Build and Test Automation at Livermore Computing

National Center for Computational Sciences Seminar Presented at Oak Ridge National Laboratory

Todd Gamblin Center for Applied Scientific Computing



Modern software developers employ a range of collaborative tools.

Collaborative web applications:

- Wikis (MediaWiki, Trac, Confluence)
- Issue trackers (RoundUp, Bugzilla, JIRA)
- Repository systems (Stash, Bitbucket, GitHub, GitLab)

• Automated Testing:

- Build & Test / Continuous Integration (Jenkins, Bamboo, Travis CI)
- Also generally involves a web dashboard.
- Package Management / automated build:
 - Homebrew, MacPorts, RPM, apt-get, yum, BSDPorts, Emerge/Gentoo
 - For HPC: Spack, Smithy, Easybuild

For many open source projects, this infrastructure is freely available.

Not widely available inside HPC centers.





This talk gives an overview of two tools currently in use at Livermore Computing

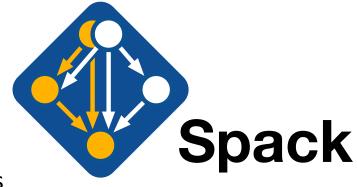
1. Atlassian Bamboo Continuous Integration

- Security challenges for CI
- How Bamboo was deployed securely at LLNL



2. The Spack Package Manager

- Developed at LLNL
- Handles combinatorial build explosion
- Now in use to build/test production codes



Web-based tools are often difficult to deploy in HPC environments

 Two-factor authentication often hard to integrate with many web applications.



- Security policies require more strict permissions than most open source tools offer.
 - Tools often assume trust among users.
 - Many tools don't have fine-grained access controls.
- Maintenance costs are higher with security
 - With no permissions, need an instance per team
 - Centers can't maintain all the instances.
 - Small teams have no resources to deploy tools.
 - HPC developers (for the most part) lack web skills.
 - Most centers prohibit running arbitrary web services.



LLNL Networks are a challenge for deployment

Organization	Network/ URL	Identity management		Accessible from						SFNs can use				
		Username	Authentication	Groups	Internet (no VPN)	VPN VPN-C	VPN-B	Blue	Yellow	cz	RZ	iSRD/ SCF	On-site	From home
Institutional	Yellow / Blue atlassian.llnl.gov	OUN	AD	Custom, Managed by admins	×	•	•	•	0	1	A	×	•	×
Livermore Computing (LC)	Collaboration Zone (CZ)	LC Username	RSA SecurID	LC Unix Groups	0	0	0	•	0	•	•	×	0	0
	Restricted Zone (RZ) rzlc.llnl.gov		CryptoCard		×	0	0	•	0	0	•	×	×	×
	Classified (SCF)		RSA SecurID		×	×	×	×	×	×	×	•	×	×

- Maximum consolidation is one tool per network
- Can't merge across identity systems or security levels.
 - Exception: LANL & Sandia users have federated login with LC, can use own credentials.

Livermore Computing (LC) has deployed Atlassian Tools for all users

X Confluence

- Wiki software for collaborative projects
- Collaborative meeting notes, design documents, documentation, other projects



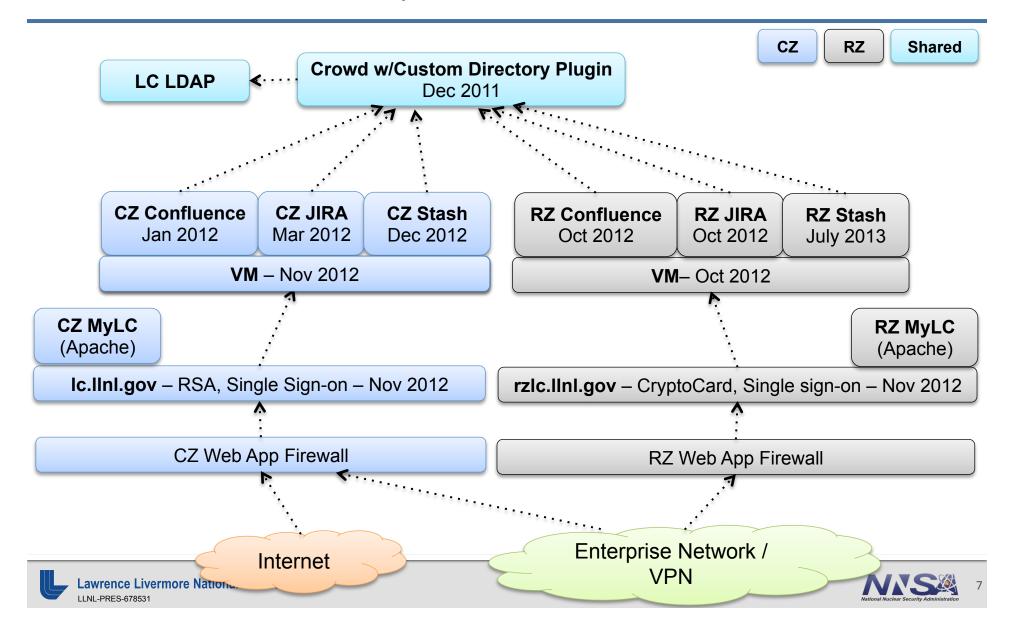
- Issue tracking for software and other projects
- Agile project management tools



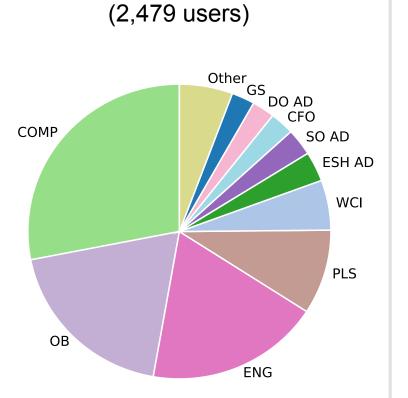
- Git repository hosting;
- Like github or sourceforge
- Cheaper and inside the firewall

Atlassian deployment has been ongoing since 2011

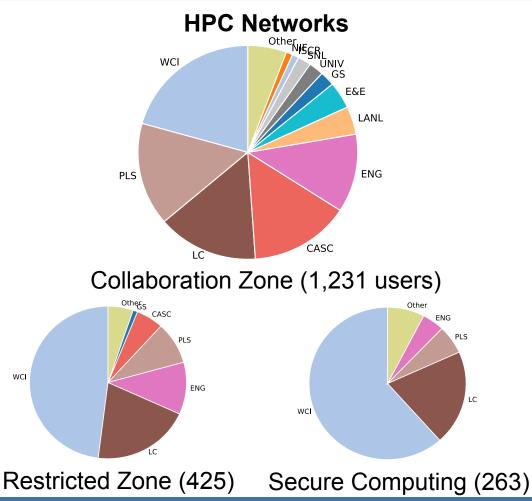
This shows how our ecosystem evolved.



Atlassian tools have become extremely popular at LLNL



Enterprise Network



These 4 instances consolidated hundreds of disparate web tools across the lab.





Why Atlassian Tools?

Excellent support for fine-grained permissions across tools

- Easily conforms to LLNL security plans.
- Projects can be private or share via unix groups.

Scalable to many teams with low maintenance

- Users can create their own projects on demand; no admin involved.
- Nice UI and online documentation makes them easy to adopt

Single integration point (Crowd), single sign-on.

- Crowd is our interface to LC's (rather esoteric) LDAP directory
- One custom directory developed for all tools.
- Offers single sign-on user types two-factor auth once per day.

Consolidation, collaboration, support for small teams.

NOT FREE or OSS, but customers do get access to the source.

Tools have broken down organizational silos and lowered maintenance burden. Some free tools are starting to catch up (GitLab).



HPC developers need better Build and Test tools.

Bleeding-edge machines need the most testing

- Newest hardware
- Least stable OS
- Newly ported software
- Constantly changing environment

Hard to run build/test suites on these machines

- Some centers don't even allow cron jobs.
- Job submission systems are different across HPC centers
 - Extra porting work
- Raises barrier to entry for software

Many code teams need to run in multiple environments

Manual testing for so many configurations is intractable

HPC Centers must lower barriers to entry for end users!





Continuous Integration (CI) Tools can help

- CI systems monitor repositories for changes, then:
 - Build latest version(s)
 - Run tests
 - Generate reports



Travis CI

- Automate common development workflows
 - Provide nice GUIs for constructing test workflows
 - Integrate with bug trackers, repository systems
- Examples:
 - Jenkins: Java server with remote "agents"
 - Bamboo: Java server with remote "agents"
 - Travis CI: Hosts CI builds in the cloud (mostly Ubuntu)



Continuous Integration tools pose a number of security challenges for centers.

- They launch real jobs on machines.
- 2. May launch jobs on remote machines.
- Job launch is automated, without a user present.
- 4. Typically need to check out code from a repository.
 - May store credentials for that repository.
- Need access to resource manager to submit parallel jobs.
- 6. Build agents may share data between builds.
 - Can't allow users' jobs to share data.

LLNL code teams currently run their own CI systems

- Resource-intensive maintenance
 - Each team has many single-node Jenkins instances
 - Each instance has its own web dashboard with a strange URL
 - https://clusternode2134:7777/jenkins/
- URLs are only accessible on the local network
 - Most users launch a browser over X11 to administer (extremely slow)
 - More sophisticated users can access via SSH tunnel
- Teams only use local, single-node agents
 - HPC code teams not have the knowhow to secure SSL remote agents
 - Insecure agents would result in spurious builds.
- Teams are responsible for security of their Jenkins instances

We started by listing our requirements for CI systems.

- 1. LC users are able to log into the system with a web browser using their LC username and two-factor authentication.
- 2. LC users can set up suites of build and test jobs to run regularly using a simple UI.
- 3. LC Users can collaborate on test configurations using LC Unix groups and permissions.
- 4. LC Unix groups and permissions can be used to restrict access to viewing and editing test configurations.
- 5. Server can launch build/test jobs on cluster front-end nodes.
- 6. Build/test jobs must run only as a user authorized by the creator of a test configuration.
- Network traffic between the server and build agents must be encrypted.

Comparison of Jenkins, Bamboo, & Travis

Product	Hosting Options	User Interface	Plugins	Remote Build	Price	Atlassian integration	Users/ Groups	Permissions	Agent security	Node Isolation
Bamboo	Hosted or internal	Easy, clean	Some	Build agents	\$\$	JIRA, Stash	Crowd	Per project	SSL	Can dedicate agents to a project.
Jenkins	Internal server	Complex, cluttered. ROSE team wants something simpler (currently use Jenkins).	Lots (1k+)	Build agents	Free	Partial	Crowd	Matrix- based, or Role strategies. Configuring per project seems complex.	SSL/ SSH	Projects can restrict jobs to particular slaves and vice versa.
Travis CI	Hosted only	Simple, but based on yaml + git		Hosted only	Free	N/A	Github	N/A	N/A	N/A

The Bamboo web application can be configured to satisfy LC's security requirements.

1. Authentication

Use Atlassian Crowd for two-factor (already deployed)

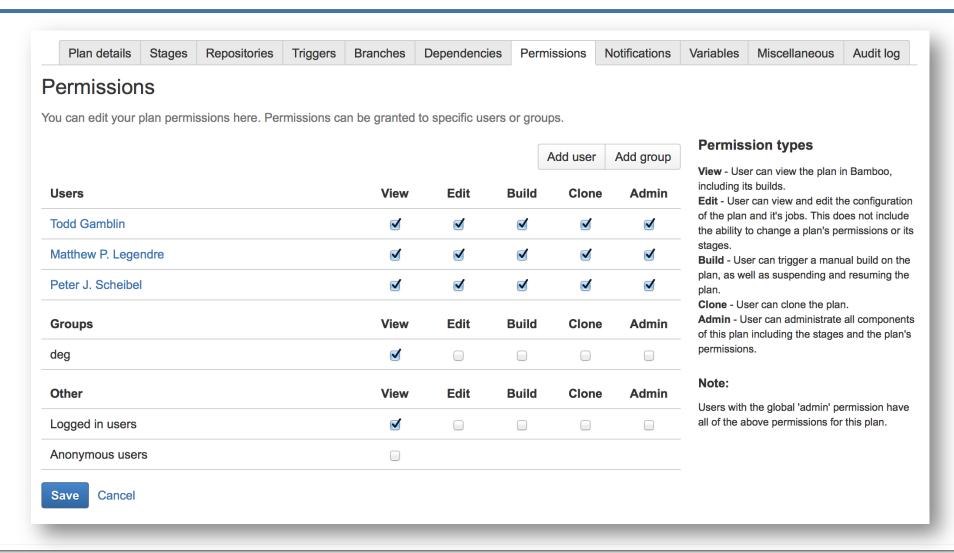
2. Per-project configuration

- Bamboo allows users to set up Projects and Plans
- Users only see projects and plans they're added to

3. Permissions

- Bamboo essentially has 3 levels of in-application permissions:
 - a. System administrator (manages Bamboo)
 - b. Plan creator/administrator (team lead, manages members)
 - c. Plan user/developer (team member)
- Many users can share the same web server.
- Users can mostly self-manage on this system, using Unix groups.
- No sys-admin support needed for setting permissions.

Bamboo permissions are configurable per build plan.



Job launch starts to get more complicated.

Bamboo can launch jobs locally on the server

- Local jobs would run as the web application user, but server is shared.
- We disable local agents and do not run local jobs.

Bamboo can also run jobs in Amazon EC2 cloud

- We've disabled this.
- Could be interesting for testing open software in the future

Bamboo can send jobs to remote agents.

- LC only uses remote agents on cluster login nodes.
- Jobs launched by agents run as same user as agent.
- How to secure remote agents?

Remote Agents: Plan A: Dedicated agents (currently deployed)

Launch:

- Agents are launched by LC users
- Agents run on login nodes as the user who started them

Use control:

1. Dedication

- Agents must be "dedicated" to specific build plans
- Dedicated agents will only run builds for specific plans.
- Agents are typically owned by the same user as the build plan.

2. Authorization

- Can require sysadmins to *authorize* agents before they can do any builds
- Sysadmin has to first approve each agent and ensure that it's dedicated to the right plan.

Transport:

- Agents use SSL with client authentication to connect to the server
- Only agents with LC-signed certificate can connect.

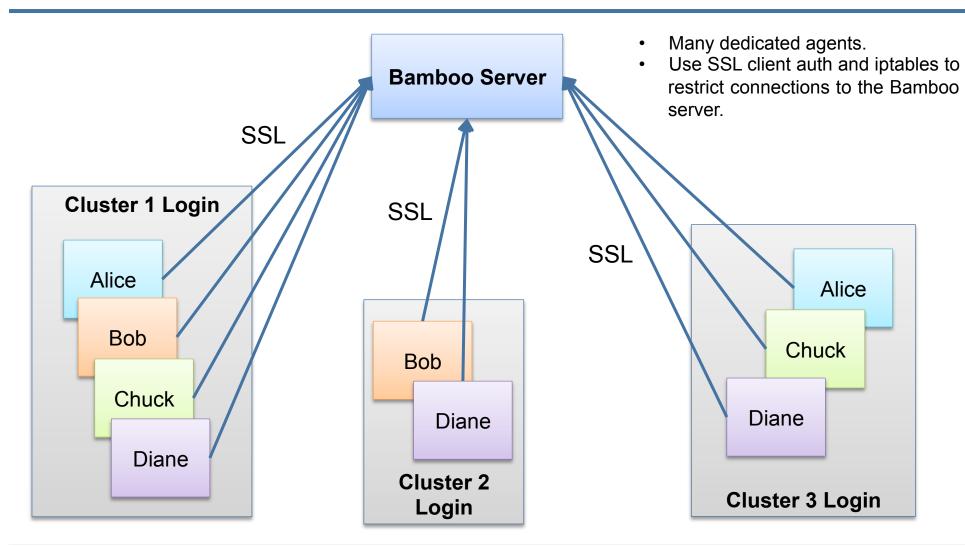
Pros: Requires no special customization of Bamboo.

Pitfalls: Requires one-time administrator effort for each agent.

Requires many per-user agents on the same node. Can get expensive.



Remote Agents: Plan A: Dedicated agents (currently deployed)



Remote Agents: Plan B: Setuid agents (needs plugin support)

Launch:

- Agents are launched as system services.
- Agents run on login nodes as root.

Use control:

- Agents run as root until they receive a job, then:
 - 1. Change permissions for working directory to the job's user
 - 2. setuid to appropriate user and run job
 - 3. Die and automatically restart
 - need to be able to force agent to die with requestShutdown().
 - Would rely on wrapper script to autmatically restart as root.
 - Need to investigate how unix permissions would be managed in the agent directory.
- No repeated authorization and dedication required
- User sees each LC cluster as an agent (or several)

Transport:

- Agents use SSL with client authentication to connect to the server
- Only agents with LC-signed certificate can connect.

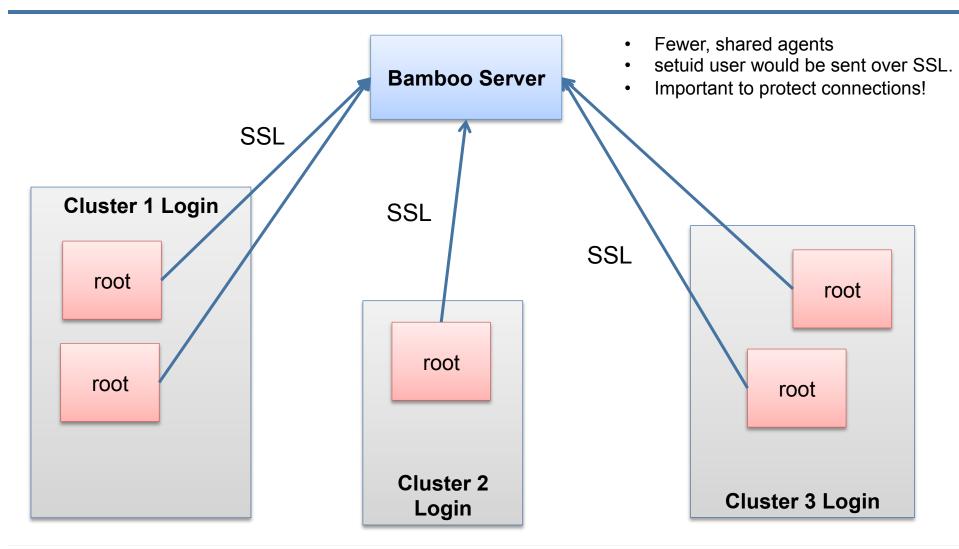
Pros: One-time agent setup, no user involvement.

Pitfalls: Requires developing plugins for the agents, may require building/maintaining a custom agent (could be brittle).





Remote Agents: Plan B: Setuid agents (in development)



Remote Agents: Plan C: Integration with Local Resource Manager

Launch:

- Bamboo could launch elastic agents through SLURM (http://slurm.schedmd.com)
 - Could support other resource managers as well (MOAB, LSF, LoadLeveler, etc.)
- User agent runs as is controlled by Bamboo server via some interface

Use control:

1. Dedication

No need for dedication – agents are elastic and SLURM (or other RM) handles secure agent launch.

2. Authorization

- No need for agent authorization.
- Project owner would need to select a user for agents to run as.
- User would need to approve it.
- User selection and approval could be implemented as a Bamboo UI plugin.

Transport:

- Bamboo could talk to SLURM through some generic elastic agent launch interface.
- SSL communication between agents and server as usual.

Pros: Integrates with SLURM, which can securely launch agents on hundreds

of thousands of cluster nodes at LLNL.

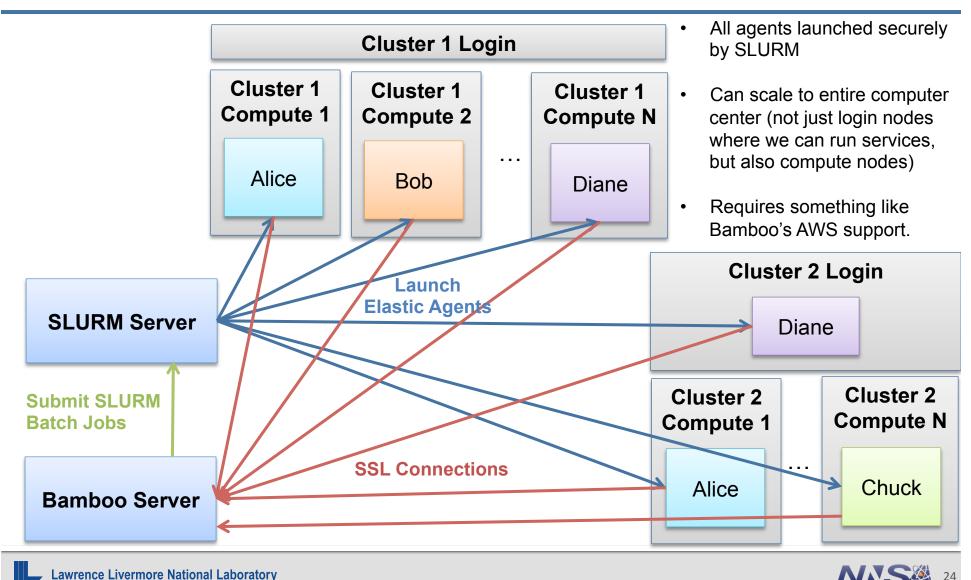
Pitfalls: Would require additional support from Bamboo.

Bamboo has an AWS interface; this would need to be a plugin point so

that we could plug in our own thing.



Remote Agents: Plan C: Integration with Local Resource Manager



Current Status of Bamboo deployment

Deployed for users in 2 zones: Collaboration Zone and Restricted Zone

- Easy web access is appealing: many have started switching from Jenkins.
- Users can now test on more LC front-end nodes with remote agents.

Issues

- 1. Bamboo only has security isolation at the **plan** (not **project**) level.
 - Agents must be dedicated to each plan individually under Plan A.
 - Requires administrative action every time user creates a new plan.
 - Project is essentially just an empty label in Bamboo... no project permissions.
- 2. Some issues with IBM JDK on Blue Gene/Q front-end
 - Had to switch to OpenJDK to support Blue Gene/Q Power Linux.
- 3. Many users have repos in shared FS that can't be polled by Bamboo server.
 - Had to mount the shared file system on the server to fix this.
 - Bamboo assumes that agents & server can access the same networks/mounts.

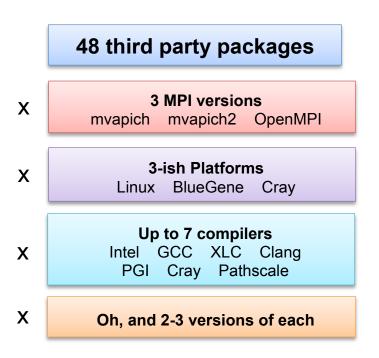
Future Directions

- 1. Agent setup needs more automation (signing certs, dedication, etc.)
- Users want to run LOTS of combinatorial tests.



Users want to experiment with many different configurations of their code.

- Every machine and app has a different software stack (or several)
- We want to experiment quickly with many architectures, compilers, MPI versions
- All of this is necessary to get the best performance



$= \sim 7,500$ combinations

- OK, so we don't build all of these
 - Many combinations don't make sense
- We want an easy way to quickly sample the space
 - Build a configuration on demand!



How do HPC sites deal with combinatorial builds?

- OS distribution does not deal with this
 - OS typically has one version of each package, installed in a common prefix: /usr
- HPC software typically installed manually in a directory hierarchy.
 - Hierarchy often doesn't give you all the information you need about a build.
 - Typically run out of unique names for directories quickly.
- Environment modules allow you to enable/disable packages.

Site	Naming Convention
LLNL	/ usr / global / tools / \$arch / \$package / \$version / usr / local / tools / \$package-\$compiler-\$build-\$version
Oak Ridge	/ \$arch / \$package / \$version / \$build
TACC	/ \$compiler-\$comp_version / \$mpi / \$mpi_version / \$package / \$version





Spack handles combinatorial version complexity.

```
spack/opt/
    linux-x86_64/
        gcc-4.7.2/
        mpileaks-1.1-0f54bf/
    bgq/
        gcc-4.5.1/
        libelf-0.8.13-251fqb/
    ...
```

- Each unique DAG is a unique configuration.
- Many configurations can coexist.
- Each package configuration is installed in a unique directory.
- Hash appended to each prefix allows versioning of full dependency DAG.
- Installed packages will automatically find their dependencies
 - Binaries are installed with proper RPATHs
 - No need to use modules or customize LD_LIBRARY_PATH
 - Things continue to work the way you built them
- Installation works just as well in \$HOME as in shared FS.





`spack list` shows what's available

	<pre>\$ spack list ==> 219 packages.</pre>							
1			1		•			
	adept-utils	dyninst	lcms	mesa	pixman	py-pypar	spindle	
	arpack	extrae	libarchive	metis	pmgr_collective	py-pyparsing	sqlite	
	asciidoc	exuberant-ctags	libcircle	Mitos	postgresql	py-pyqt	stat	
	atk	flex	libdrm	mpc	ppl	py-pyside	sundials	
	atlas	flux	libdwarf	mpe2	py-basemap	py-python-daemon	swig	
	autoconf	fontconfig	libelf	mpfr	py-biopython	py-pytz	task	
	automaded	freetype	libevent	mpibash	py-cffi	py-rpy2	taskd	
	automake	gasnet	libffi	mpich	py-cython	py-scientificpython	tau	
	bear	gcc	libgcrypt	mpileaks	py-dateutil	py-scikit-learn	tcl	
	bib2xhtml	gdk-pixbuf	libgpg-error	mrnet	py-epydoc	py-scipy	the_silver_searcher	
	binutils	geos	libjpeg-turbo	munge	py-genders	py-setuptools	thrift	
	bison	git	libjson-c	muster	py-gnuplot	py-shiboken	tk	
	boost	glib	libmng	mvapich2	py-h5py	py-sip	tmux	
	boxlib	global	libmonitor	nasm	py-ipython	py-six	tmuxinator	
	bzip2	gmp	libNBC	ncurses	py-libxml2	py-sympy	uncrustify	
	cairo	gnutls	libpciaccess	netcdf	py-lockfile	py-virtualenv	util-linux	
	callpath	gperf	libpng	netgauge	py-mako	py-yapf	vim	
	cblas	gperftools	libsodium	netlib-blas	py-matplotlib	python	vtk	
	cgm	graphlib	libtiff	nettle	py-mock	ghull	wget	
	clang	gtkplus	libtool	ompss	py-mpi4py	at	wx	
	cloog	harfbuzz	libunwind	opari2	py-mx	athreads	wxpropgrid	
	cmake	hdf5	libuuid	openmpi	py-nose	R	xcb-proto	
	coreutils	hwloc	libxcb	openssl	py-numpy	ravel	XZ	
	cppcheck	hypre	libxml2	otf	py-pandas	readline	yasm	
	cram	icu	libxshmfence	otf2	py-pexpect	rose	zeroma	
	cscope	icu4c	libxslt	pango	py-pil	ruby	zlib	
	cube	ImageMagick	llvm	papi	py-pmw	SAMRAI	zsh	
	czmą	isl	ll∨m-lld	paraver	py-pychecker	scalasca	23	
	dbus	jdk	lua	parmetis	py-pycparser	scorep		
	docbook-xml	jpeg	lwgrp	parpack	py-pyelftools	scotch		
	dri2proto	lapack	lwm2	pcre	py-pygments	scr		
	dtcmp	launchmon	memaxes	petsc	py-pylint	silo		
				F	F) F)			

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

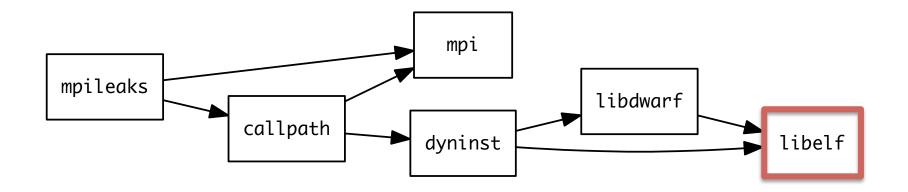
```
default: unconstrained
$ spack install tool
$ spack install tool@3.3
                                                @ custom version
$ spack install tool@3.3 %gcc@4.7.3
                                                % custom compiler
$ spack install tool@3.3 %gcc@4.7.3 +threads
                                               +/- build option
$ spack install tool@3.3 =bgqos_0
                                                = cross-compile
```

- 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!
- Package authors can use same syntax within package files
 - Makes it easy to parameterize build by version, compiler, arch, etc.





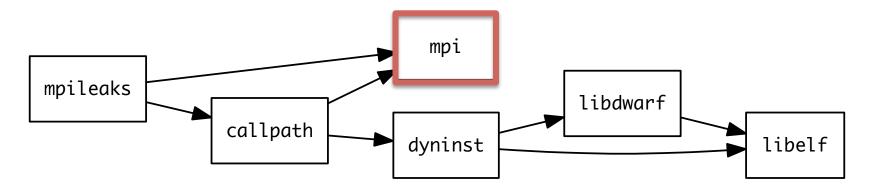
Specs can constrain dependency versions



- \$ spack install mpileaks %intel@12.1 ^libelf@0.8.12
- Spack ensures that all packages in the same install are built with the same version of libraries, like **libelf**.
- Spack can ensure that builds use the same compiler
 - Can also mix compilers but it's not default



Spack handles ABI-incompatible, versioned interfaces like MPI



Ask specifically for mvapich 1.9

\$ spack install mpileaks ^mvapich@1.9

Ask for openmpi 1.4 or higher

\$ spack install mpileaks ^openmpi@1.4:

These install separately, in unique directories

Ask for an MPI that supports MPI-2 interface

\$ spack install mpileaks ^mpi@2

Spack chooses an MPI version that satisfies constraint





Spack packages are simple Python

```
from spack import *
class Dyninst(Package):
                                                                                                                   Metadata
    """API for dynamic binary instrumentation. Modify programs while they
      are executing without recompiling, re-linking, or re-executing."""
   homepage = "https://paradyn.org"
                                                                                                                  Version/URLs
   version('8.2.1', 'abf60b7faabe7a2e', url="http://www.paradyn.org/release8.2/DyninstAPI-8.2.1.tgz")
version('8.1.2', 'bf03b33375afa66f', url="http://www.paradyn.org/release8.1.2/DyninstAPI-8.1.2.tgz")
   version('8.1.1', 'd1a04e995b7aa709', url="http://www.paradyn.org/release8.1/DyninstAPI-8.1.1.tqz")
   depends_on("libelf")
                                                                                                                   Dependencies
   depends_on("libdwarf")
    depends_on("boost@1.42:")
                                                                                                              Patches (not shown)
   # new version uses cmake
   def install(self, spec, prefix):
        libelf = spec['libelf'].prefix
        libdwarf = spec['libdwarf'].prefix
        with working_dir('spack-build', create=True):
           cmake('...',
                  '-DBoost_INCLUDE_DIR=%s' % spec['boost'].prefix.include,
                  '-DBoost_LIBRARY_DIR=%s' % spec['boost'].prefix.lib,
                  '-DBoost_NO_SYSTEM_PATHS=TRUE'
                  '-DLIBELF_INCLUDE_DIR=%s'
                                             % join_path(libelf.include, 'libelf'),
                  '-DLIBELF_LIBRARIES=%s'
                                             % join_path(libelf.lib, 'libelf.so'),
                                                                                                                    Commands for install
                  '-DLIBDWARF INCLUDE DIR=%s' % libdwarf.include.
                  '-DLIBDWARF_LIBRARIES=%s' % join_path(libdwarf.lib, 'libdwarf.so'),
                 *std_cmake_args)
           make()
           make("install")
                                                                                                                   Access build config
   # Old version uses configure
                                                                                                                   through spec.
   @when('@:8.1')
   def install(self, spec, prefix):
        configure("--prefix=" + prefix)
       make()
        make("install")
```

- Package files live in repositories.
- 'spack create' command generates boilerplate package given a URL.



Spack supports optional dependencies

Based on user-enabled variants:

```
variant("python", default=False, "Build with python support")
depends_on("python", when="+python")
```

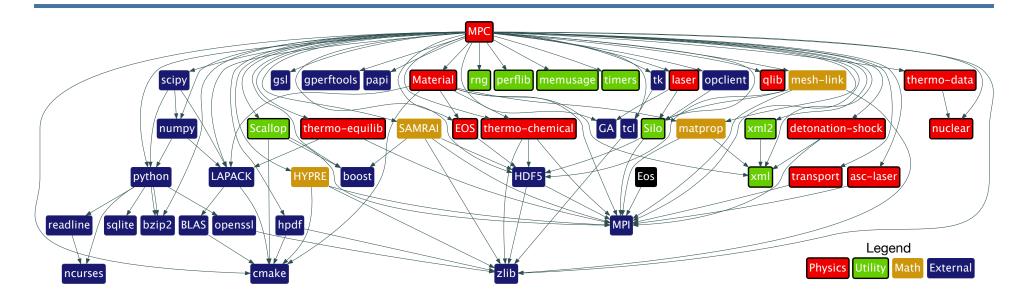
spack install vim +python

 And according to other spec conditions e.g., gcc dependency on mpc from 4.5 on:

```
depends_on("mpc", when="@4.5:")
```

DAG is not always complete before concretization!

Example: Spack has recently been adopted by an LLNL production code.



Dependencies shown above

- 47 component packages
- ~50% physics + math
- ~50% open source
- Build suite runs many parallel test jobs with up to 128 processes.
- Spack automates this build of code and its dependencies
 - Also being used to automate post-build testing.

Our production code team uses Spack to test 36 different configurations

		Linux	BG/Q	Cray XE6	
	MVAPICH	MVAPICH2	<i>OpenMPI</i>	BG/Q MPI	Cray MPI
GCC	CPLD			CPLD	
Intel 14	CPLD				
Intel 15	CPLD	D			
PGI		D	CPLD		CLD
Clang	CPLD			CLD	
XL				CPLD	

- Above are nightly builds on machines at LLNL and LANL
 - · Zin (Linux), Sequioa (BG/Q), Cielo (Cray)
- 4 code versions:

• (C)urrent Production (L)ite

• (P)revious Production (D)evelopment

Team is currently porting to the new Trinity machine at LANL

Spack has a growing community.

- Spack is starting to be used in production at LLNL
 - Used for tool installation at Livermore Computing (LC)
 - Used by code teams at LLNL, starting to be adopted by more.
 - Will enable a common deployment environment for LC and codes.
- Spack has a growing external community
 - NERSC working with us to use Spack on Cori XC40
 - Kitware is working with us to package ParaView and develop core features.
 - NNSA: Participation in Spack calls by Sandia, LANL
 - Argonne, IIT, INRIA, Krell Institute, Stowers Medical Research Center
- Sites can easily leverage efforts by sharing builds.
- Get Spack!

Github: http://bit.ly/spack-git

Mailing List: http://groups.google.com/d/spack



Future directions for Spack

Dependencies on Compiler features

- Profusion of new compiler features frequently causes build confusion:
 - C++11 feature support
 - OpenMP language levels
 - CUDA compute capabilities

```
require('cxx11-lambda')
require('openmp@4:')
```

Automatic ABI Checking

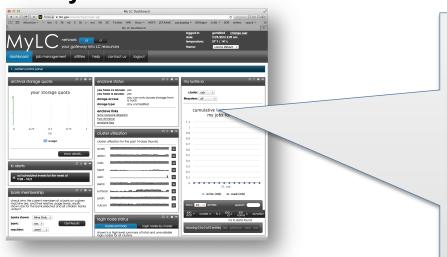
- Ensure that Spack-built packages are ABI-compatible with system versions.
- Working with RedHat to use libabigail for this
- Have used Spack + libabigail to find ABI bugs in clang

Compiler wrappers for tools

- Spack will allow our largest codes to be used with source instrumentation
- LLVM tools like thread sanitizers can be applied to more than toy problems.

We are looking at providing secure web interfaces for other user services.

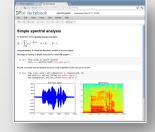
MyLC Web Portal



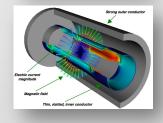


- Services run securely as the owning user
- User discovers services through Lorenz.
- No need to set up servers/ connect to obscure ports

My Running Services



IPython Notebook



In-situ Physics Visualization



Performance/ debug data

We are prototyping a system to securely connect users with running services on clusters

