

# Building things: Spack, Software, and Sustainable Communities in HPC

ATPESC: Argonne Training Program on Extreme-Scale Computing



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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

LLNL-PRES-747560



### Scientific software is becoming extremely complex



#### Even proprietary codes are based on many open source libraries



- Half of this DAG is external (blue); more than half of it is open source
- Nearly all of it needs to be built specially for HPC to get the best performance











#### The Exascale Computing Project is building an entire *ecosystem*



#### = up to **1,260,000** combinations!

- Every application has its own stack of dependencies.
- Developers, users, and facilities dedicate (many) FTEs to building & porting.
- Often trade reuse and usability for performance.

#### We must make it easier to rely on others' software!













#### How to install software on a Mac laptop, circa 2013

(gluon):~\$ port install libelf

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







#### How to install software on a supercomputer, circa 2013



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### What about modules?

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

```
$ gcc
-bash: gcc: command not found
$ module load gcc/7.0.1
$ gcc -dumpversion
7.0.1
```

- Modules don't handle installation!
  - They only modify your environment (things like PATH, LD\_LIBRARY\_PATH, etc.)
- Someone (likely a team of people) has already installed gcc for you!
  - Also, you can only `module load` the things they've installed







# What's a package manager?

#### Package manager

- **Does not** a replace Cmake/Autotools
- Packages built by Spack can have any build system they want
- PMs manage *dependencies* 
  - Drive package-level build systems
  - Or installs pre-built binaries
  - Ensures consistent configuration
- Determining magic configure lines takes time
  - PMs cache the work of others
  - Provide a way to encode recipes so that you can reuse others' effort!

Package Manager	<ul> <li>Manages package installation</li> <li>Manages dependency relationships</li> <li>Drives package-level build systems</li> </ul>
High Level Build System	<ul> <li>Cmake, Autotools</li> <li>Handle library abstractions</li> <li>Generate Makefiles, etc.</li> </ul>
Low Level Build System	<ul> <li>Make, Ninja</li> <li>Handles dependencies among commands in a single build</li> </ul>







# So why didn't these things catch on in HPC?

- Traditional binary package managers don't support combinatorial versioning
  - 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
- Neither, typically, do port systems
  - BSD Ports, portage, Macports, Homebrew, Gentoo portage, etc.
  - Minimal support for builds parameterized by compilers, dependency versions.
- Issues:
  - HPC people want to experiment
  - Many of these typically require root access, can't have root on a supercomputer
  - Binaries aren't optimized
    - typically built for lowest-common-denominator hardware
- System package managers mostly used for low level system, not the HPC stack







### HPC needed a better way to build software

#### My frustrations:

- 1. Constantly rebuilding graduate students' software for them
- 2. Facilities spend lots of time building a comparatively small number of software packages
  - Quickly goes out of date
  - Not built with the right compiler, MPI, dependency version, etc.
  - App teams end up rebuilding anyway!
- 3. Hard to distribute performance tools!
  - My research was going unused because it was hard to install.
- Requirements for a good solution:
  - Target users, admins, and developers (many roles in HPC)
  - Easy to use commands, no tedious build steps
  - Easy to contribute: package recipes should be in a language that HPC people already know
  - Rapidly build many different versions of software, experiment with performance options







# **Spack is a flexible package manager for HPC**

- How to install Spack (works out of the box):
- \$ git clone <u>https://github.com/spack/spack</u>
- \$ . spack/share/spack/setup-env.sh
- How to install a package:

\$ spack install hdf5

- HDF5 and its dependencies are installed within the Spack directory.
- Unlike typical package managers, Spack can also install many variants of the same build.
  - Different compilers
  - Different MPI implementations
  - Different build options











#### Spack provides the spec syntax to describe custom configurations

<pre>\$ spack install mpileaks</pre>	unconstrained
<pre>\$ spack install mpileaks@3.3</pre>	<pre>@ custom version</pre>
<pre>\$ spack install mpileaks@3.3 %gcc@4.7.3</pre>	% custom compiler
<pre>\$ spack install mpileaks@3.3 %gcc@4.7.3 +threads</pre>	+/- build option
<pre>\$ spack install mpileaks@3.3 cppflags="-03 -g3"</pre>	setting compiler flags
<pre>\$ spack install mpileaks@3.3 os=CNL10 target=haswell</pre>	setting target for X-compile
<pre>\$ spack install mpileaks@3.3 ^mpich@3.2 %gcc@4.9.3</pre>	^ dependency information

- Each expression is a *spec* for a particular configuration
  - Each clause adds a constraint to the spec
  - Constraints are optional specify only what you need.
  - Customize install on the command line!
- Spec syntax is recursive
  - Full control over the combinatorial build space









#### `spack list` shows what packages are available

\$ spack lis	t									
==> 303 pac	kages.									
activeharmony	cgal	fish	gtkplus	libgd	mesa	openmpi	py-coverage	py-pycparser	qt	tcl
adept-utils	cgm	flex	harfbuzz	libgpg-error	metis	openspeedshop	py-cython	py-pyelftools	gthreads	texinfo
apex	cityhash	fltk	hdf	libjpeg-turbo	Mitos	openssl	py-dateutil	py-pygments	Ŕ	the_silver_searcher
arpack	cleverleaf	flux	hdf5	libjson-c	mpc	otf	py-epydoc	py-pylint	ravel	thrift
asciidoc	cloog	fontconfig	hwloc	libmng	mpe2	otf2	py-funcsigs	py-pypar	readline	tk
atk	cmake	freetype	hypre	libmonitor	mpfr	pango	py-genders	py-pyparsing	rose	tmux
atlas	cmocka	gasnet	icu	libNBC	mpibash	papi	py-gnuplot	py-pyqt	rsync	tmuxinator
atop	coreutils	gcc	icu4c	libpciaccess	mpich	paraver	py-h5py	py-pyside	ruby	trilinos
autoconf	cppcheck	gdb	ImageMagick	libpng	mpileaks	paraview	py-ipython	py-pytables	SAMRAI	uncrustify
automaded	cram	gdk-pixbuf	isl	libsodium	mrnet	parmetis	py-libxml2	py-python-daemon	samtools	util-linux
automake	cscope	geos	jdk	libtiff	mumps	parpack	py-lockfile	py-pytz	scalasca	valgrind
bear	cube	gflags	jemalloc	libtool	munge	patchelf	py-mako	py-rpy2	scorep	vim
bib2xhtml	curl	ghostscript	jpeg	libunwind	muster	pcre	py-matplotlib	py-scientificpython	scotch	vtk
binutils	czmq	git	judy	libuuid	mvapich2	pcre2	py-mock	py-scikit-learn	scr	wget
bison	damselfly	glib	julia	libxcb	nasm	pdt	py-mpi4py	py-scipy	silo	WX
boost	dbus	glm	launchmon	libxml2	ncdu	petsc	py-mx	py-setuptools	snappy	wxpropgrid
bowtie2	docbook-xml	global	lcms	libxshmfence	ncurses	pidx	py-mysqldb1	py-shiboken	sparsehash	xcb-proto
boxlib	doxygen	glog	leveldb	libxslt	netcdf	pixman	py-nose	py-sip	spindle	xerces-c
bzip2	dri2proto	glpk	libarchive	ll∨m	netgauge	pkg-config	py-numexpr	py-six	spot	XZ
cairo	dtcmp	gmp	libcerf	ll∨m-lld	netlib-blas	pmgr_collective	py-numpy	py-sphinx	sqlite	yasm
callpath	dyninst	gmsh	libcircle	lmdb	netlib-lapack	postgresql	py-pandas	py-sympy	stat	zeromq
cblas	eigen	gnuplot	libdrm	lmod	netlib-scalapack	ppl	py-pbr	py-tappy	sundials	zlib
cbtf	elfutils	gnutls	libdwarf	lua	nettle	protobuf	py-periodictable	py-twisted	swig	zsh
cbtf-argonavis	elpa	gperf	libedit	lwgrp	ninja	py-astropy	py-pexpect	py-urwid	szip	
cbtf-krell	expat	gperftools	libelf	lwm2	ompss	py-basemap	py-pil	py-virtualenv	tar	
cbtf-lanl	extrae	graphlib	libevent	matio	ompt-openmp	py-biopython	py-pillow	py-yapf	task	
cereal	exuberant-ctags	graphviz	libffi	mbedtls	opari2	py-blessings	py-pmw	python	taskd	
cfitsio	fftw	gsl	libgcrypt	memaxes	openblas	py-cffi	py-pychecker	qhull	tau	

Spack has over 2,800 packages now.







# `spack find` shows what is installed



- All the versions coexist!

   Multiple versions of same package are ok.
- Packages are installed to automatically find correct dependencies.
- Binaries work regardless of user's environment.
- Spack also generates module files.
  - Don't have to use them.







# Users can query the full dependency configuration of installed packages.

<pre>\$ spack find callpath ==&gt; 2 installed packages.  linux-x86_64 / clang@3.4 callpath@1.0.2</pre>		linux-x86_64 / gcc@4.9.2 callpath@1.0.2		
Expand dependencies with spack find -d	<pre>\$ spack f ==&gt; 2 ins  linux- xv2clz2 ckjazss 3ws43m4 ft7znm6 qqnuet3 3ws43m4 g65rdud cj5p5fk cj5p5fk g65rdud cj5p5fk cj5p5fk cj5p5fk</pre>	Find -dl callpath stalled packages. -x86_64 / clang@3.4 callpath@1.0.2 ^adept-utils@1.0.1 ^boost@1.59.0 ^mpich@3.1.4 ^dyninst@8.2.1 ^boost@1.59.0 ^libdwarf@20130729 ^libelf@0.8.13 ^libelf@0.8.13 ^libelf@0.8.13	linux- udltshs rfsu7fb <b>ybet64y</b> aa4ar6i tmnnge5 <b>ybet64y</b> g2mxrl2 ynpai3j ynpai3j g2mxrl2 ynpai3j ynpai3j	<pre>x86_64 / gcc@4.9.2 callpath@1.0.2     ^adept-utils@1.0.1</pre>
	ft7znm6	^mpich@3.1.4	aa4ar6i	^mpich@3.1.4

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







#### Spack packages are *templates*: they define how to build a spec









# Spack handles combinatorial software complexity.



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- Each unique dependency graph is a unique configuration.
- Each configuration installed in a unique directory.
   Configurations of the same package can coexist.
- Hash of entire directed acyclic graph (DAG) is appended to each prefix.
- Installed packages automatically find dependencies
   Spack embeds RPATHs in binaries.
  - No need to use modules or set LD\_LIBRARY\_PATH
  - Things work the way you built them







# **Depend on interfaces (not implementations)** with virtual dependencies

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

\$ spack install mpileaks ^mvapich

\$ spack install mpileaks ^openmpi@1.4:

- Virtual deps are replaced with a valid implementation at resolution time.
  - If the user didn't pick something and there are multiple options, Spack picks.



Virtual dependencies can be versioned:

class	<pre>Mpileaks(Package):</pre>	
d	epends_on("mpi@2:")	

dependent

class Mvapich(Package): provides("mpi@1" when="@:1.8") provides("mpi@2" when="@1.9:")

provider

class Openmpi(Package): provider provides("mpi@:2.2" when="@1.6.5:")







### **Concretization fills in missing parts of requested specs.**

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



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

#### Workflow:

- 1. Users input only an *abstract* spec with some constraints
- 2. Spack makes choices according to policies (site/user/etc.)
- 3. Spack installs *concrete* configurations of package + dependencies
- Dependency resolution is an NP-complete problem!
  - Different versions/configurations of packages require different versions/configurations of dependencies
  - Concretizer searches for a configuration that satisfies all the requirements
  - This is basically a SAT/SMT solve



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#### **Dependency Resolution is an NP-complete problem!**



Unsatisfiable!

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https://research.swtch.com/version-sat

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Different versions of packages require different versions of dependencies

- Concretizer searches for a configuration that satisfies all the requirements
- Can show that SAT/SMT solve is equivalent problem
- Resolution is NP-complete for \*just\* package and version metadata
  - Concretization also includes compilers, variants, architecture, optional dependencies, virtual dependencies
  - We have some leeway because multiple stacks can coexist within Spack (unlike system PMs)
  - Even within one DAG there can be issues!









**Contributions to Spack have taken off** 

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LLNL packages comprise < 20% of total</p>



Documentation



uly 2, 2018 – Au	gust 2, 2018		Period: 1 month -	
Overview				
206 Active Pull Request	ts	98 Active Issues		#16 most contributed-to Python project on GitHu
រ៉ <b>ា 161</b> Merged Pull Requests	¥ 45 Proposed Pull Requests	<b>58</b> Closed Issues	<b>! 40</b> New Issues	

Excluding merges, 55 authors have pushed 202 commits to develop and 251 commits to all branches. On develop, 761 files have changed and there have been 14,324 additions and 4,332 deletions.



11 161 Pull requests merged by 52 people

https://krihelinator.xyz/languages/Python









# Spack is now used worldwide!

- 400-500 downloads per day
- Over **2,800** package recipes
- 7,800 unique users on docs site in the past year
  - Probably a (large) overestimate
  - Hard to get good numbers
- There is steady interest in Spack!





Users

190





# Spack is being used on many of the top HPC systems

- At HPC sites for reproducible software stack+ modules
  - Reduced Summit deploy time from 2 weeks to 12 hrs.
  - EPFL deploys its software stack with Jenkins + Spack
  - NERSC, LLNL, ANL, other US DOE sites
  - SJTU in China
- Within ECP as part of their software release process
  - ECP-wide software distribution
  - SDK workflows
- Within High Energy Physics (HEP) community
  - HEP (Fermi, CERN) have contributed many features to support their workflow
- Many others





They wouldn't let me put a sticker on it...

@spackpm

github.com/spack





# Under ECP, "SDK" teams manage releases using Spack

- xSDK pioneered the SDK concept
  - 8 member projects, 22 required dependencies
  - Includes many major solver library teams
  - Next release will have 10+ additional packages
- Teams work together on regular releases
  - Helps to work out compatibility issues
  - Gets developers talking to each other
  - Encourages teams to factor into smaller libraries
- ECP is establishing more SDKs for different areas
  - SDKs will be released using Spack
  - Each will be its own meta-package like xSDK









# How did we build a community?

- Mostly luck, and also by lowering barriers for people to join.
- Without git & GitHub, we wouldn't be able to manage contributions from nearly as many people
  - Git handles concurrent development easily with forks and branches
- Many people are familiar with how to contribute to github projects
  - Pull requests are well understood and accessible

LLNL / spack		⊙ Unwatch -	51 🛨 Unstar 191 😵 Fork 1
<>Code (!) Issues 373	1) Pull requests 77 III Projects 2	🗉 Wiki  Pulse 👔	🗓 Graphs 🔅 Settings
flexible package manager - Edit	designed to support multiple versions, co	onfigurations, platforms, and	d compilers. http://llnl.github.io/spa
© 5,162 commits	پ <b>78</b> branches	♥ 10 releases	103 contributors
Branch: develop - New pull	request	Create new file Uplo	pad files Find file Clone or downloa
davydden committed with	tgamblin slepc/petsc: fix python dependency (	#2560)	Latest commit fab9af7 8 hours a
bin	Add a test to ensure package names hav	e the right case. (#2562)	8 hours a
etc/spack/defaults	add ACLOCAL_PATH updates for packag	es that register m4 macros (#	2518) 6 days a
lib/spack	Add a test to ensure package names hav	re the right case. (#2562)	8 hours a
share/spack	Allow shell support to work when set -u i	is set (#2418)	14 days a
var/spack	slepc/petsc: fix python dependency (#25	560)	8 hours a
coveragerc	Move args to .coveragerc		7 months a
.flake8	Some flake8 settings weren't documente	ed	4 months a
.gitignore	Abinit: Added package(s) (#1995)		2 months a
.mailmap	Update mail map. So many email aliases.		2 months a
.travis.yml	Remove CYAML tests from Spack now th	at the DB is JSON. (#2487)	8 days a
	Correct LLNL LGPL license template for	clarity.	7 months a



build passing coverage 65%

Spack is a package management tool designed to support multiple versions and configurations of software on a wide variety of platforms and environments. It was designed for large supercomputing centers, where many users and application teams share common installations of software on clusters with exotic architectures, using libraries that do not have a standard ABI. Spack is non-destructive: installing a new version does not break existing installations, so many configurations can coexist on the same system.



github.com/spack





### **Documentation is critical for recruiting users and contributors**

- Recent GitHub survey showed that users are much more inclined to use a well documented project Obvious? Maybe.
- readthedocs.org makes hosting documentation easy
  - Sphinx .rst files are fairly easy to write
  - Auto-generate docs from the main **GitHub** repository
  - Built-in versioning
- Remember that users can contribute docs!
  - Make it easy for them.







C Edit on GitHub

#### **Spack Documentation**

Spack is a package management tool designed to support multiple versions and configurations of software on a wide variety of platforms and environments. It was designed for large supercomputing centers, where many users and application teams share common installations of software on clusters with exotic architectures, using libraries that do not have a standard ABI. Spack is non-destructive: installing a new version does not break existing installations, so many configurations can coexist on

Most importantly, Spack is *simple*. It offers a simple *spec* syntax so that users can specify versions and configuration options concisely. Spack is also simple for package authors: package files are written in pure Python, and specs allow package authors to maintain a single file for many different

See the Feature Overview for examples and highlights.

Get spack from the github repository and install your first package:

\$ git clone https://github.com/llnl/spack.git

If you're new to spack and want to start using it, see Getting Started, or refer to the full manual

- Simple package installation
- Custom versions & configurations
- Customize dependencies
- Non-destructive installs
- Packages can peacefully coexist

#### spack.readthedocs.io







# Testing and Continuous Integration are critical for scaling a large project.

- Spack currently uses Travis CI to test Spack itself.
  - Every contribution is tested against regression tests in the cloud.
  - We only merge pull requests if they pass Spack's test suite
  - Also enforce style guidelines
- The contribution process is also documented.
- Travis is free and easy!
  - Commit a single, short .travis.yml file to your repo
  - Tests are run automatically
- We would never be able to handle so many contributions if we had to do all this manually.













#### Spack Roadmap

#### 1. Infrastructure for binary distribution

- Source mirror with archives for all projects in Spack
- Cloud-based build farm for relocatable binary packaging

#### 2. "Environments" for developer dependency management

- Ability to have separate contexts in Spack
- Manifest/lockfile model supported in Spack

#### 3. We are developing a new concretizer for Spack

Needed to support the above two roadmap elements









# We are building more extensive CI infrastructure to enable testing real package *builds*





# Through ECP, we are working with Onyx Point to deliver continuous integration for HPC centers







- CI at HPC centers is notoriously difficult
  - Security concerns prevent most CI tools from being run by staff or by users
  - HPC centers really need to deploy trusted CI services for this to work
- Contracted Onyx Point to develop a secure CI system for HPC centers:
  - Setuid runners (run CI jobs as users); Batch integration (similar, but parallel jobs); multi-center runner support
- This effort required cooperation from 6 labs and ECP!
- Getting everyone on the same page about requirements was key to enabling the project.









# Package managers are a key part of reproducible workflows



- Package managers are used to install packages needed before a build
- Also used by HPC facilities to manage system software on supercomputers
  - OS level (RPM, yum, yast, OpenHPC, etc.)
  - Scientific software level (increasingly Spack, Easybuild)
- Manifest / Lockfile model pioneered by Bundler is becoming standard
  - Lockfile can be used to exactly reproduce a prior installation
  - Many language-specific examples: Bundler, Cargo, npm, pipenv, etc.
- This model is very similar to Spack's concretization!





gnupg2
cmake
r-base

- perl

install:

r-base-corer-base-dev

- perl-base

- pip install --upgrade pip

- pip install --upgrade six

- pip install --upgrade flake8

pip install --upgrade setuptoolspip install --upgrade codecov

Excerpt from a .travis.yml file



# Spack environments will support the manifest/lockfile model



github.com/spack

- Ability to manage multiple environments independently
  - On the command line with regular spack commands, or
  - Projects can have a spackfile.yaml describing dependencies
- Lock file contains complete provenance

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- Lock file can be used to reproduce the same build on the same machine
- Or to reproduce a "close as possible" build on a different machine



@spackpm



# Binary packaging and environments require improvements to concretization

- Currently, Spack looks only at command line and package files for constraints
  - Does not make special efforts to reuse already-installed binaries
- For both environments and binary packaging, we need to reuse:
  - Available packages in a binary mirror
  - Available packages in the current environment
- New concretizer needs to do solves not just for package/version but also:
  - Build options (potentially multi-valued)
  - Compilers and compiler versions
  - Virtual dependencies
  - Binary compatibility and compiler constraints
- This is like existing manifest/lockfile solvers, but with many more constraints







# **Summary: Insights from Spack**

- Don't be afraid to tackle problems that are somewhat outside your primary domain.
  - I didn't expect to be working on a build system!
- If you think your project could have impact, build a community!
  - Think about more than just your use case
  - Even if your contributors' needs are different, they can help your project
  - Every new Spack package gets us more core contributions, more robustness
- General open source guidelines:
  - Documentation!

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- Continuous integration!
- Use a language the community knows
- Delegate and spread the work out to your contributors

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Be open to putting more work in. You could get much more out.



#### Get stickers!













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