Getting Scientific Software Installed BOF
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Spack is a flexible package manager for HPC

- How to install Spack:
  
  ```
  $ git clone https://github.com/scalability-llnl/spack.git
  ```

- How to install a package:
  
  ```
  $ cd spack/bin
  $ ./spack install hdf5
  ```

- HDF5 and its dependencies are installed within the Spack directory.

- No additional setup required!
$ spack compilers

```bash
>>> Available compilers
-- gcc --
gcc@4.4.7
-- intel
intel@16.0.0 intel@14.0.3 intel@13.1.0 intel@12.1.2 intel@10.0
intel@15.0.3 intel@14.0.2 intel@13.0.1 intel@12.1.0 intel@9.1
intel@15.0.1 intel@14.0.1 intel@13.0.0 intel@12.0.4
intel@15.0.0 intel@14.0.0 intel@12.1.5 intel@11.1
intel@14.0.4 intel@13.1.1 intel@12.1.3 intel@10.1
-- clang
clang@3.6.2 clang@3.4 clang@3.3 clang@3.2 clang@3.1
-- pgi
pgi@15.5-0 pgi@14.3-0 pgi@13.1-1 pgi@11.1-0 pgi@8.0-1
pgi@15.1-0 pgi@13.10-0 pgi@12.8-0 pgi@10.9-0 pgi@7.1-3
pgi@14.10-0 pgi@13.6-0 pgi@12.1-0 pgi@10.2-0 pgi@7.0-6
pgi@14.7-0 pgi@13.2-0 pgi@11.10-0 pgi@9.0-4
```

- Spack searches PATH
  - Can also give it a prefix
  - Searching modules coming soon

- Any package can be built with any compiler.
  - Swapping is easy and automatic.
  - Not guaranteed to work, but exploring the space is easy.

- Spack will also build compilers like gcc and clang for you, but it doesn’t have to.
Spack can install the same package many different ways

- These are called **spec expressions**
  - Concise and expressive language for describing builds.

- Specs describe a configuration of a package.
  - Arbitrary configurations are possible and can coexist.
  - Install it your way!

```bash
$ spack install mpileaks          default
$ spack install mpileaks@3.3     @ custom version
$ spack install mpileaks@3.3 @gcc@4.7.3 @ custom compiler
$ spack install mpileaks@3.3 @gcc@4.7.3 +threads +/- build option
$ spack install mpileaks@3.3 =bgq = cross-compile
```
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.

`spack find` shows what is installed

$ spack find

```bash
$ spack find
```
Spack tracks detailed provenance for every build.

- Every configuration is a new dependency graph.
  - Spack hashes the graph to make a version id.
  - Full graph information is stored with each build.

- Spack allows arbitrary composition of packages
  - Build Python with different compilers and BLAS implementations.
  - Build your code with different compiler/MPI/dependency versions.

```yaml
spec:
  - mpi:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      - callpath: boh5f4h4d2n47mgycej2mtrnrivvxy77
        mpich: aao406ifji23yijmddakpejcli7t3
        hash: 33mijhjxi7pbyyosptghyesaghyiprj
        variants: {}
      - version: "1.0"
        - adept-utils:
          arch: linux-x86_64
          compiler:
            name: gcc
            version: 4.9.2
          dependencies:
            - boost: teesjv7epe5ksspjin5dk43a7gnwq
              mpich: aao406ifji23yijmddakpejcli7t3
              hash: kszrtgbzoc3a2licjkorleybnptp
              variants: {}
              version: 1.8.1
            - boost:
              arch: linux-x86_64
              compiler:
                name: gcc
                version: 4.9.2
              dependencies: {}
              hash: teesjv7epe5ksspjin5dk43a7gnwq
              variants: {}
              version: 1.59.0
            ...
Spack allows Python extensions to be activated and deactivated on demand

```
$ spack install python@2.7.10
>>> Building python.
>>> Successfully installed python.
Fetch: 5.01s. Build: 97.16s. Total: 103.17s.
[+] /home/gamblin2/spack/opt/spack/linux-x86_64/gcc-4.9.2/python-2.7.10-y2zr767
```

```
$ spack extensions python@2.7.10
>>> python@2.7.10@gcc@4.9.2=linux-x86_64-y2zr767
>>> 49 extensions:
geos   py-h5py   py-numpy   py-ppar   py-setuptools
libxml2 py-ipython py-pandas   py-pparsing py-shiboken
py-bosemap py-libxml2 py-pexpect py-pyqt   py-sip
py-biopython py-lockfile py-pil   py-psyide py-six
py-fftw py-mako   py-pmw   py-python-daemon py-sphinx
py-cython py-matplotlib py-ppchecker py-pytz   py-sympy
py-doteutil py-mock   py-pycparser py-rrpy2 py-virtualenv
py-epydoc py-mpi4py py-pyelftools py-scientificpython py-yapf
py-genders py-mx   py-pygments py-scikit-learn thrift
py-gnuplot py-nose   py-pylint py-scipy

>>> 3 installed:
-- linux-x86_64 / gcc@4.9.2 ------------------------------------
py-nose@1.3.6  py-numpy@1.9.2  py-setuptools@18.1

>>> None currently activated.
```

```
$ spack activate py-numpy
>>> Activated extension py-setuptools@18.1-gcc@4.9.2-ru7w3lx
>>> Activated extension py-nose=1.3.6-gcc@4.9.2-vudjpwc
>>> Activated extension py-numpy=1.9.2-gcc@4.9.2-45hjazt
```

```
$ spack deactivate -a py-numpy
>>> Deactivated extension py-numpy@1.9.2-gcc@4.9.2-45hjazt
>>> Deactivated extension py-nose@1.3.6-gcc@4.9.2-vudjpwc
>>> Deactivated extension py-setuptools@18.1-gcc@4.9.2-ru7w3lx
```

**Many interpreted languages have their own mechanisms for modules, e.g.:**

- Require installation into interpreter prefix
- Breaks combinatorial versioning

**Spack installs each Python package in its own prefix**

**“Activating” links an extension into the interpreter directory on demand**

- Supports .egg, merging .pth files
- Mechanism is extensible to other languages
- Similar to virtualenv, but Spack allows much more build customization.
Get Involved with Spack!

- **Come to our SC15 Talk:**
  *The Spack Package Manager: Bringing Order to HPC Software Chaos*
  Wednesday, 11:30am
  Hall 18AB

- **Spack is starting to be used in production at LLNL**
  - Build, test, and deployment by code teams.
  - Build research projects for students, postdocs.

- **Spack has a rapidly growing external community.**
  - NERSC is working with LLNL on Cray support for Cori.
  - Argonne/IIT cluster challenge project.
  - Kitware contributing ParaView builds & features.
  - Users at INRIA, EPFL, U. Oregon, Sandia, LANL, others.

Get Spack!


Unwatch 28  Unstar 51  Fork 55

1,043 commits  25 contributors
8 releases  25 branches
