

Spack in Shared Environment

2018 Scalable Tools Workshop

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The Program Runtime Env. Team

We support:

- 4 Compilers (GCC, Intel, PGI, cray)
- 4 MPI libraries (openmpi, mvapich2, intel-mpi, cray-mpich)
- ~64 packages total in production
- Continuous release schedule
- Package Life = System Life

No root access

Multiple Customers, Shared Environment





About our Environment

- > 12 systems
- 25000 Compute Nodes
- 3 OS's
- 5 Interconnects
- Many CPU architectures
- GPU clusters
- Lmod and Env Mod module systems



It's all under control

- Solid, readable build scripts for everything
- Smart modules
 - Hide and manage the dep chain automatically, even under Env. Mod
- Shared builds (when it's easy)





What Do We Lack?

- No automated inventory
- Each project is an island.
- Many (mostly) identical builds
- No definition of what 'should be'





What Should be in our Environment?

Environment Definition

Build System

Programming Environment Q3 2018





Spack Package Manager

- Automated building
 - Multiple configurations of the same thing
- Dependency management
- Module management/auto-generation
- Comes with a large library of packages.







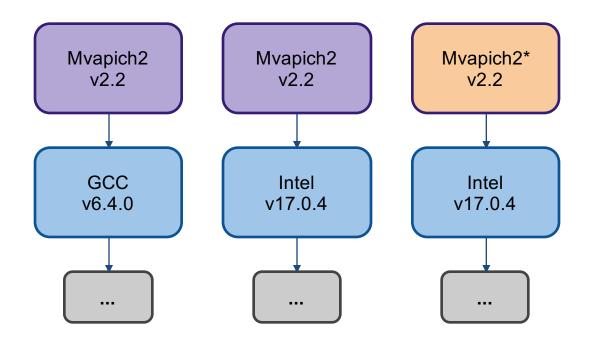
Does Spack Actually Help?

- Automated inventory Awareness
- Each project is an island Uniformity
- ✓ Many (mostly) identical builds
- X No definition of what 'should be'
- → Efficiency
- ___





The Problem with Spack...





Non-Conflicting Environments?

It's Multiplicative:

- 12 systems
- * 3 compilers
- * 3 MPI's
- * (assorted versions)
- * (other oddities)
- = Just too much





Spack, as the Foundation

Spack is good at what it does.

Build everything else around it.







Wrapping Spack, Requirements

- Per (Environment Version) environment definitions
- Automated building of each environment
 - Host awareness
 - Scheduler awareness
- Separation of User Modules from Spack Modules





Spack Environment Wrapper

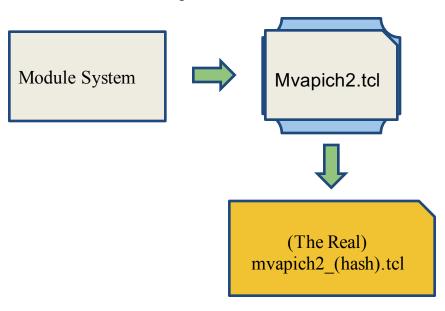
Environment Spack Wrapper Definition Programming Spack Environment (shared) Q3 2018





Module Separation

bash \$ module load myapich2





- Which environment?
- What dependencies?
- Dependency defaults?
- Module default?

Spack Wrapper





Famous Last Words

This should be easy!





Questions

