DS 7347 High-Performance Computing (HPC) and Data Science Session 4

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Research and Data Sciences Services Office of Information Technology Center for Research Computing Southern Methodist University

Outline



Session Question

Introduction to UNIX and Shell Scripting

Application and Package Management

Lmod

Spack

Readings and Assignments

Session Question

Session Question



Question

Why are there so many package managers?

Sub-Question

Why are there so many UNIX(-like) variants?

Sub-Sub-Question

Why are there so many Linux distributions?

Introduction to UNIX and Shell

Scripting

Introduction to Unix



Introduction to UNIX

Introduction to Scripting with Bash



Introduction to Scripting with Bash

Management

Application and Package

Lmod Environment Module System



Lmod

Spack



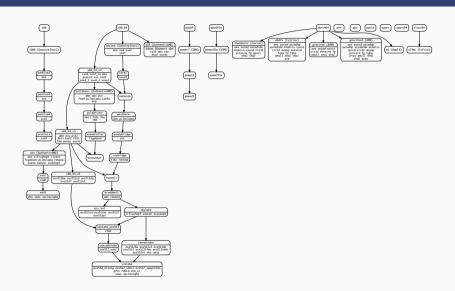
Spack

Bootstrap



```
#!/usr/bin/env bash
cd $WORK
git clone -c feature.manyFiles=true https://github.com/spack/spack.git
# Do for each new shell or add to shell configuration
module purge
module load gcc-9.2 python-3.8.6-gcc-9.2.0-6pic63r
export SPACK_PYTHON=$(which python3)
source $WORK/spack/share/spack/setup-env.sh
# End do
spack compiler find
spack compilers
```





Spack Environments



```
spack:
      config:
        install missing compilers: true
      view: true
      definitions:
      - compilers: [gcc@10.3.0, gcc@11.2.0]
      - packages: [openblas threads=openmp, python@3.8.12, py-numpy+blas+lapack]
      - targets: [target=broadwell. target=zen2. target=x86 64 v3]
      specs:
9
10
      - matrix:
        - [$%compilers]
11
        - [$packages]
12
        - [$targets]
13
14
```

Readings and Assignments

Readings and Assignments



Readings

- Introduction to Writing Module Files
- Spack Basic Usage

Readings and Assignments



Lab

- · Setup Spack installation in **\$WORK**.
- Install a version of the GCC compiler toolchain.
- Install Python with Matplotlib and Pandas using a Spack environment file, i.e. spack.yaml.
- Detail reasons for specific choices in assignments/lab_01.md and notes during peer review
- Commit assignments/lab_01.{yaml,md} to your class repo
- · Due 12:00 AM Central, Thursday, May 19, 2022