OAK RIDGE National Laboratory

Spack at the OLCF

Matt Belhorn
OLCF User Assistance Group

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

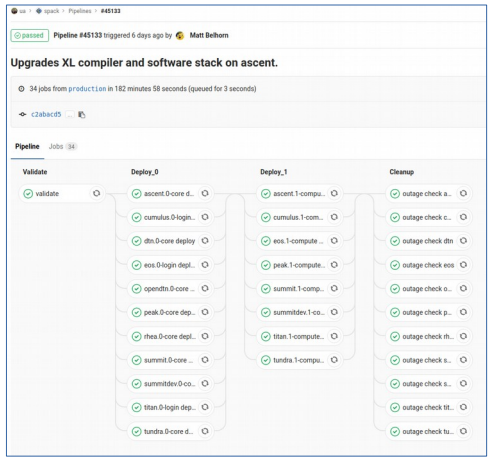
U.S. DEPARTMENT OF ENERGY

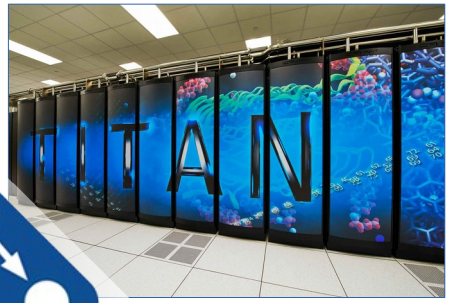
In 2016, the OLCF needed a new userspace package manager...

- Adopted Spack to replace unmaintained in-house developed homebrew clone *smithy*.
- At the time, Spack was a nearly feature-complete replacement
  - Custom OLCF [s]package repo; to augment builtin repo with site-specific tuning.
  - Larger community of package maintainers.
  - Multi-toolchain support, modulefile support.
- Multiple Spack instances per host, used sequentially in *tiers*.
  - When toolchains (PGI, older XL) have difficulty building low-level, non-linked or C-only common dependencies
  - Lowest tier uses OS compiler only.
  - Higher tiers reference specific lower-tier builds as *unbuildable external packages*.

Software ecosystem management: Spack + DevOps

- Spack configs and list of desired explicit specs for each machine kept in VCS
- CI/CD scripts automatically build software manifests.
  - CI runner on each machine login node;
    exact build environment as runtime.
  - Staging area with private module tree for testing prior to production deployment.
- Can upgrade or redeploy
  - 1333 repeatable explicit builds*
  - of 75 explicit software* titles
  - on 11 OLCF machines* at the push of a button.





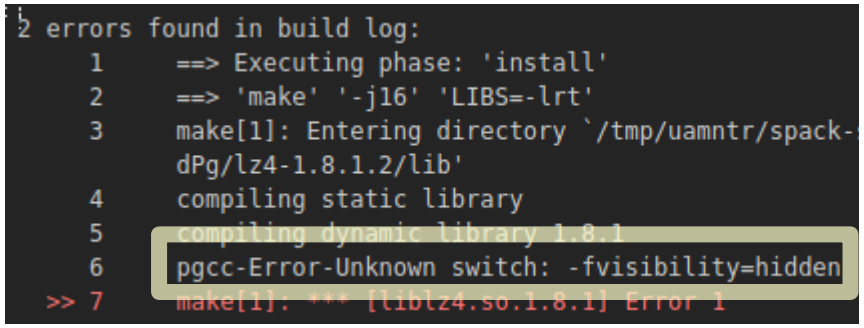
***not including staff-only research clusters or NCRC machines and older versions of software previously deployed.

Customized Modulefile deployment

- Must manually generate TCL modulefiles on Cray; painful.
- Use spack-generated LMOD modulefiles on Summit, new machines; fantastic.
- Users prefer minimal, hash-less modulefile names:
  - Carefully check builds in staging area, set defaults, specs, and suffixes to prevent collisions.
  - Expose only modules for explicitly installed specs with custom modulefile class and post-install hooks.
  - LMOD makes this easier, but future may be to expose all builds with alternative unique suffixes (serial id, install datetime,)?
- Spack binary not exposed to users for modulefile management.
  - Longtime users not interested in learning new interface to module system.

We’d like to see (and contribute to) continued improvements

- Play nicer with CrayPE
  (or rather, CrayPE play nicer with all other build systems…)
- Finer grained constraints on spec at site config scope
  - Express packages as unbuildable on per-compiler basis until all packages have such constrainsts added to them
  - Concretize mixed toolchain common link- vs. build-dependencies separately.
  - Use acceptable compiler for build-time dependencies even with different toolchain.
  - Package variant and version defaults on per-compiler basis



- Nightly build testing for major packages on HPC resources (ECP project)
- Deploy modulefile tree to multiple roots for same type of modulefile
- Mark package as explicit or implicit build prior to DB commit (useful in hooks)

  Spack Chains to allow users to build off of what we provide (licensed, tuned dependencies such as MPI).
- Support for toolchains as providers (eg, BLAS shipped with PGI).