HPS

artur.wachtel@gwdg.de

Artur Wachtel

Provisioning of an Environment for Parallel Computing

How to manage conflicting requirements from users

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Learning Objectives

- What are environment modules
- Manage software with Spack
- Set up Lmod and Spack
- Install software and provide module files

Conflicts of interest

Having many users can raise conflicts:

- Among the users
  - Software versions
  - Configurations
- For the admins
  - Manual software compilation
  - Maintenance of multiple versions

Environment Modules with Lmod

Dynamically modify environment of the user via commands!

- User A
  - $ module load python/3.6
- User B
  - $ module load python/3.8
- Catalogue of available software
  - $ module avail python
  - $ module spider gromacs

Lmod module files

tar.lua

```
-- -*- lua -*-
whatis([[Name : tar]])
whatis([[Version : 1.34]])
whatis([[Target : x86_64_v3]])
whatis([[Short description : GNU Tar provides the ability to create tar archives, as well as various other kinds of manipulat
whatis([[Configure options : --with-libiconv-prefix=/opt/sw/spack/linux-centos8-x86_64_v3/gcc-8.5.0/libiconv-1.16-muqy73jovyw

help([[GNU Tar provides the ability to create tar archives, as well as various
other kinds of manipulation.]])


depends_on("bzip2/1.0.8")
depends_on("libiconv/1.16")
depends_on("pigz/2.7")
depends_on("xz/5.2.7")
depends_on("zstd/1.5.2")

prepend_path("PATH", "/opt/sw/spack/linux-centos8-x86_64_v3/gcc-8.5.0/tar-1.34-k4iylbi6ss4ic6jhrrh2gxcnnwfl5qwg/bin", ":")
prepend_path("MANPATH", "/opt/sw/spack/linux-centos8-x86_64_v3/gcc-8.5.0/tar-1.34-k4iylbi6ss4ic6jhrrh2gxcnnwfl5qwg/share/man"
prepend_path("CMAKE_PREFIX_PATH", "/opt/sw/spack/linux-centos8-x86_64_v3/gcc-8.5.0/tar-1.34-k4iylbi6ss4ic6jhrrh2gxcnnwfl5qwg/
```

What is Spack

- Package manager designed for HPC
- Compiles and installs software
  - Multiple versions and configurations
  - Manages build-time and run-time dependencies
  - Utilizes different compiler sets as needed
- Automatically generates module files

How to use Spack

Spack is written in Python so requires no installation.
Sourcing the setup script provides shell integration.

- `source spack/setup-env.sh`
- `spack list <search_term>`
- `spack info <name>`
- `spack spec <SPEC>`
- `spack install <SPEC>`

Spack's SPEC format

- `name`
- `name@version`
- `name@version %compiler@compilerver`
- `name@version +option1 ~option2 key=value1,value2`
- `name@version ^dependency@dependencyver`

Spack's SPEC format

- `openmpi`
- `openmpi@4.1.4`
- `openmpi@4.1.4 %gcc@12.2.0`
- `gcc@12.2.0 +strip ~bootstrap languages=c,c++,fortran,go,objc`
- `gromacs@2022.3 ^openmpi@4.1.4`

Exercise

- Install Lmod
- Install Spack
- Use spack to install software and provide module files