Spack
Supercomputer PACKage Manager

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CCS-2: Computational Physics and Methods

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2018-01-17

Overview

1. What is Spack?
2. What does Spack do?
3. How does Spack work?
4. Why Use Spack?

Challenge: Install Spack, GSL

1. Clone Spack
2. Install GNU Scientific Library (GSL)

Challenge: Install Spack, GSL

1. Clone Spack
2. `cd` to new directory
3. Set environment variables
4. Install GNU Scientific Library (GSL)

Challenge: Install Spack, GSL

1. `$ git clone https://github.com/spack/spack mySpack`
2. `$ cd mySpack`
3. `$ . share/spack/setup-env.sh`
4. `$ Spack install gsl`

Results: Clone Spack

```
$ git clone https://github.com/spack/spack mySpack
Cloning into 'mySpack'...
remote:  Counting objects:  98699, done.)
remote:  Compressing objects:  100% (14/14), done.
remote:  Total 98699 (delta 9), reused 1 (delta 1), pack-reused
98684
Receiving objects:  100% (98699/98699), 34.05 MiB | 15.80 MiB/s,
done.
```

Results: Install GSL - Summary

```
$ spack install gsl
==> Installing gsl
==> .   .   .
==> Successfully installed gsl
  Fetch:  3.59s.  Build:  2m 29.58s.  Total:  2m 33.17s.
[+] /Users/l127914/mySpack/opt/spack/darwin-sierra-x86_64/
clang-9.0.0-apple/ gsl-2.4-2sems7ybkixmyqmxu6hp4z4nlhpgqkrl
```

Results: Install GSL

```
$ spack install gsl
==> Installing gsl
==> Fetching http://mirror.switch.ch/ftp/mirror/gnu/gsl/...
######################################################################## 100.0%
==> Staging archive:  /Users/l127914/mySpack/var/spack/stage/...
==> Created stage in /Users/l127914/mySpack/var/spack/stage/...
==> No patches needed for gsl
==> Building gsl [AutotoolsPackage]
==> Executing phase:  'autoreconf'
==> Executing phase:  'configure'
==> Executing phase:  'build'
==> Executing phase:  'install'
==> Successfully installed gsl
  Fetch:  3.59s.  Build:  2m 29.58s.  Total:  2m 33.17s.
[+] /Users/l127914/mySpack/opt/spack/darwin-sierra-x86_64/
clang-9.0.0-apple/ gsl-2.4-2sems7ybkixmyqmxu6hp4z4nlhpgqkrl
```

Results: Install GSL- Verify

```
$ spack find
==> 1 installed package
-- darwin-sierra-x86_64 / clang@9.0.0-apple ------
gsl@2.4
```

Hash Encodes Version, Compiler, Architecture

Package Version

Package Variants

Hardware Architecture

Compiler Version

Package Dependencies

Package Build Type

Compiler Flags

Operating System

Package Patches

CCS Net: spack find -ldf hypre

```
-- linux-rhel7-x86_64 / gcc@6.4.0 ----------------

ppqpzkf    hypre@2.13.0%gcc                    3ff6771    hypre@2.13.0%gcc
qmqnjy6        ^openblas@0.2.20%gcc            qmqnjy6        ^openblas@0.2.20%gcc
nw4jyek        ^openmpi@1.10.5%gcc             lwe5lft        ^openmpi@2.1.2%gcc
nul7v5e            ^hwloc@1.11.8%gcc           nul7v5e            ^hwloc@1.11.8%gcc
o53uqv7                ^libpciaccess@0.13.5%gcc o53uqv7               ^libpciaccess@0.13.5%gcc
pnpcuxa                ^libxml2@2.9.4%gcc      pnpcuxa                ^libxml2@2.9.4%gcc
pfw5gjb                    ^xz@5.2.3%gcc       pfw5gjb                    ^xz@5.2.3%gcc
w43e56t                    ^zlib@1.2.11%gcc    w43e56t                    ^zlib@1.2.11%gcc
```

Hash Encodes Full Provenance

Package Version

Package Variants

Hardware Architecture

Compiler Version

Package Dependencies

Package Build Type

Compiler Flags

Operating System

Package Patches

About Spack

- Supercomputer PACKage Manager
- Open source
- Started by Todd Gamblin (LLNL)
- Best hope for HPC software control
- Version 0.11

Spack Introduction - SC15

The Spack Package Manager: Bringing Order to HPC Software Chaos

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ABSTRACT

Large HPC centers spend considerable time supporting software for thousands of users, but the complexity of HPC software is quickly outpacing the capabilities of existing software management tools. Scientific applications require specific versions of compilers, MPI, and other dependency libraries, so using a single, standard software stack is infeasible. However, managing many configurations is difficult because the configuration space is combinatorial in size.

We introduce Spack, a tool used at Lawrence Livermore National Laboratory to manage this complexity. Spack provides a novel, recursive specification syntax to invoke parametric builds of packages and dependencies. It allows any number of builds to coexist on the same system, and it ensures that installed packages can find their dependencies, *regardless of the environment*. We show through real-world use cases that Spack supports diverse and demanding applications, bringing order to HPC software chaos.

Worse, the space of required builds grows combinatorially with each new configuration parameter. As a result, LLNL staff spend countless hours dealing with build and deployment issues.

Existing package management tools automate parts of the build process [2, 10, 11, 12, 23, 24, 38, 39, 41]. For the most part, they focus on keeping a single, stable set of packages up to date, and they do not handle installation of multiple versions or configurations. Those that *do* handle multiple configurations typically require that package files be created for each combination of options [10, 11, 12, 23], leading to a profusion of files and maintenance issues. Some allow limited forms of composition [11, 12, 23], but their dependency management is overly rigid, and they burden users with combinatorial naming and versioning problems.

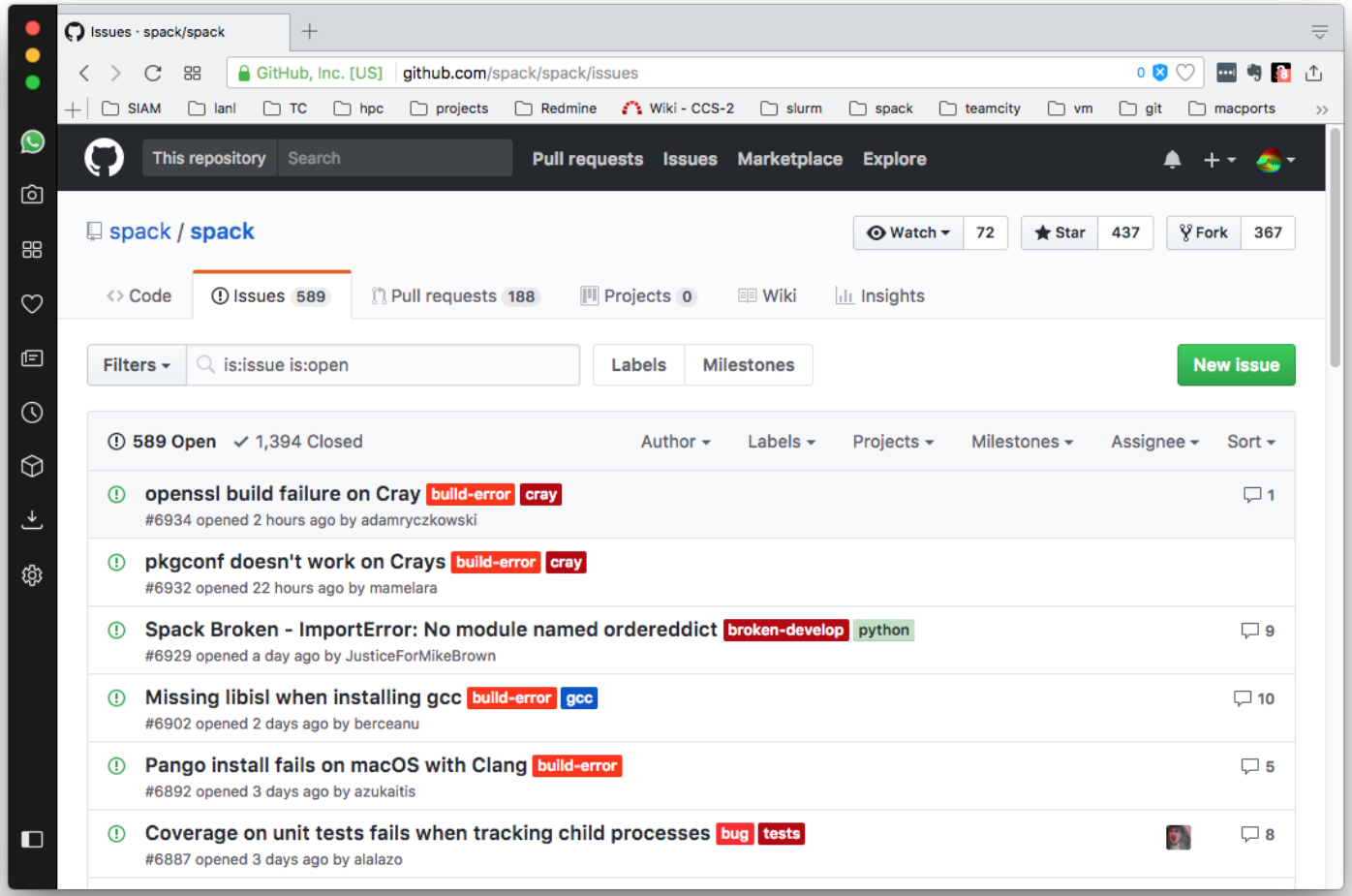
This paper describes our experiences with the *Spack* package manager, which we have developed at LLNL to manage increasing software complexity. It makes the following contributions:

Spack: A Path to Exascale

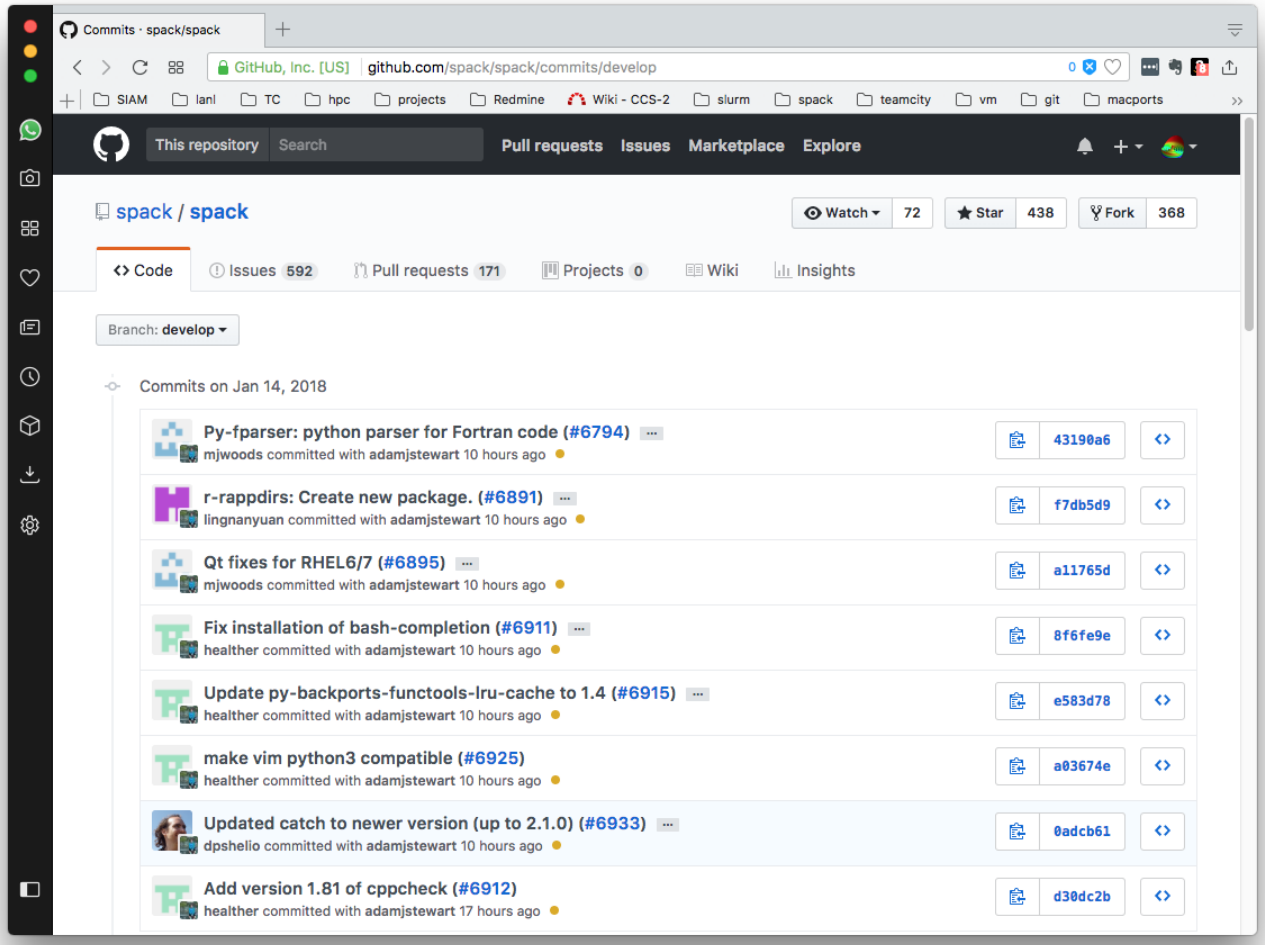
Vibrant Development Community

- GitHub Issue Tracking
- Google Discussion Group
- Weekly Teleconference
- New User Guide
- Tutorials
- LANL: user_contrib

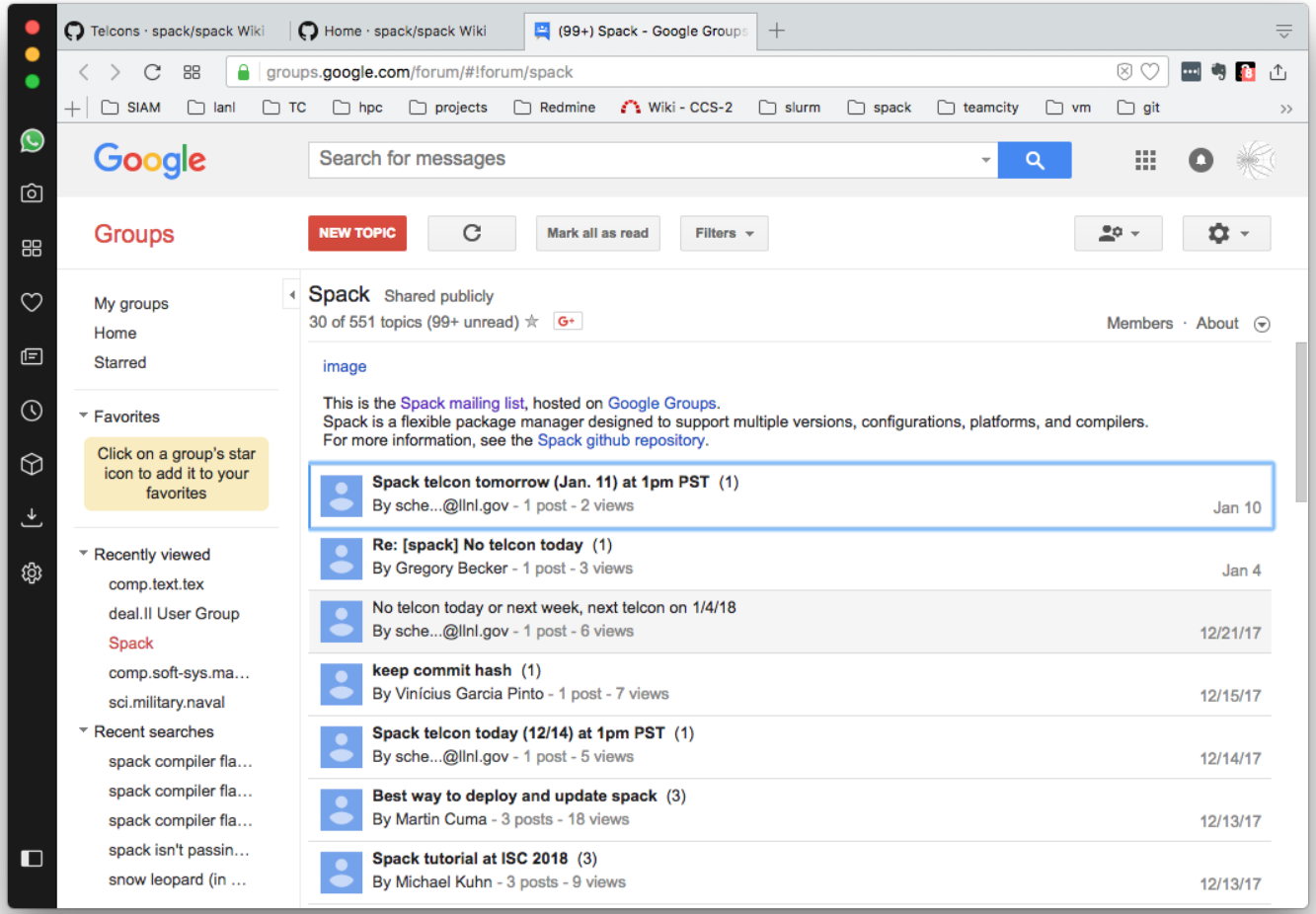
Github Issue Tracking



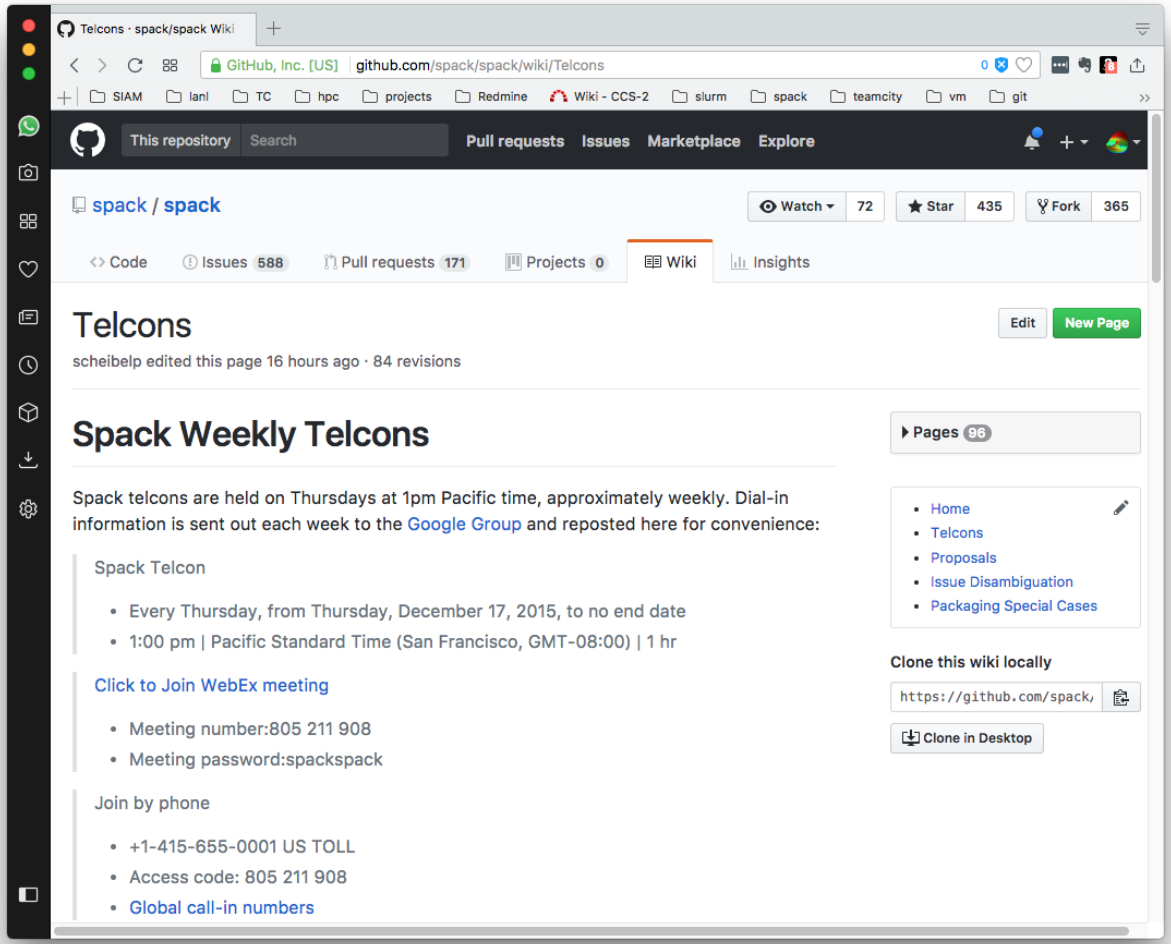
Dynamic Development Team



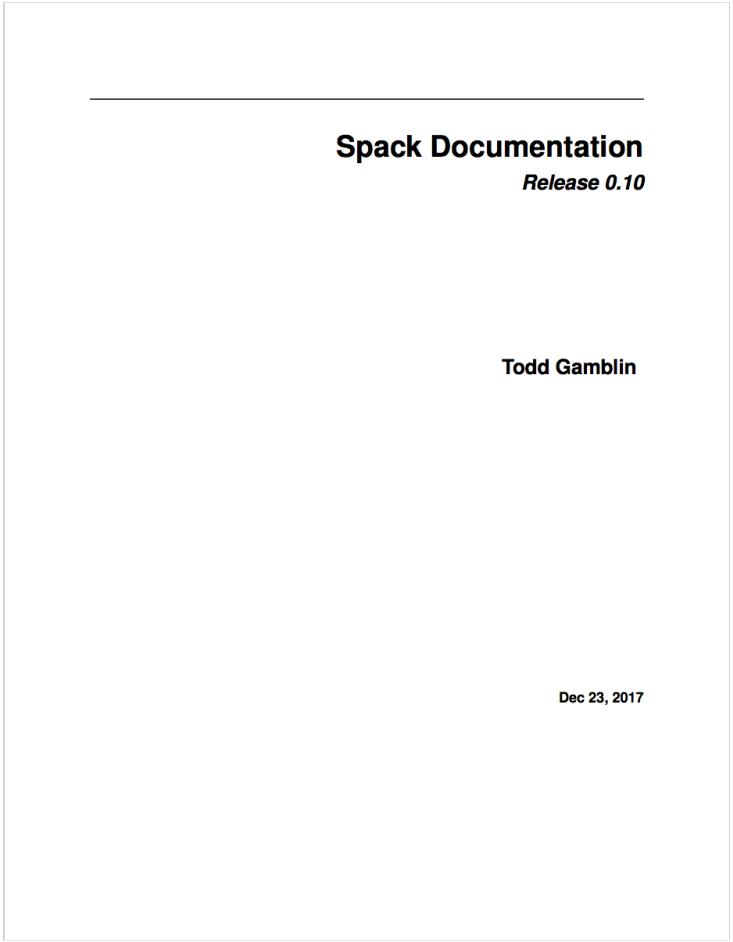
Spack Google Group



Weekly Teleconference



Spack User Guide: 600+ pp



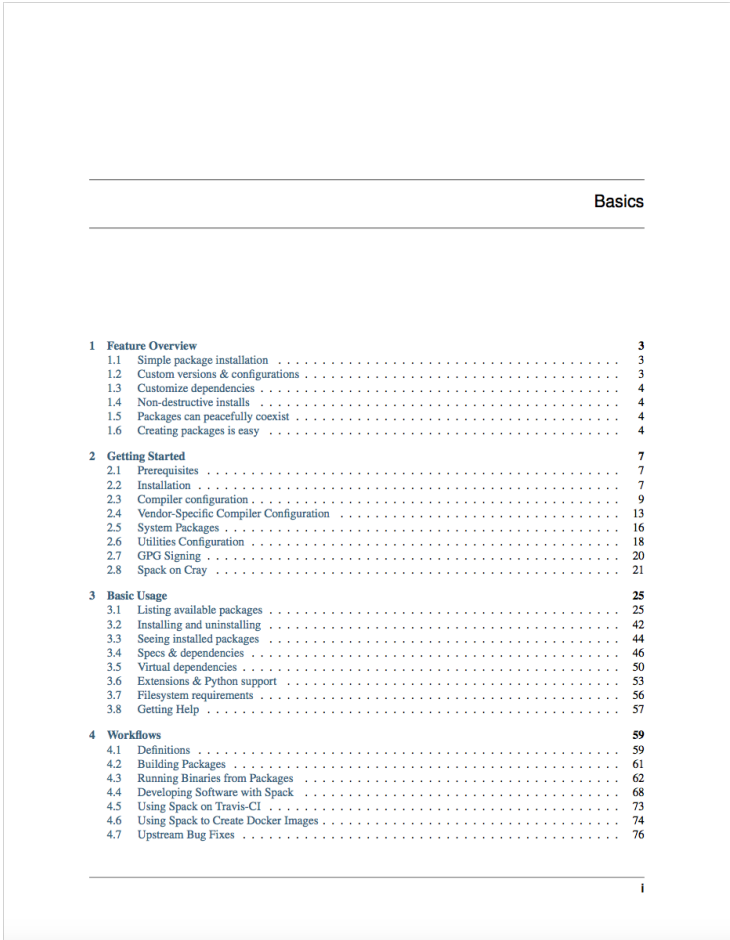
Spack Documentation

Release 0.10

Todd Gamblin

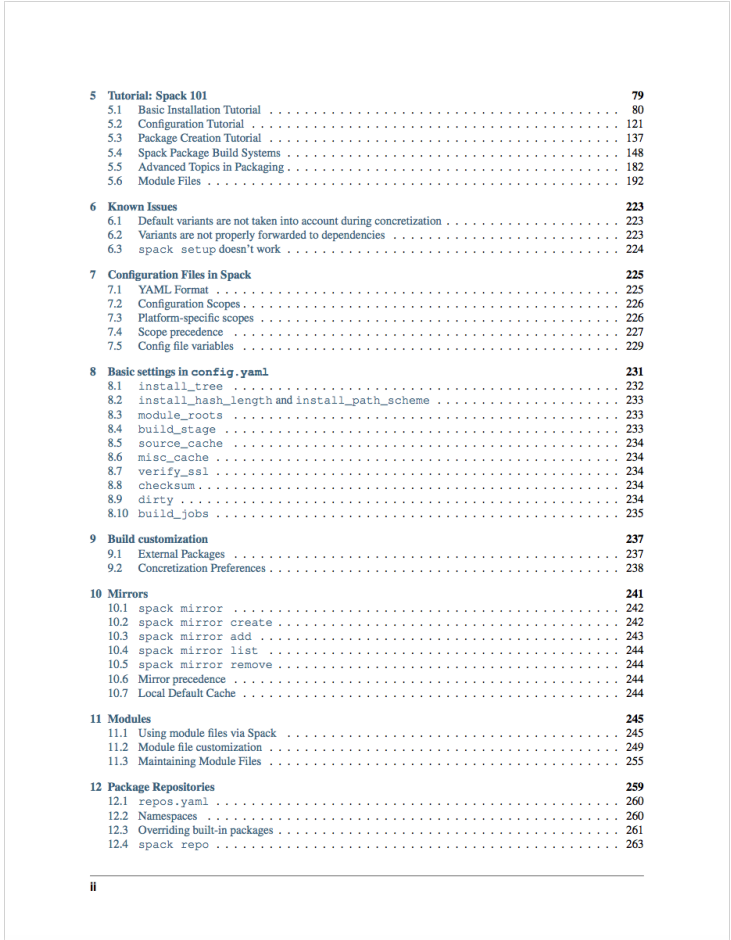
Dec 23, 2017

Spack User Guide: Part I - Users



Basics

i



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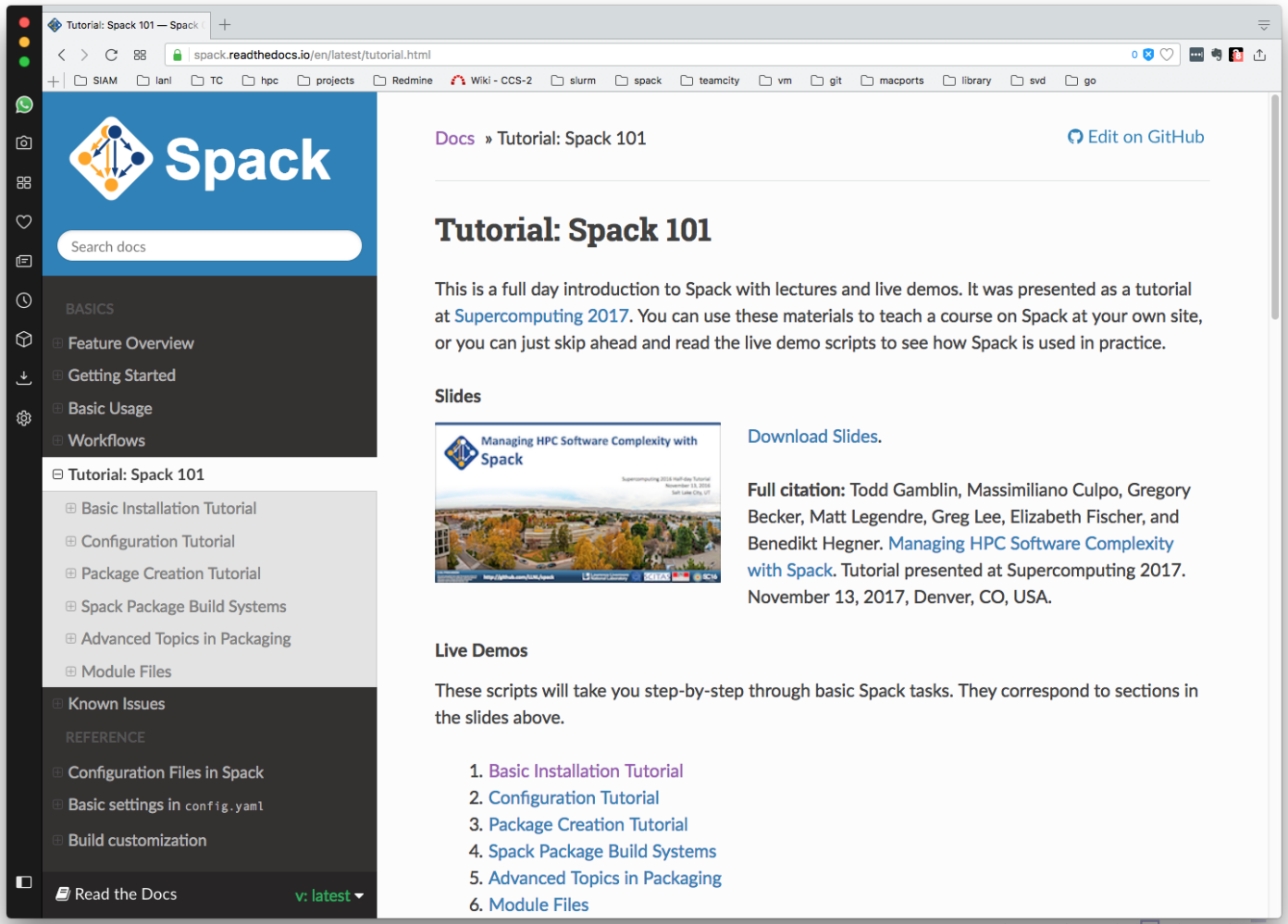
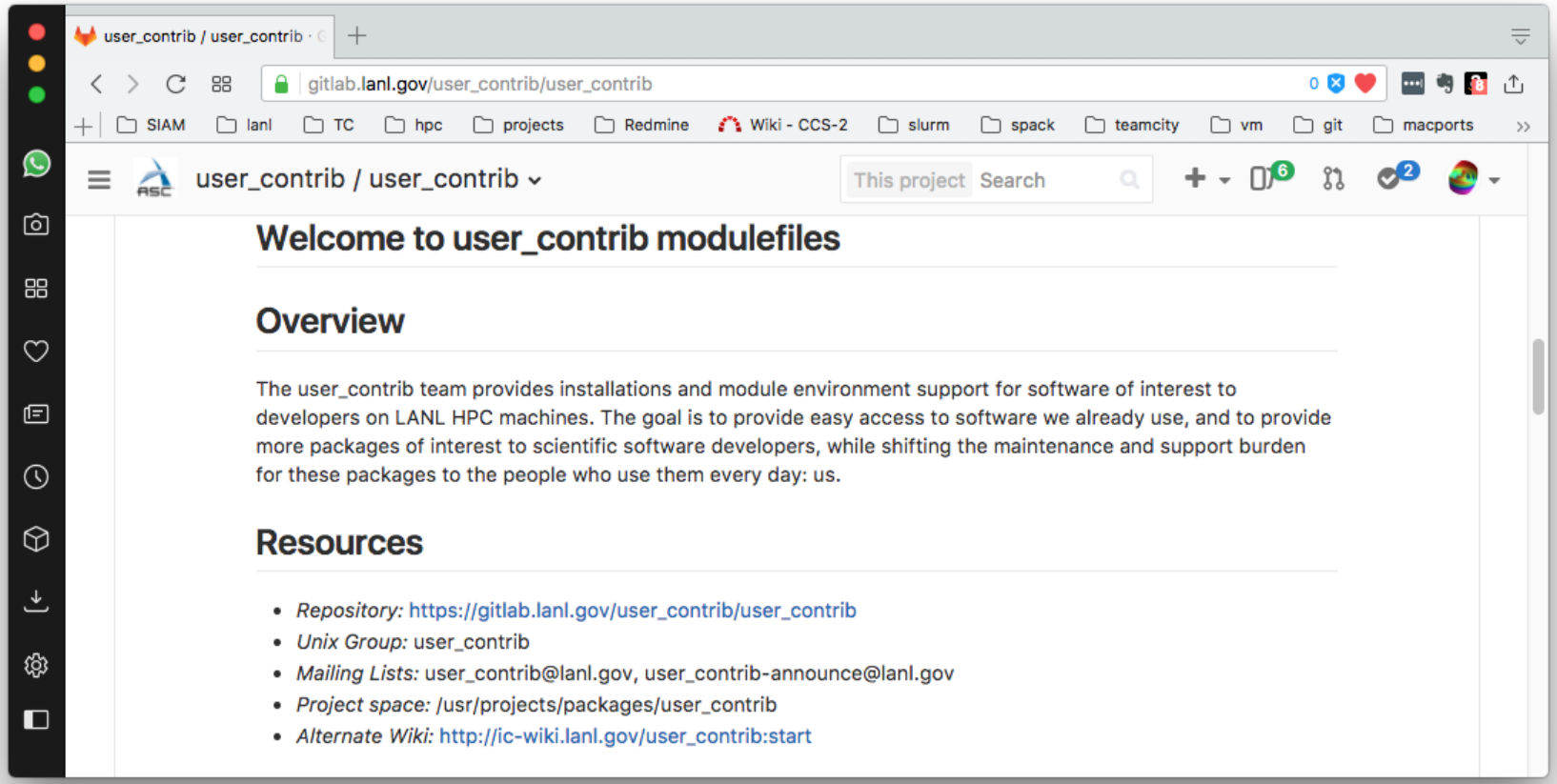
Spack User Guide: Part II - Developers

Spack Tutorial



Spack Tutorial SC17

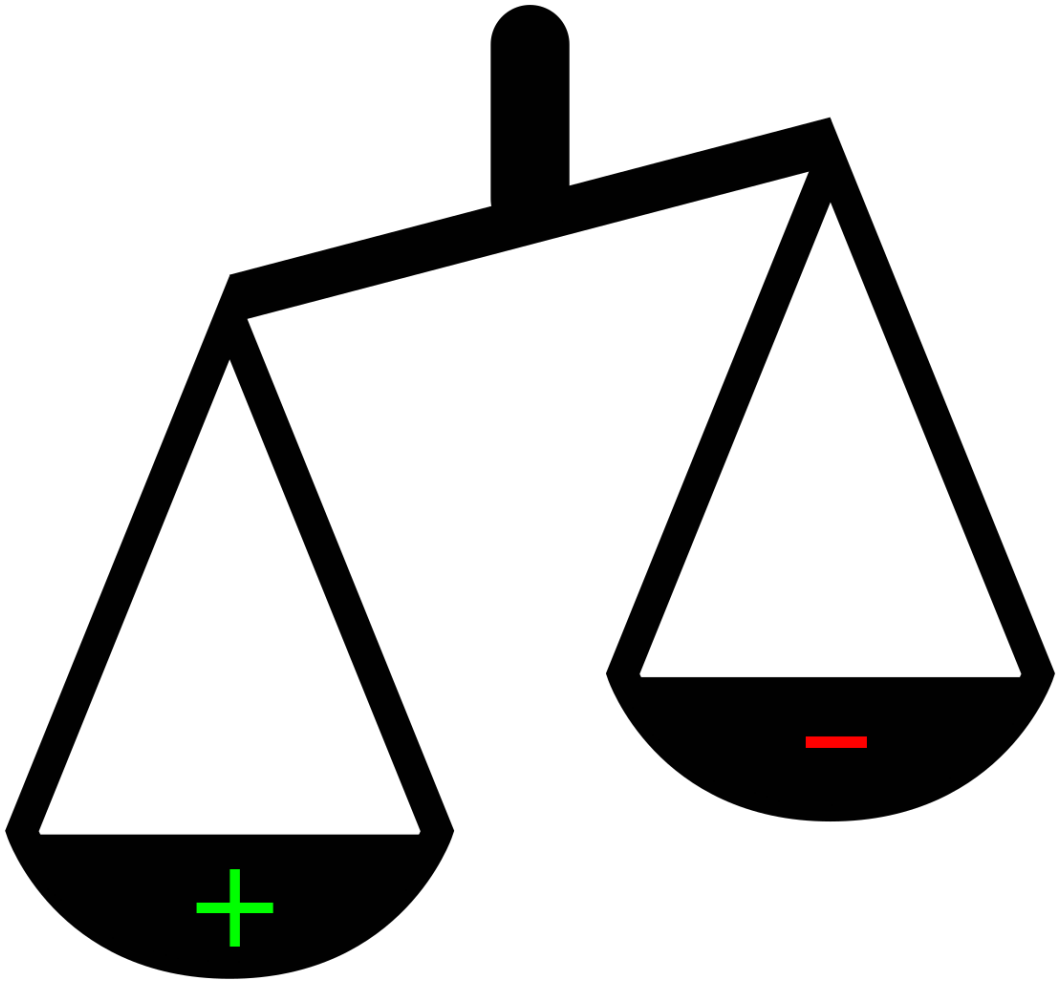
LANL: user_contrib



Caveat Emptor

- Pre-beta
- # issues > # developers
- Punished for our sins
- Success demands discipline

Benefits >> Inconveniences



A Simple Script to Build a Software Stack

1. Select 4 Compilers
2. Build 2 Versions of Python
3. Install, Activate Several Python Packages
4. Build Trilinos against 3 Versions of OpenMPI

Simplicity: Script I

```
#!/bin/bash

ver_mpi="1.10.5 2.1.2 3.0.0"; ver_gcc="5.3.0 6.4.0 7.2.0"

for v in ${ver_gcc}; do
  spack install gcc @ ${v}
done
```

Simplicity: Script II

```
#!/bin/bash

ver_mpi="1.10.5 2.1.2 3.0.0"; ver_gcc="5.3.0 6.4.0 7.2.0"

for v in ${ver_gcc}; do
  spack install gcc @ ${v}
done

for v in ${ver_gcc}; do
  spack install python @ 2.7.14 % gcc @ ${v}
  spack install python          % gcc @ ${v}
  for m in ${ver_mpi}; do
    spack install trilinos % gcc @ ${v} ^openmpi @ ${m}
  done
done
```

Trilinos: 4 Compilers, 3 OpenMPIs, 2 Pythons

```
-- linux-rhel7-x86_64 / gcc@4.8.5 ----------------
  autoconf@2.69       libbsd@0.8.6            netlib-scalapack@2.0.2   py-pyparsing@2.2.0
  automake@1.15.1     libedit@3.1-20170329    openblas@0.2.20          py-pytz@2017.2
  binutils@2.29.1     ibiconv@1.15            openmpi@1.10.5           py-requests@2.14.2
  bison@3.0.4         libjpeg-turbo@1.5.0     openmpi@2.1.2            py-setuptools@35.0.2
  boost@1.65.1        libpciaccess@0.13.5     openmpi@3.0.0            py-setuptools@35.0.2
  bzip2@1.0.6         libpng@1.6.29           openssl@1.0.2n           py-six@1.10.0
  cmake@3.10.1        libpthread-stubs@0.4    parmetis@4.0.3           py-six@1.10.0
  curl@7.56.0         libsigsegv@2.11         parmetis@4.0.3           py-sympy@1.0
  expat@2.2.2         libtool@2.4.6           parmetis@4.0.3           py-sympy@1.0
  flex@2.6.4          libx11@1.6.5            pcre@8.41                python@2.7.14
  freetype@2.7.1      libxau@1.0.8            pcre@8.41                python@3.6.2
  gcc@5.3.0           libxcb@1.12             perl@5.24.1              qhull@2015.2
  gcc@6.4.0           libxdmcp@1.1.2          pkgconf@1.4.0            readline@7.0
  gcc@7.2.0           libxml2@2.9.4           py-appdirs@1.4.3         sqlite@3.21.0
  gdbm@1.14.1         llvm@5.0.0              py-appdirs@1.4.3         suite-sparse@5.1.0
  gettext@0.19.8.1    m4@1.4.18               py-configparser@3.5.0    superlu-dist@5.2.2
  git@2.15.1          matio@1.5.9             py-cycler@0.10.0         superlu-dist@5.2.2
  glm@0.9.7.1         matio@1.5.9             py-cycler@0.10.0         superlu-dist@5.2.2
  gmp@6.1.2           matio@1.5.9             py-dateutil@2.5.2        swig@3.0.12
  gsl@2.4             metis@5.1.0             py-enum34@1.1.6          tar@1.29
  hdf5@1.10.1         mpc@1.0.3               py-gnuplot@1.8           tcl@8.6.6
  hdf5@1.10.1         mpfr@3.1.5              py-lit@0.5.0             tk@8.6.6
  hdf5@1.10.1         mumps@5.1.1             py-lit@0.5.0             trilinos@12.12.1
  help2man@1.47.4     mumps@5.1.1             py-mpmath@0.19           trilinos@12.12.1
  hwloc@1.11.8        mumps@5.1.1             py-mpmath@0.19           trilinos@12.12.1
```

Trilinos: 4 Compilers, 3 OpenMPI, 2 Python

```
  hypre@2.13.0          nasm@2.11.06              py-numpy@1.13.3       util-macros@1.19.1
  hypre@2.13.0          ncurses@6.0               py-numpy@1.13.3       xcb-proto@1.12
  hypre@2.13.0          netcdf@4.4.1.1            py-packaging@16.8     xextproto@7.3.0
  inputproto@2.3.2      netcdf@4.4.1.1            py-packaging@16.8     xproto@7.0.31
  isl@0.14              netcdf@4.4.1.1            py-pbr@1.10.0         xtrans@1.3.5
  isl@0.18              netlib-scalapack@2.0.2    py-pillow@3.2.0       xz@5.2.3
  kbproto@1.0.7         netlib-scalapack@2.0.2    py-pyparsing@2.2.0    zlib@1.2.11

- linux-rhel7-x86_64 / gcc@5.3.0 ----------------

  autoconf@2.69         libpciaccess@0.13.5       openmpi@3.0.0         py-setuptools@35.0.2
  automake@1.15.1       libpng@1.6.29             openssl@1.0.2n        py-setuptools@35.0.2
  binutils@2.29.1       libpthread-stubs@0.4      parmetis@4.0.3        py-six@1.10.0
  bison@3.0.4           libsigsegv@2.11           parmetis@4.0.3        py-six@1.10.0
  boost@1.65.1          libtool@2.4.6             parmetis@4.0.3        py-sympy@1.0
  bzip2@1.0.6           libx11@1.6.5              pcre@8.41             py-sympy@1.0
  cmake@3.10.1          libxau@1.0.8              perl@5.24.1           python@2.7.14
  curl@7.56.0           libxcb@1.12               pkgconf@1.4.0         python@3.6.2
  expat@2.2.2           libxdmcp@1.1.2            py-appdirs@1.4.3      qhull@2015.2
  flex@2.6.4            libxml2@2.9.4             py-appdirs@1.4.3      readline@7.0
  freetype@2.7.1        m4@1.4.18                 py-configparser@3.5.0 sqlite@3.21.0
  gdbm@1.14.1           matio@1.5.9               py-cycler@0.10.0      suite-sparse@5.1.0
  gettext@0.19.8.1      matio@1.5.9               py-dateutil@2.5.2     superlu-dist@5.2.2
  git@2.15.1            matio@1.5.9               py-enum34@1.1.6       superlu-dist@5.2.2
  glm@0.9.7.1           metis@5.1.0               py-gnuplot@1.8        superlu-dist@5.2.2
```

Trilinos: 4 Compilers, 3 OpenMPI, 2 Python

```
  gsl@2.4          mumps@5.1.1    py-lit@0.5.0       tar@1.29
  hdf5@1.10.1      mumps@5.1.1    py-lit@0.5.0       tcl@8.6.6
  hdf5@1.10.1      mumps@5.1.1    py-mpmath@0.19     tk@8.6.6

- linux-rhel7-x86_64 / gcc@6.4.0 ----------------

  autoconf@2.69        libpciaccess@0.13.5    openmpi@3.0.0          py-setuptools@35.0.2
  automake@1.15.1      libpng@1.6.29          openssl@1.0.2n         py-setuptools@35.0.2
  binutils@2.29.1      libpthread-stubs@0.4   parmetis@4.0.3         py-six@1.10.0
  bison@3.0.4          libsigsegv@2.11        parmetis@4.0.3         py-six@1.10.0
  boost@1.65.1         libtool@2.4.6          parmetis@4.0.3         py-sympy@1.0
  bzip2@1.0.6          libx11@1.6.5           pcre@8.41              py-sympy@1.0
  cmake@3.10.1         libxau@1.0.8           perl@5.24.1            python@2.7.14
  curl@7.56.0          libxcb@1.12            pkgconf@1.4.0          python@3.6.2
  expat@2.2.2          libxdmcp@1.1.2         py-appdirs@1.4.3       qhull@2015.2
  flex@2.6.4           libxml2@2.9.4          py-appdirs@1.4.3       readline@7.0
  freetype@2.7.1       m4@1.4.18              py-configparser@3.5.0  sqlite@3.21.0
  gdbm@1.14.1          matio@1.5.9            py-cycler@0.10.0       suite-sparse@5.1.0
  gettext@0.19.8.1     matio@1.5.9            py-dateutil@2.5.2      superlu-dist@5.2.2
  git@2.15.1           matio@1.5.9            py-enum34@1.1.6        superlu-dist@5.2.2
  glm@0.9.7.1          metis@5.1.0            py-gnuplot@1.8         superlu-dist@5.2.2
  gsl@2.4              mumps@5.1.1            py-lit@0.5.0           tar@1.29
  hdf5@1.10.1          mumps@5.1.1            py-lit@0.5.0           tcl@8.6.6
  hdf5@1.10.1          mumps@5.1.1            py-mpmath@0.19         tk@8.6.6
```

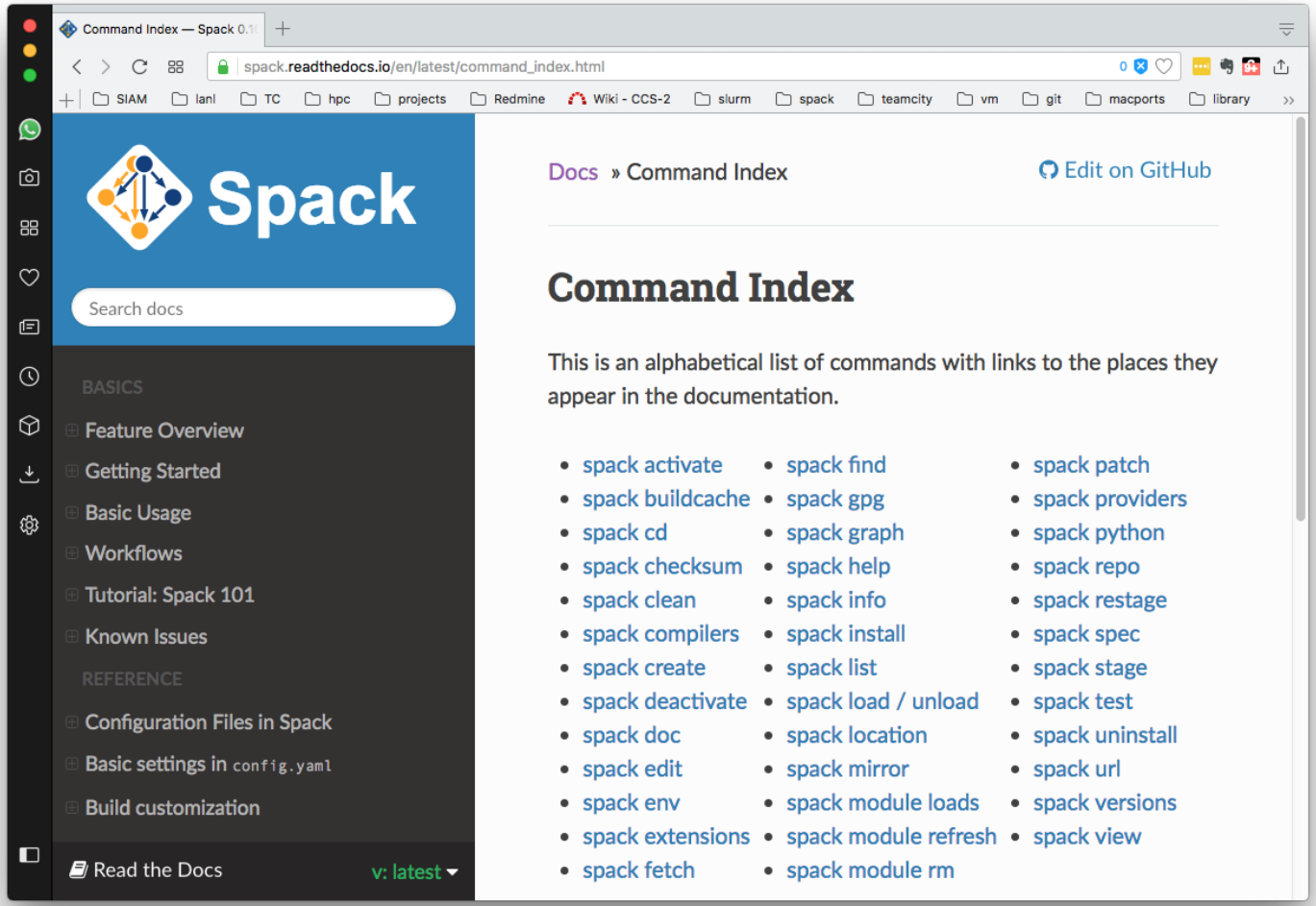
Spack Programming Elements

1. Command Set
2. Sigils
3. Configuration Files (*.yaml)
4. Either commands – Or yaml files

More Details Here:

- Configuration Files in Spack
- Build Customization

Spack Command Set



Spack Command Set

(de)activate	arch	buildcache	cd	checksum
clean	compiler	compilers	config	edit
env	extensions	fetch	find	gpg
graph	help	info	(un)install	list
(un)load	location	mirror	module	patch
providers	python	repo	spec	(re)stage
test	url	versions	view	

Spack Workhorse Commands

(de)activate	**arch**	buildcache	cd	checksum
clean	**compiler**	**compilers**	**config**	edit
env	extensions	fetch	**find**	gpg
graph	help	**info**	**(un)install**	**list**
(un)load	location	mirror	**module**	patch
providers	python	repo	**spec**	(re)stage
test	url	**versions**	view	

Info Command Examples: providers (CCS)

```
$ spack providers mpi
intel-mpi   mpich   mpich@3:   mvapich2@1.9   openmpi
openmpi@1.7.5:   spectrum-mpi   intel-parallel-studio+mpi
mpich@1:   mvapich2   mvapich2@2.0:   openmpi@1.6.5
openmpi@2.0.0:

$ spack providers lapack
atlas   intel-mkl   intel-parallel-studio+mkl
netlib-lapack   openblas   veclibfort
```

Info Command Examples: compilers (Power8+)

```
$ spack compilers
==> Available compilers

-- clang centos7-x86_64 ---------------------
clang@5.0.1 clang@5.0.0 clang@4.0.1 clang@3.9.1 clang@3.8.1 clang@3.7.1 clang@3.5.2

-- gcc centos7-x86_64 -----------------------
gcc@7.2.0 gcc@7.1.0 gcc@6.3.0 gcc@6.2.0 gcc@6.1.0 gcc@5.4.0 gcc@5.3.0 gcc@5.2.0 gcc@5.1.0
gcc@4.9.3 gcc@4.9.2 gcc@4.9.1 gcc@4.9.0 gcc@4.8.5 gcc@4.6.4

-- gcc rhel7-ppc64le ------------------------
gcc@7.2.0 gcc@7.1.0 gcc@6.3.0 gcc@5.4.0 gcc@4.8.5

-- intel centos7-x86_64 ---------------------
intel@18.0.1 intel@17.0.0 intel@16.0.1 intel@15.0.3 intel@15.0.0 intel@13.1.2 intel@13.1.0
intel@17.0.1 intel@16.0.3 intel@16.0.0 intel@15.0.1 intel@14.0.2 intel@13.1.1 intel@13.0.1

-- pgi centos7-x86_64 -----------------------

pgi@17.4 pgi@16.10 pgi@16.5 pgi@16.1 pgi@15.10 pgi@15.7

-- pgi rhel7-ppc64le ------------------------

pgi@17.5 pgi@16.10
```

Info Command Examples: versions (CCS)

```
$ spack versions hypre
==> Safe versions (already checksummed):
develop 2.13.0 2.12.1 2.11.2 2.11.1 2.10.1 2.10.0b xsdk-0.2.0
==> Remote versions (not yet checksummed):
2.13.0-28-g42e267b 2.12.0-2-ga34db78 2.12.
```

Info Command Examples: arch (CCS)

```
dantopa@cn2000:spack.power8.2018-01-13 $ spack arch
linux-rhel7-ppc64le

dantopa@tt-fey1:spack.tt.2018-01-04 $ spack arch
cray-CNL-haswell

dantopa@ccscs2.lanl.gov:spack.ccs.2018-01-114 $ spack arch
linux-rhel7-x86_64

1127914@pn1249300.lanl.gov $ spack arch
darwin-sierra-x86_64
```

Spack Sigils

sigil | ˈsijəl |

noun

an inscribed or painted symbol considered to have magical power.

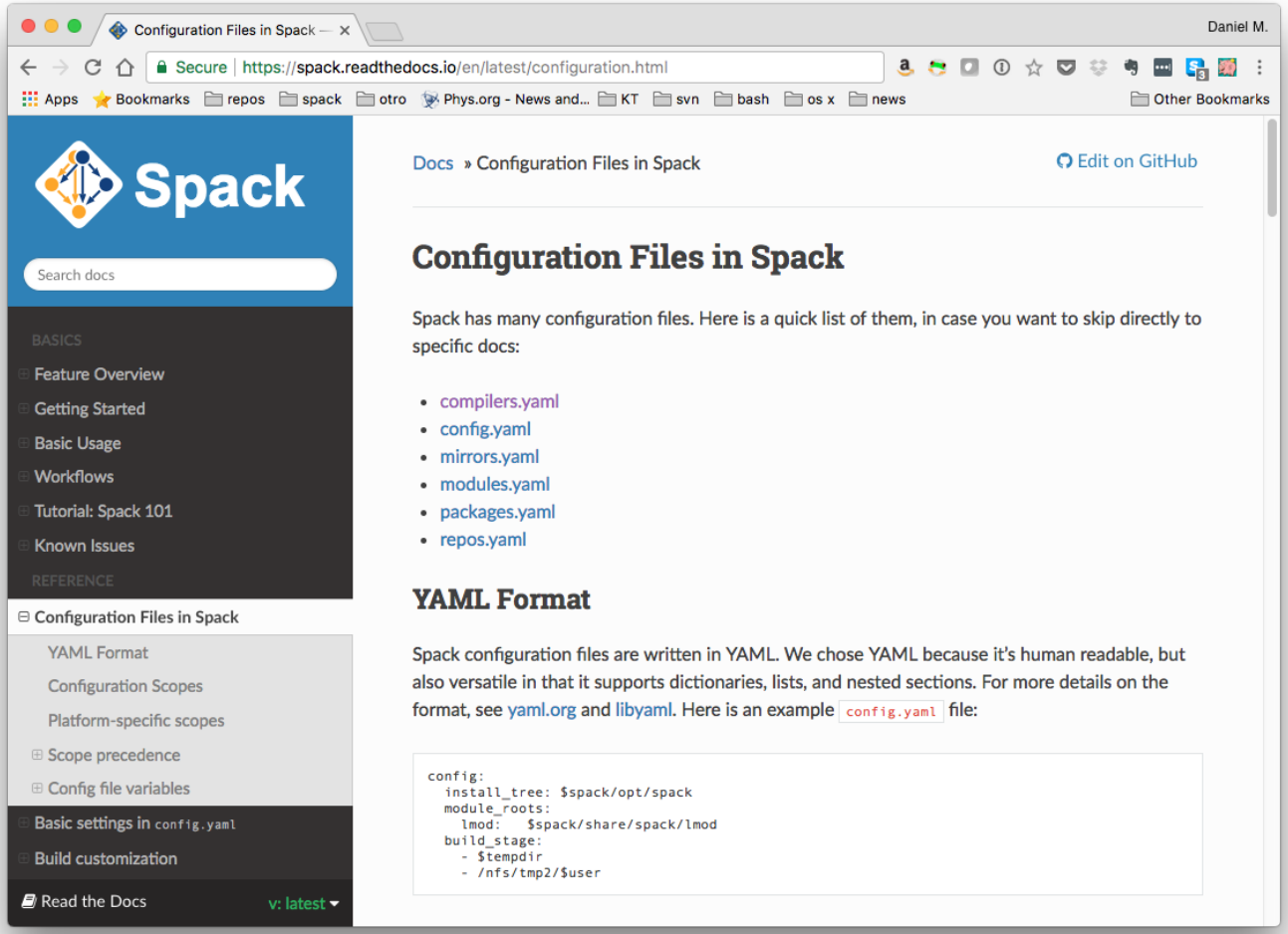
Spack Sigils

sigil	denotes
@	package version
%	compiler version
^	dependencies
+	Boolean TRUE
−, ~	Boolean FALSE
/	hash

Sigil Examples

```
spack install hypre
spack install hypre @ 2.12.1
spack install hypre % gcc @ 4.8.5
spack install hypre +mpi ^ mpich
```

You Have To Read The Manual



Spack Configuration Files

1. config.yaml
2. compilers.yaml
3. mirrors.yaml
4. modules.yaml
5. packages.yaml
6. repos.yaml

CCS: modules.yaml

```
modules:
    enable:
        - tcl
        - dotkit
    tcl:
        hash_length:  0
        naming_scheme:
'${PACKAGE}/${VERSION}-${COMPILERNAME}-${COMPILERVER}'
        all:
            suffixes:
                ^openmpi@1.10.5:  'openmpi@1.10.5'
                ^openmpi@2.1.0:  'openmpi@2.1.0'
                ^openmpi@2.2.0:  'openmpi@2.2.0'
                ^openmpi@3.0.0:  'openmpi@3.0.0'
                ^python@2.7.14:  'python@2.7.14'
                ^python@3.6.2:  'python@3.6.2'
```

CCS: packages.yaml

```
packages:
    all:
        compiler:  [gcc, intel, pgi, clang, xl, nag]
        providers:
            blas:  [openblas]
            lapack:  [openblas]
            mkl:  [intel-mkl]
            mpi:  [openmpi, mpich]
            scalapack:  [netlib-scalapack]
```

CCS: compilers.yaml I

```
compilers:
- compiler:
    environment:  {}
    extra_rpaths:  []:
    flags:  {}:
    operating_system:  rhel7
    paths:
        cc:  /usr/bin/gcc
        cxx:  /usr/bin/g++
        f77:  /usr/bin/gfortran
        fc:  /usr/bin/gfortran
    spec:  gcc4.8.5
    target:  x86_64
```

CCS: compilers.yaml II

```
compilers:
- compiler:
    environment:  {}
    extra_rpaths:  []:
    flags:  {}:
    operating_system:  rhel7
    paths:
        cc:
/scratch/dantopa/spack.ccs.developmental/spack.ccs.2018-01-11/opt/spack/linux-rhel7-x86_64/gcc-4.8.5/gcc-7
        cxx:
/scratch/dantopa/spack.ccs.developmental/spack.ccs.2018-01-11/opt/spack/linux-rhel7-x86_64/gcc-4.8.5/gcc-7
        f77:
/scratch/dantopa/spack.ccs.developmental/spack.ccs.2018-01-11/opt/spack/linux-rhel7-x86_64/gcc-4.8.5/gcc-7
        fc:
/scratch/dantopa/spack.ccs.developmental/spack.ccs.2018-01-11/opt/spack/linux-rhel7-x86_64/gcc-4.8.5/gcc-7
    spec:  gcc7.2.0
    target:  x86_64
```

spack config get ...

`spack config get` { *compilers*, *config*, *mirrors*, *modules*, *packages*, *repos*

Command Sequence

1. `spack install hypre`
2. `spack install hypre % gcc @4.8.5`
3. `spack install hypre % gcc @4.8.5 +mpi ^mpich`
4. `spack install hypre % gcc @4.8.5 +mpi ^openmpi@2.1.2`
5. `spack find -ldf hypre`
6. `spack spec /jk47cxx`

Load Compilers from MacPorts I

```
$ port select -list gcc
Available versions for gcc:
    mp-gcc47
    mp-gcc48
    mp-gcc5
    mp-gcc6
    mp-gcc7 (active)
    mp-gcc8
    none
$ sudo port select -set gcc mp-gcc8
Selecting 'mp-gcc8'for 'gcc'succeeded.  'mp-gcc8'is now
active.
```

Load Compilers from MacPorts II

```
$ spack compiler find
==> Added 1 new compiler to
/Users/l127914/.spack/darwin/compilers.yaml
    gcc@7.2.0
==> Compilers are defined in the following files:
    /Users/l127914/.spack/darwin/compilers.yaml
```

Task: Load Compilers from Modules on Darwin

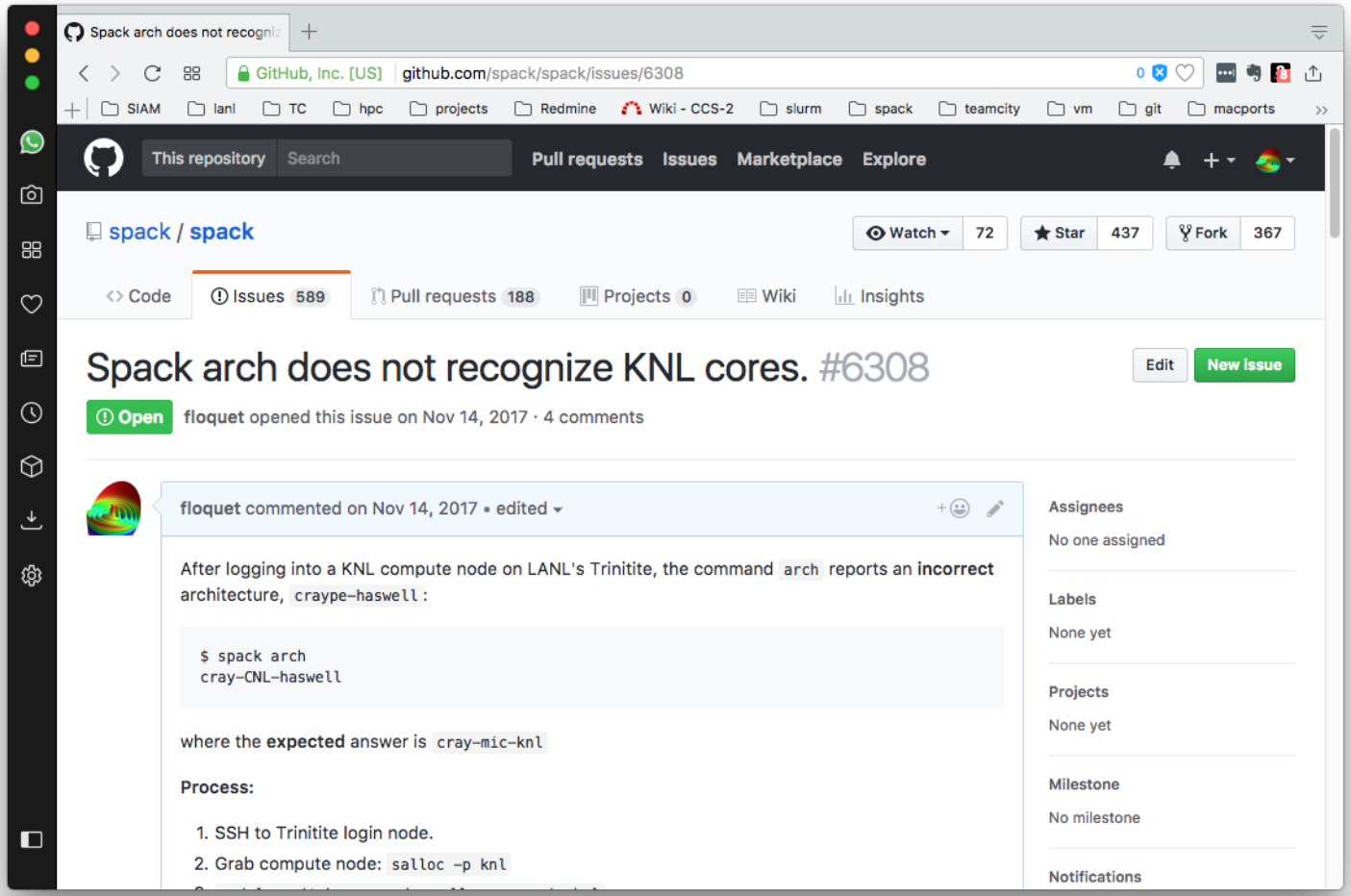
Table: module avail excerpt

clang/3.5.2	gcc/4.6.4	intel/13.0.1
clang/3.7.1	gcc/4.9.0	intel/13.1.0
clang/3.8.1	gcc/4.9.1	intel/13.1.1
clang/3.9.1	gcc/4.9.2	intel/13.1.2
clang/4.0.1	gcc/4.9.3(default)	intel/14.0.2
clang/5.0.1(default)	gcc/5.1.0	intel/15.0.0
pgi/15.10	gcc/5.2.0	intel/15.0.1
pgi/15.7	gcc/5.3.0	intel/15.0.3(default)
pgi/16.1	gcc/6.1.0	intel/16.0.0
pgi/16.10(default)	gcc/6.2.0	intel/16.0.1
pgi/16.5	gcc/6.3.0	intel/16.0.3
pgi/17.4	gcc/7.1.0	intel/17.0.0
	gcc/7.2.0	intel/17.0.1
		intel/18.0.1

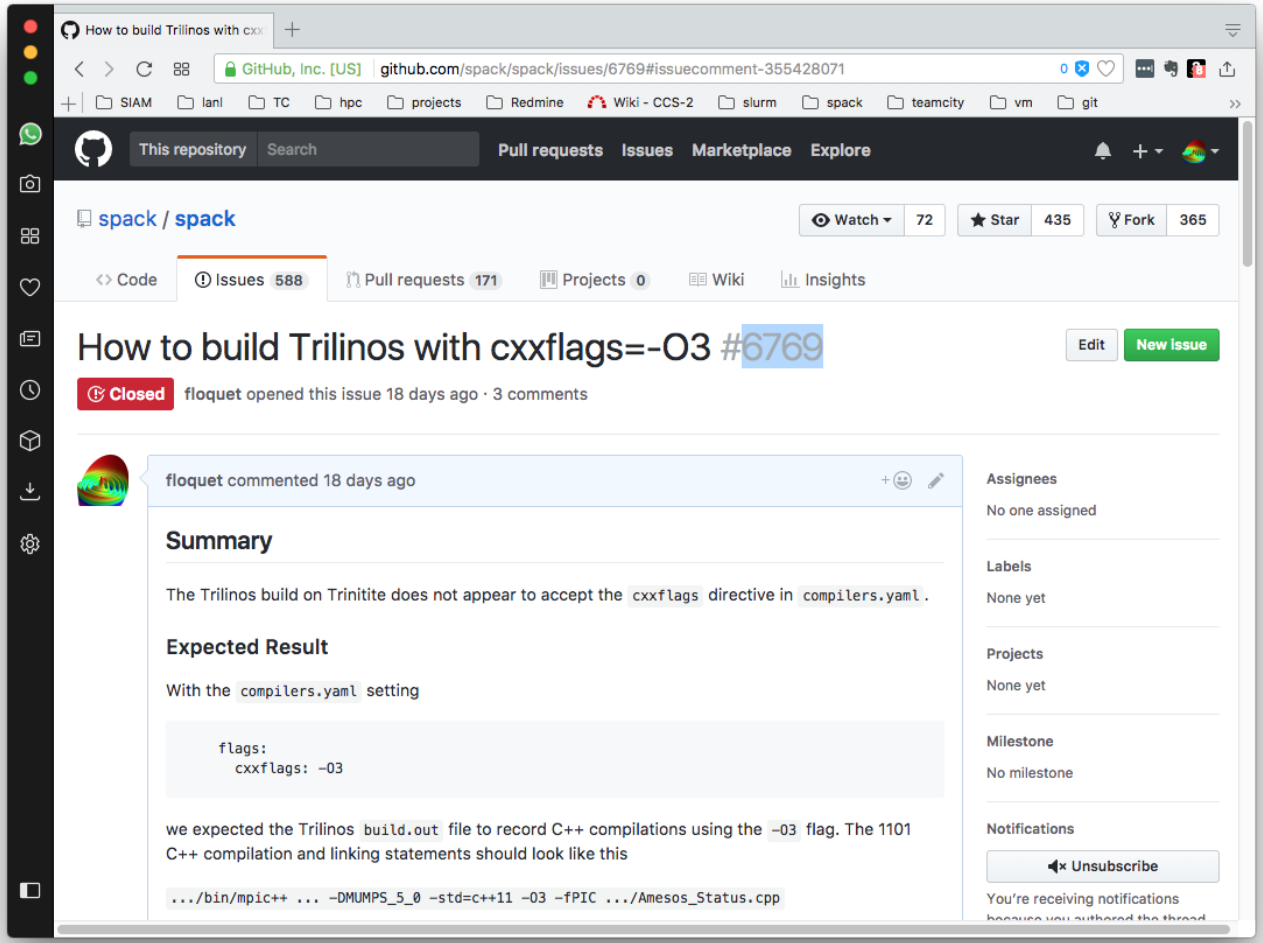
Load Compilers from Modules

```
$ module load <vendor/version>
$ spack compiler find
$ module purge
```

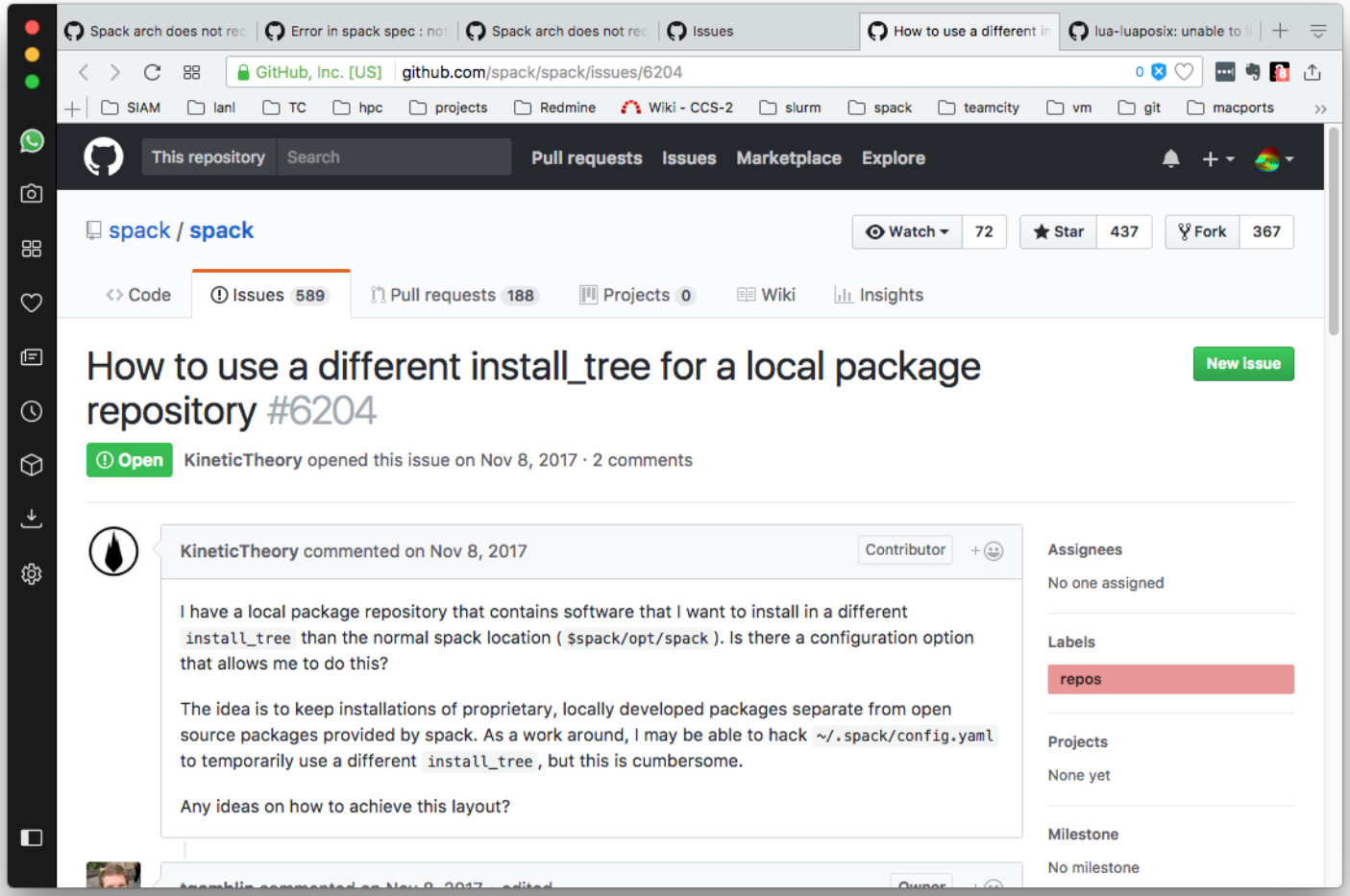
Spack doesn't recognize KNL (6308)



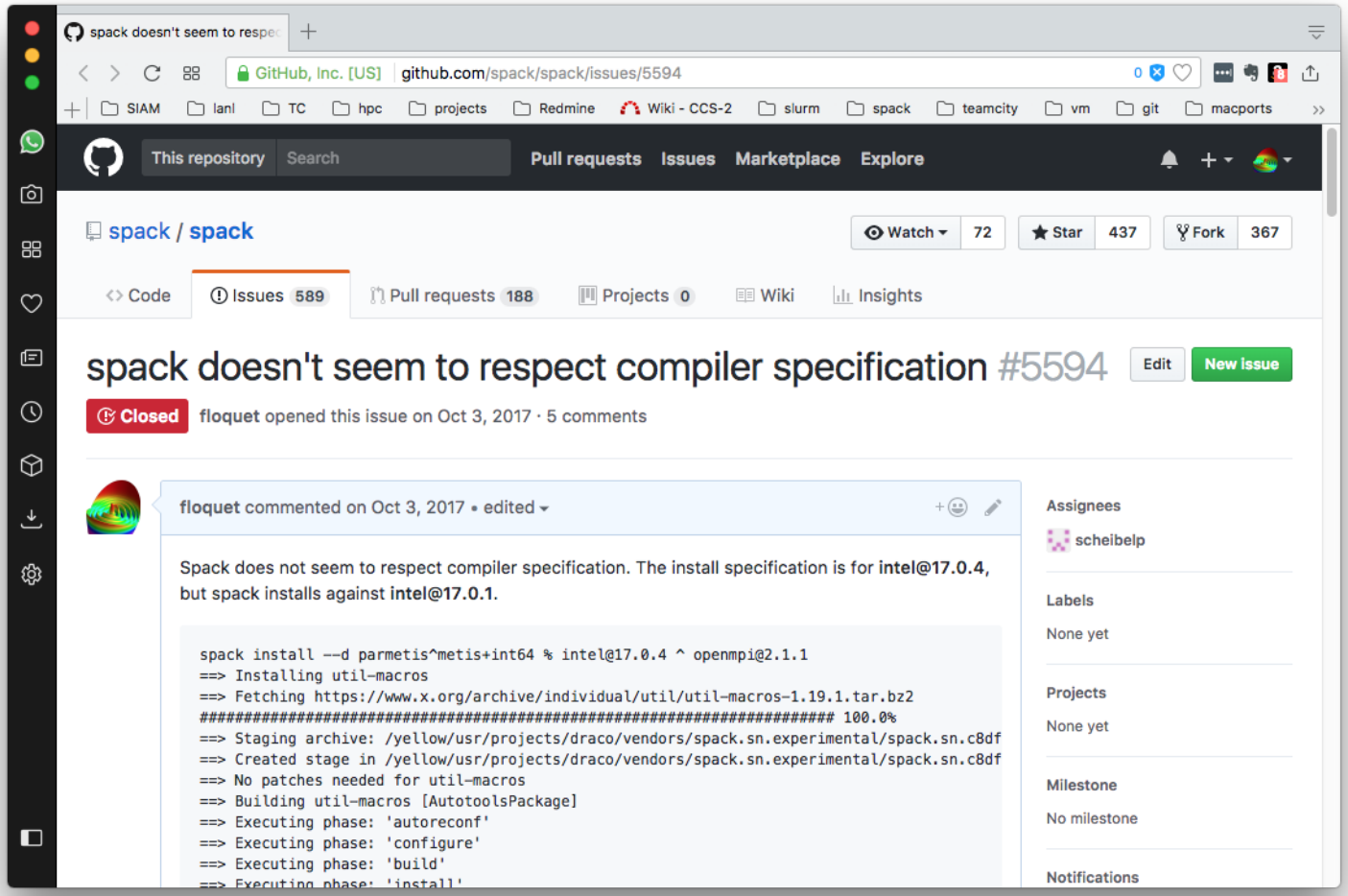
CMake won't accept compiler flags (6769)



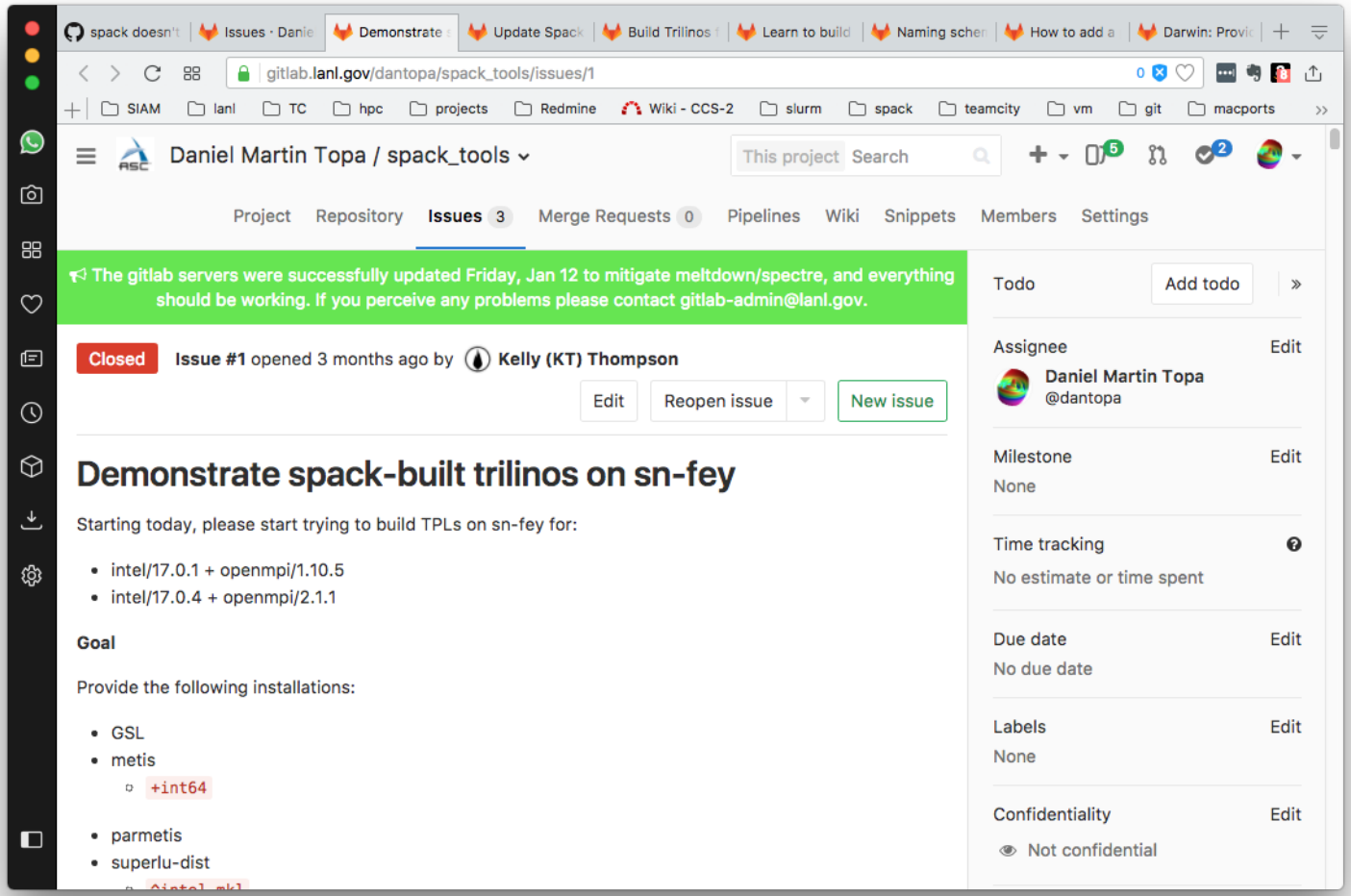
How to use a different install_tree (6204)



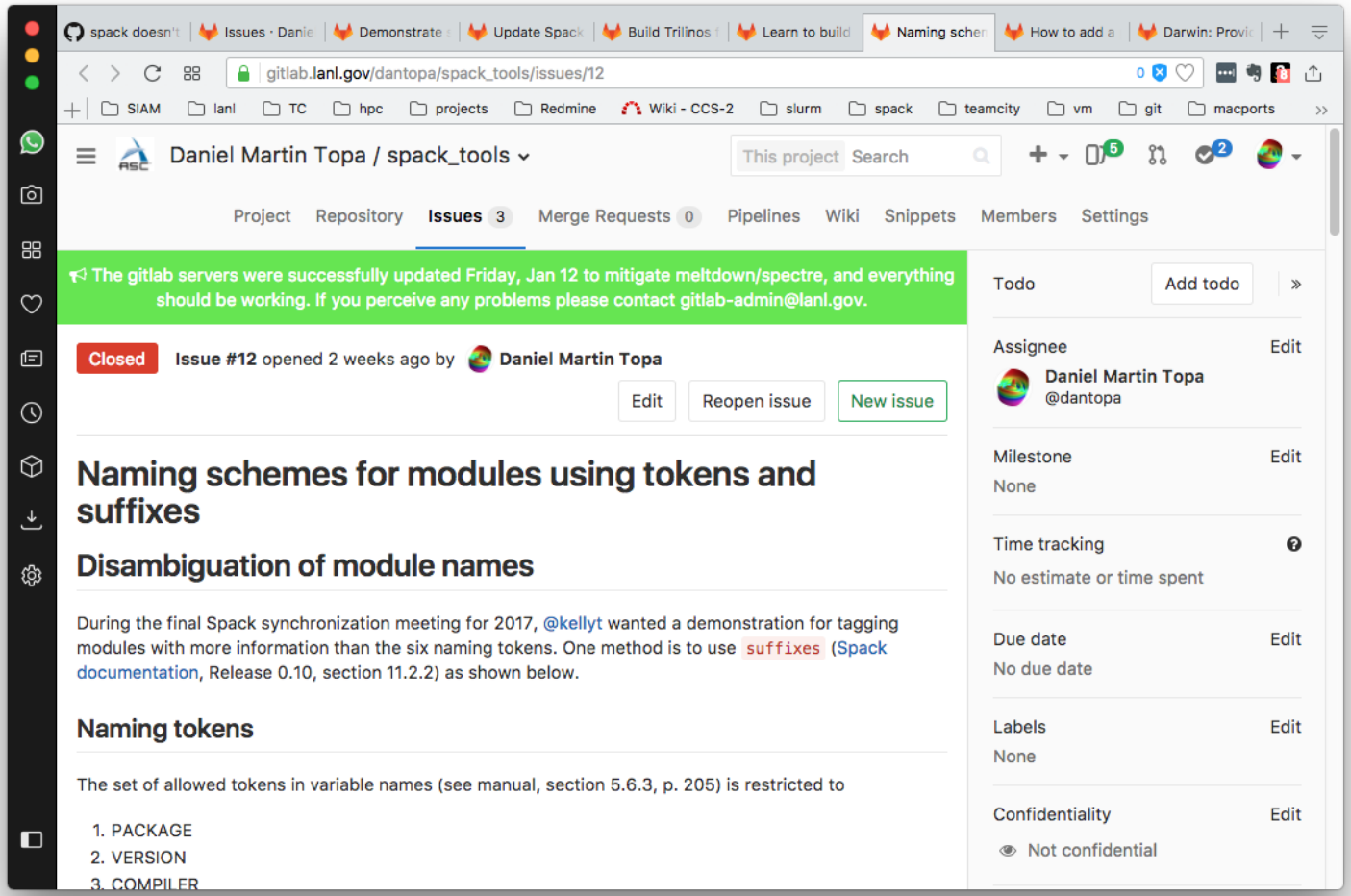
Compiler selection (5594)



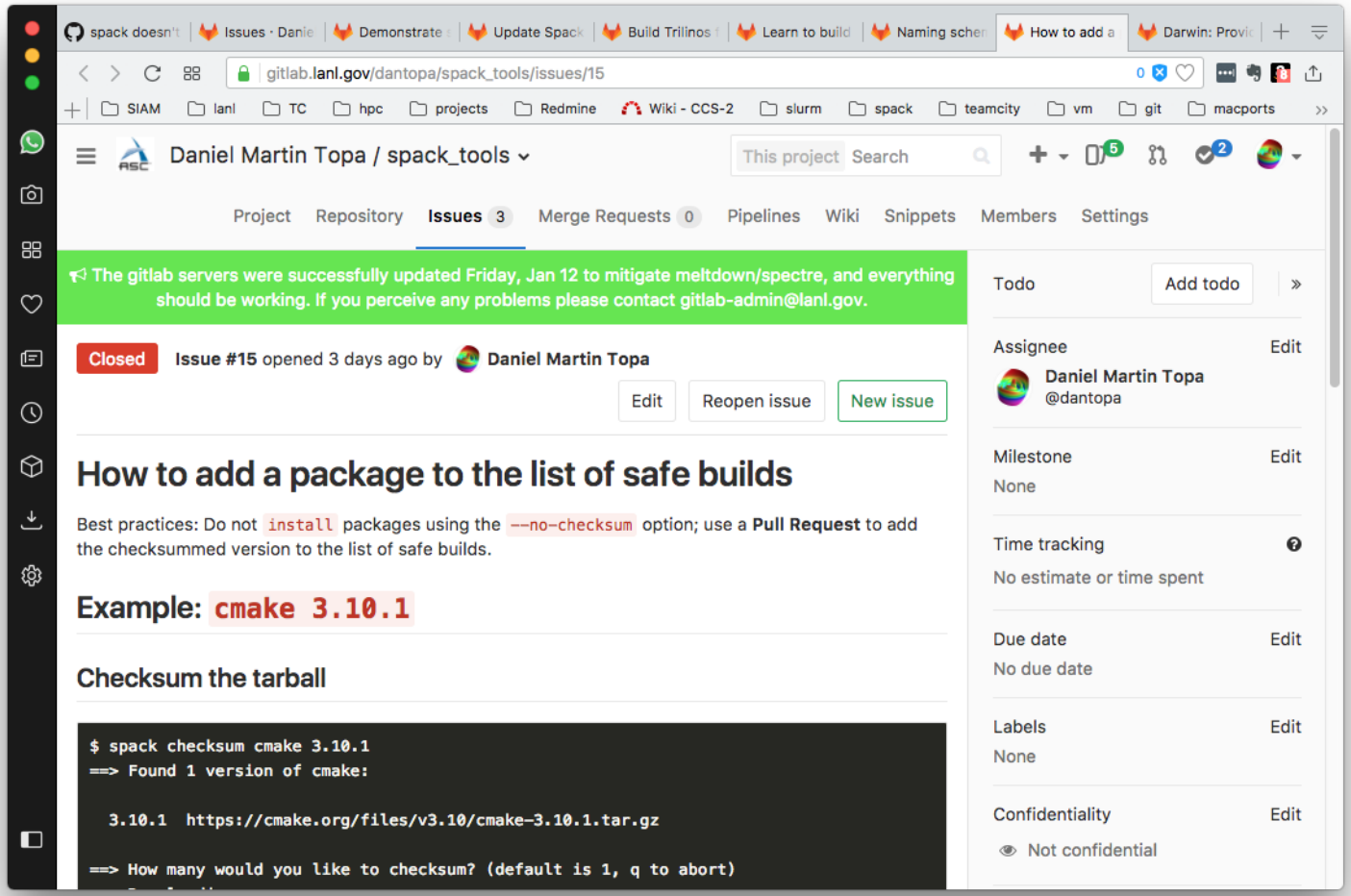
Build Trilinos on Snow (1)



Naming Spack Modules (12)



Safe Builds (15)



Spack
Supercomputer PACKage Manager

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CCS-2: Computational Physics and Methods

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2018-01-17