documentation page for 'Spack'. At the top is a blue header bar with the Spack logo and the word 'Spack' in white. Below the header is a search bar labeled 'Search docs' and a 'latest' version indicator. A sidebar on the left contains sections for 'LINKS' (Main Spack Documentation), 'TUTORIAL' (Basic Installation Tutorial, Configuration Tutorial, Package Creation Tutorial, Developer Workflows Tutorial), and 'Read the Docs' with a dropdown menu showing 'v: latest'. The main content area includes sections for 'Versions' (latest, sc18, sc17, sc16, riken19, pearc19, nsf19, lanl19, isc19, ecp19), 'Downloads', 'HTML', 'On Read the Docs' (Project Home, Builds, Downloads), 'On GitHub', 'View', 'Edit', and 'Search'. At the bottom of the page is a footer with the text 'Hosted by Read the Docs · Privacy Policy'.

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Live Demos

We provide scripts
sections in the slide

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Hands-on Time: Creating Packages

Follow script at spack-tutorial.readthedocs.io



Hands-on Time: Developer Workflows

Follow script at spack-tutorial.readthedocs.io



Hands-on Time: Binary Caches and Mirrors

Follow script at spack-tutorial.readthedocs.io



Hands-on Time: Stacks

Follow script at spack-tutorial.readthedocs.io



Hands-on Time: Scripting

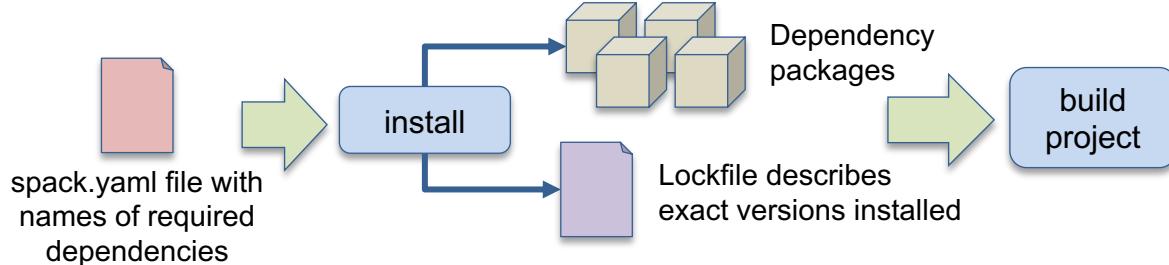
Follow script at spack-tutorial.readthedocs.io



More Features and the Road Ahead



Spack environments are the basis for complex workflows



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
```

- Two files:
 - `spack.yaml` describes project requirements
 - `spack.lock` records installed versions and configurations exactly
 - Enables reproducibility for many configurations
- Can use environments for:
 - Creating containers (`spack containerize`)
 - Auto-generate continuous integration builds (`spack ci`)
 - Deployment (`matrix`, `spack stacks`)
 - **Developer workflows (new!)**

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": {}  
      }  
    }  
  }  
}
```



Generate container images from environments (0.14)

```
spack:  
  specs:  
    - gromacs+mpi  
    - mpich  
  
  container:  
    # Select the format of the recip  
    # singularity or anything else t  
    format: docker  
  
    # Select from a valid list of im  
    base:  
      image: "centos:7"  
      spack: develop  
  
    # Whether or not to strip binari  
    strip: true  
  
    # Additional system packages tha  
    os_packages:  
    - libgomp  
  
    # Extra instructions  
    extra_instructions:  
      final: |  
RUN echo 'export PS1="\[$(tput bold)  
  
# 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  
  # as specified in a manifest file (spack.yaml)  
  RUN mkdir /opt/spack-environment  
  RUN (echo "spack:" \  
  echo "  specs:" \  
  echo "    - gromacs+mpi" \  
  echo "    - mpich" \  
  echo "    concretization: together" \  
  echo "    config:" \  
  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 --  
  
  # 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_en  
  
  # Update the system  
  RUN yum update -y && yum install -y epel-release && yum update -y  
  RUN rm -rf /var/cache/yum && yum clean all  
  
RUN echo 'export PS1="\[$(tput bold)\]\[$(tput setaf 1)\][gromacs]\[$(tput setaf 2)\]\u\[$(tpu
```

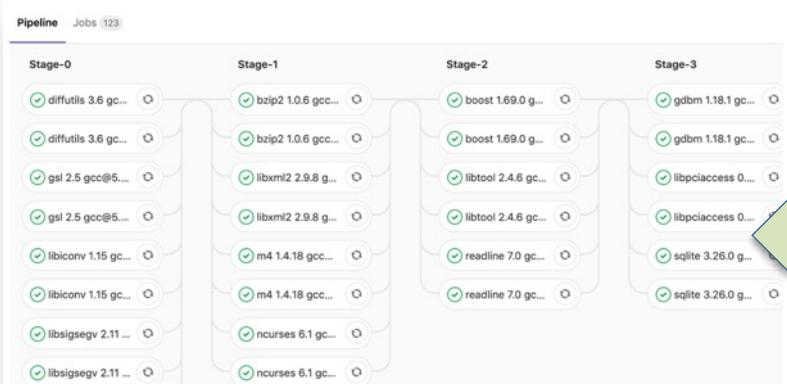


spack containerize

- Any Spack environment can be bundled into a container image
 - Optional container section allows finer-grained customization
- Generated Dockerfile uses multi-stage builds to minimize size of final image
 - Strips binaries
 - Removes unneeded build deps with `spack gc`
- Can also generate Singularity recipes

Spack can generate CI Pipelines from environments

- User adds a gitlab-ci section to environment
 - Spack maps builds to GitLab runners
 - Generate gitlab-ci.yml with `spack ci` command
- Can run in a Kube cluster or on bare metal at an HPC site
 - Sends progress to CDash



spack ci

```
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
```

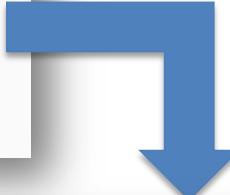
spack external find

```
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))
```

Logic for finding external installations in package.py



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

packages.yaml configuration

- Spack has had compiler detection for a while
 - Finds compilers in your PATH
 - Registers them for use
- We can find any package now
 - Package defines:
 - possible command names
 - how to query the command
 - Spack searches for known commands and adds them to configuration
- Community can easily enable tools to be set up rapidly

spack test: write tests directly in Spack packages, so that they can evolve with the software

```
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%{prefix.include}',
                '-L%{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')
```

Tests are part of a regular Spack recipe class

Easily save source code from the package

User just defines a `test()` method

Retrieve saved source.
Link a simple executable.

Spack ensures that cc is a compatible compiler

Run the built smoke test and verify output

Run programs installed with package



spack develop lets developers work on many packages at once

- Developer features so far have focused on single packages
 - spack dev-build, etc.
- New spack develop feature enables development environments
 - Work on a code
 - Develop multiple packages from its dependencies
 - Easily rebuild with changes
- Builds on spack environments
 - Required changes to the installation model for dev packages
 - dev packages don't change paths with configuration changes
 - Allows devs to iterate on builds quickly

```
$ spack env activate .
$ spack add myapplication
$ spack develop axom@0.4.0
$ spack develop mfem@4.2.0

$ ls
spack.yaml      axom/      mfem/

$ cat spack.yaml
spack:
  specs:
    - myapplication      # depends on axom, mfem
  develop:
    - axom @0.4.0
    - mfem @develop
```



Spack helped streamline the AML team's development environments.

- **Before Spack**

- Everybody built their own python/pytorch from scratch
- People wrote scripts and passed them around
- Scripts slowly accumulated modifications and magic
- **Days were spent trying to debug build differences**

- **After spack**

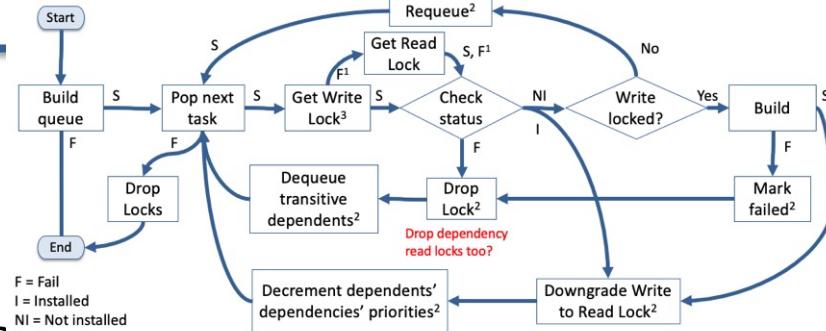
- Versioned reproducible spack environments in a repo
- Standard environments in a shared team directory
- **Any team member can get a customizable working environment in ~20 minutes.**
 - Change python version, change pytorch version, etc.

```
spack:  
  specs:  
    - py-horovod  
    - py-torch  
    - python  
    - py-h5py  
  packages:  
    all:  
      providers:  
        mpi:  
          - mvapich2@2.3  
        lapack:  
          - openblas threads=openmp  
        blas:  
          - openblas threads=openmp  
      buildable: true  
      variants: [+cuda cuda_arch=37]  
      compiler: [gcc@7.3.0]  
    python:  
      version: [3.8.6]  
    cudnn:  
      version:  
        - 8.0.4.30-11.1-linux-x64  
    py-torch:  
      buildable: true  
      variants: +cuda +distributed  
    mvapich2:  
      externals:  
        - spec: mvapich2@2.3.1%gcc@7.3.0  
          prefix: /usr/tce/packages/mvapich2/mvapich2-2.3-gcc-7.3.0  
  compilers:  
    - compiler:  
        operating_system: rhel7  
        paths:  
          cc: /usr/tce/packages/gcc/gcc-7.3.0/bin/gcc  
          cxx: /usr/tce/packages/gcc/gcc-7.3.0/bin/g++
```

Configure and build complex software stacks with a single `spack.yaml` file

Spack's parallel build support can complete 297 E4S packages in 85 minutes on a single node

srun -N 1 -n 8 spack install .



Distributed locking algorithm

```
spack:  
  spec:  
    - openmpi+api  
    - py-libensemble@python3.7.3  
    - hydra  
    - athena  
    - trilinos@12.14.1+dtk+intrepid2+shards  
    - sundials  
    - libfabric  
    - superlu-dist  
    - superlu  
    - taosian  
    - mercury  
    - hdf5  
    - aegis  
    - dyninst  
    - pdt  
    - tau  
    - hecrotkit  
  packages:  
    all:  
      providers:  
        mpi: [spectrum-mpi]  
        target: [ppc64le]  
      cuda:  
        buildable: false  
        version: [10.1.243]  
        modules: [cuda@10.1.243: cuda@10.1.243]  
      spectrum-mpi:  
        buildable: false  
        version: [18.3.1.2]  
        modules:  
          - spectrum-mpi@18.3.1.2: spectrum-mpi@18.3.1.2-20200122  
  config:  
    misc:  
      spack.cache  
      build_stages: $spack/build-stage  
      install_tree: $spack/install-tree  
    view: false  
    concretization: separately|
```

E4S Manifest



Build configuration is its own many-dimensional constraint optimization problem

- The new concretizer in v0.16.0 allows us to solve this problem
 - Uses *Answer Set Programming* – framework for solving NP-hard optimization problems
 - Unlike other systems, package manager has insight into build details and configuration
- ASP program has 2 parts:
 - Large list of facts
 - generated from our package repositories
 - 20,000 – 30,000 facts is typical
 - includes dependencies, versions, options, etc.
 - Small logic program
 - ~800 lines of ASP code
 - 300 rules + 11 optimization criteria

```
%-----  
% 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").
```

Sample ASP input for Spack solver



The new concretizer enables significant simplifications to packages, particularly complex constraints in SDKs

- Dependencies and other constraints within SDKs could get very messy
- The new concretizer removes the need for some of the more painful constructs
- Also allows for new constructs, like specializing dependencies
 - When conditions are now much more general
 - Can be solved together with other constraints.

In some cases we needed cross-products of dependency options:

Before

```
depends_on('foo+A+B', when='+a+b')
depends_on('foo+A~B', when='+a~b')
depends_on('foo~A+B', when='~a+b')
depends_on('foo~A~B', when='~a~b')
```

After

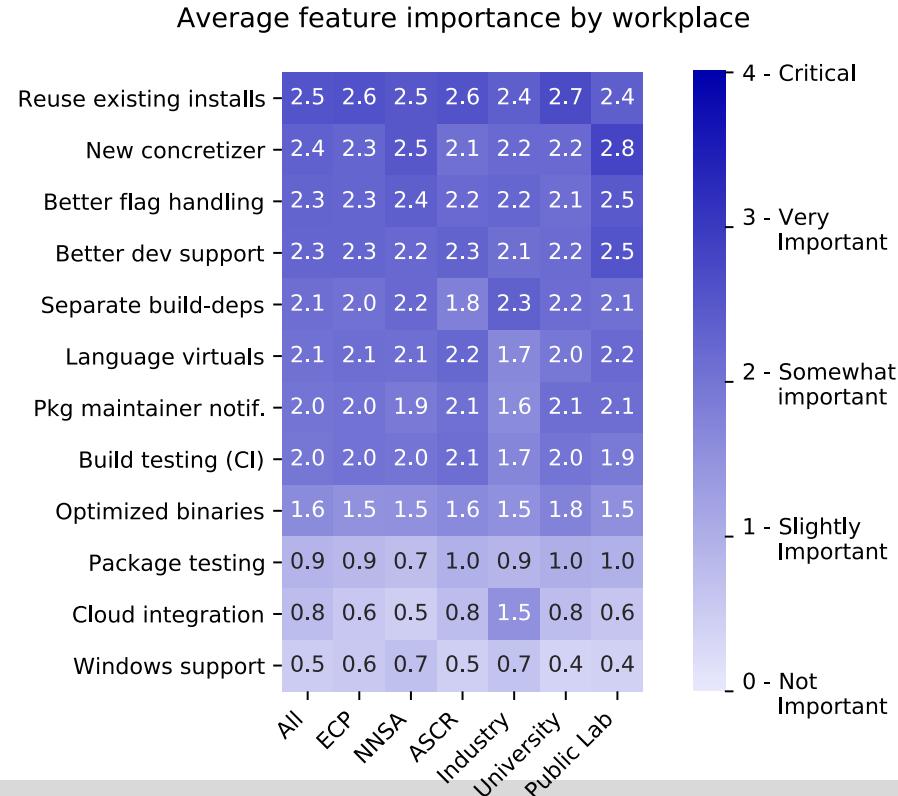
```
depends_on('foo')
depends_on('foo+A', when='+a')
depends_on('foo+B', when='+b')
```

Specializing a virtual did not previously work:

```
depends_on('blas')
depends_on(
    'openblas threads=openmp', when='^openblas'
)
```



Four of the top six most wanted features in Spack are tied to the new concretizer

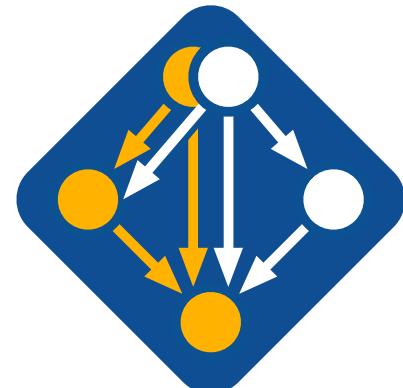


- Complexity of packages in Spack is increasing
 - many more package solves require backtracking than a year ago
 - Many variants, conditional dependencies, special compiler requirements
- More aggressive reuse of existing installs requires better dependency resolution
 - Need to be able to analyze how to configure the build to work with installed packages
- Separate resolution of build dependencies also requires a more sophisticated solver
 - Makes the solve even more combinatorial
 - Needed to support mixed compilers, version conflicts between different package's build requirements

We will be releasing v0.17 soon

Main goals:

1. Get rid of the old concretizer, make the new concretizer default
2. Improve and harden binary cache workflows
3. Make Spack able to optimize for reuse of installed packages and packages from binary mirrors
4. Make “shared” spack instances for facilities more manageable
5. Get rid of pain points like `~/.spack configuration`



Spack 0.17 Roadmap: permissions and directory structure

- **Sharing a Spack instance**

- Many users want to be able to install Spack on a cluster and `module load spack`
- Installations in the Spack prefix are shared among users
- Users would `spack install` to their home directory by default.
- This requires us to move most state ***out*** of the Spack prefix
 - Installations would go into `~/.spack/...`

- **Getting rid of configuration in `~/.spack`**

- While *installations* may move to the home directory, *configuration* there is causing issues
- User configuration is like an unwanted global (e.g., `LD_LIBRARY_PATH` 😬)
 - Interferes with CI builds (many users will `rm -rf ~/.spack` to avoid it)
 - Goes against a lot of our efforts for reproducibility
 - Hard to manage this configuration between multiple machines
- Environments are a much better fit
 - Make users keep configuration like this in an environment instead of a single config

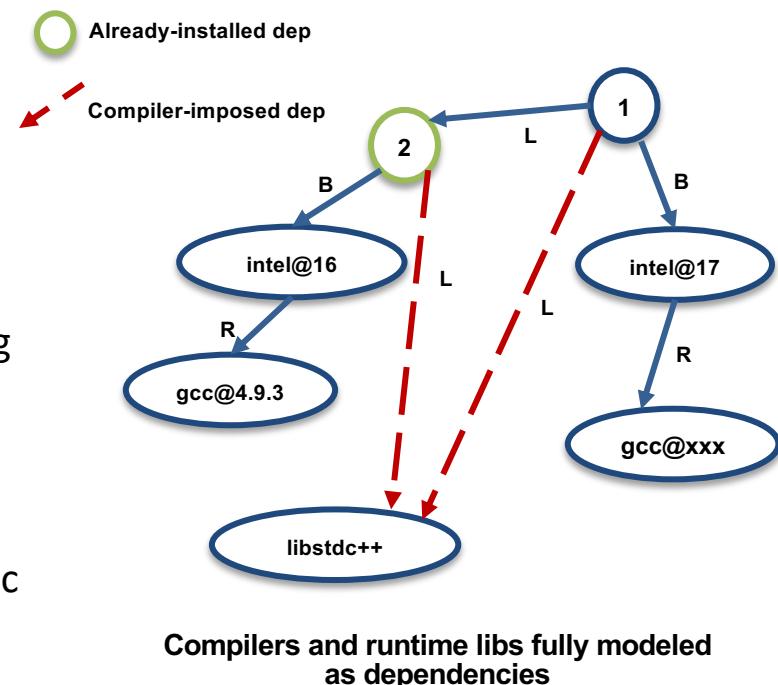


Spack 0.18 Roadmap: compilers as dependencies

- We need deeper modeling of compilers to handle compiler interoperability
 - libstdc++, libc++ compatibility
 - Compilers that depend on compilers
 - Linking executables with multiple compilers

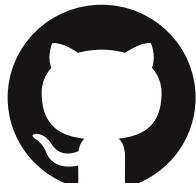
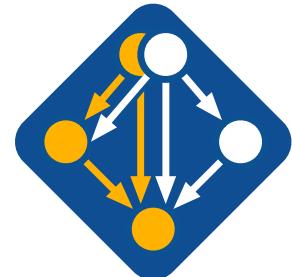
- First prototype is complete!
 - We've done successful builds of some packages using compilers as dependencies
 - We need the new concretizer to move forward!

- 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



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!
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We hope to make distributing & using HPC software easy!



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