Spack Package Manager

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Reusing this material

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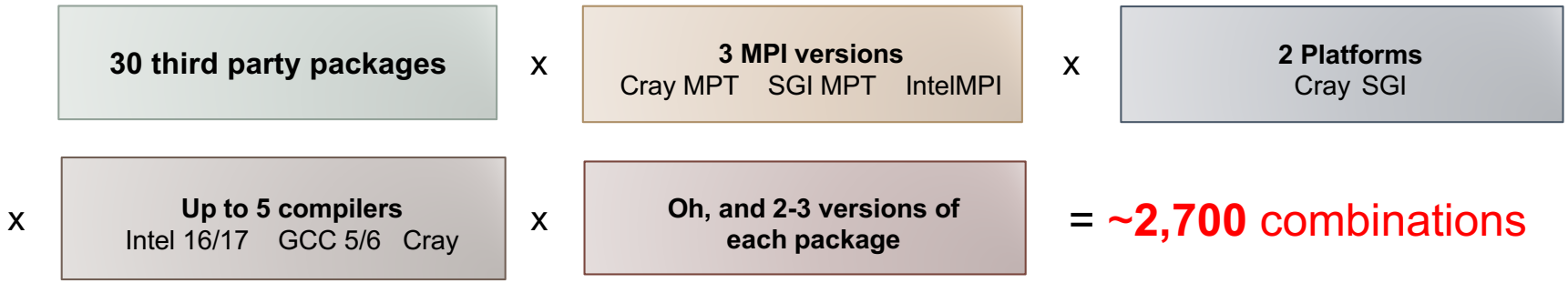
Thanks to Todd Gamblin, LLNL for much of the technical material

HPC package management issues

- Not much standardization in HPC: every machine/app has a different software stack
  - Usually source compilation is required
- Sites share unique hardware among teams with *very* different requirements
  - May want to experiment with many exotic architectures, compilers, MPI versions
  - All of this is necessary to get the best ***performance***
- Example environment for EPCC national services:



We want an easy way to quickly sample the space and to build configurations on demand

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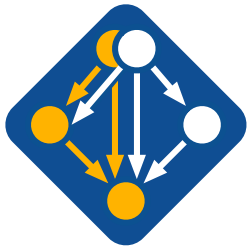
Existing tools

- Do not really support combinatorial versioning…
- Traditional binary package managers
  - RPM, yum, APT, yast, etc.
  - Designed to manage a single stack for standard hardware
  - 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 parameterised by compilers, dependency versions.
- Virtual Machines and Linux Containers
  - 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 – maybe a route past this with Singularity…



Spack approach

- *Simple* package management based on source compilation
  - Support for multiple compilers and versions
- Automatically resolve (and build) dependencies
  - Reuse already installed dependencies
  - Support pre-installed dependencies (e.g. vendor MPI, MKL)
- Capture compilation instructions in natural way
  - Open Source to share with community
- Integration with various environment module solutions
- Focus on simplicity of implementation and use

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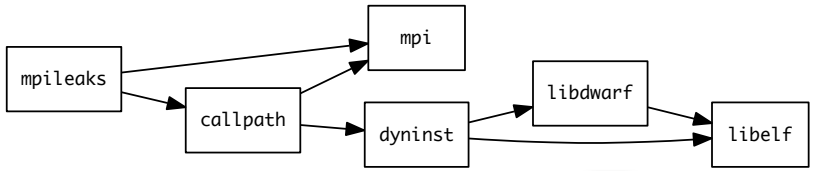
Spack – handling combinations

Dependency DAG



Installation Layout

Hash

```
spack/opt/
    linux-x86_64/
        gcc-6.2.0/
            mpileaks-1.1-
0f54bf34cadk/
        intel-17.0.2/
            hdf5-1.8.15-lkf14aq3nqiz/
    bgq/
        xl-12.1/
            hdf5-1-8.16-fqb3a15abrwx/
    ...
```

- 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*

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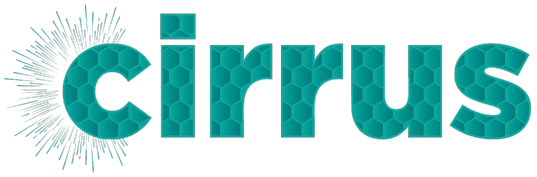
spec syntax to describe configurations

```
$ spack install gromacs                          unconstrained
$ spack install gromacs@2016.3                   @ custom version
$ spack install gromacs@2016.3 %gcc@6.2.0        % custom compiler
$ spack install gromacs@2016.3 %gcc@6.2.0 +double   +/- build option
$ spack install gromacs@2016.3 %intel@17 target=knl   target=<cpu target>
```

- 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.
  - Customise install on the command line!
- Syntax abstracts details in the common case
  - Makes parameterisation by version, compiler, and options easy when necessary

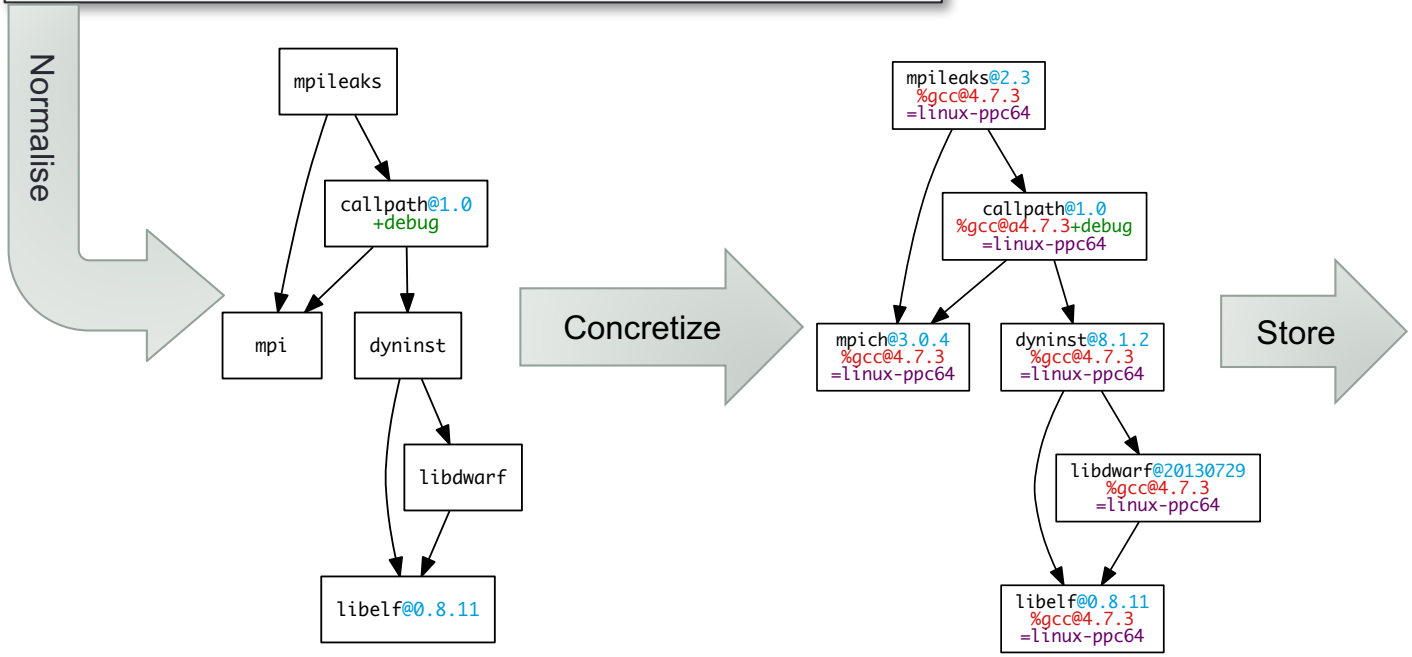


Concretization

- Fills in missing configuration details when user is not explicit

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

User input: *abstract* spec with some constraints



Abstract, normalised spec with some dependencies.

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

spec.yaml

```
spec:
- mpileaks:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      adept-utils: kszrtkpbzac3ss2ixcjkcorlaybnptp4
      callpath: bah5f4h4d2n47mgycej2mtrnrivvxy77
      mpich: aa4ar6ifj23yijqmdabeakpejcli72t3
    hash: 33hjjhxi7p6gyzn5ptgyes7sghyprujh
    variants: {}
    version: '1.0'
- adept-utils:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      boost: teesjv7ehpe5ksspjim5dk43a7qnowlq
      mpich: aa4ar6ifj23yijqmdabeakpejcli72t3
    hash: kszrtkpbzac3ss2ixcjkcorlaybnptp4
    variants: {}
    version: 1.0.1
- boost:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies: {}
    hash: teesjv7ehpe5ksspjim5dk43a7qnowlq
    variants: {}
    version: 1.59.0
...
```

Detailed provenance is stored with the installed package

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Spack packages are simple Python scripts.

- Scripts closely mirror the commands you would usually type on the command line
- Easy to understand what is going on and modify

```
from spack import *

class Dyninst(Package):
    """API for dynamic binary instrumentation."""

    homepage = "https://paradyn.org"

    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.tgz")

    depends_on("libelf")
    depends_on("libdwarf")
    depends_on("boost@1.42:")

    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'
                  *std_cmake_args)
            make()
            make("install")

    @when('@:8.1')
    def install(self, spec, prefix):
        configure("--prefix=" + prefix)
        make()
        make("install")
```

Metadata

Versions and URLs

Dependencies

Patches, variants (not shown)

Commands for installation

Access build config through the *spec* parameter.

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Demo!

Spack and Easybuild

- Similar tools but underlying philosophy slightly different
  - Easybuild focus on *reproducibility* of binaries – loses some simplicity
  - Spack focus on *simplicty* of use – loses full reproducibility
- Both widely used across HPC centres worldwide
- Both have active developer communities
- Both support a wide range of software
- Suspect that personal preference will decide which one is more useful for you
  - Probably the one that most matches your team mentality…
  - …in our case the simplicity of Spack and particularly the package scripts made our minds up after playing with both of them

Python and R

- Both have their own package dependency chain
  - Can have their own package managers: e.g. conda, pip
- On HPC systems some of modules/packages have to be compiled
  - Usually parallel/performance modules
  - Cannot usually be managed using tools such as conda
- Often the distro Python/R and modules are too out of date
- Spack supports source installation of Python/R and many common scientific modules
  - Can also be linked into controlled environments to ensure people only access the correct packages for that installation

Conclusions

- Spack has proven very useful to us on Cirrus
- Simplified our central installation of packages
  - Easy stuff just installs with single command
  - Some tweaking needed for some packages
  - Some packages still compiled and supported outwith Spack…
  - …but the dependency chain is often mostly met using Spack
- Allows us to focus on more difficult installations
  - Less time spent resolving source compiled dependency chains
- Next steps:
  - Get Spack up and running on ARCHER
  - Explore Python and R support