

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



Session Question

Introduction to UNIX and Shell Scripting

Application and Package Management

- Lmod

- Spack

Readings and Assignments

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 Scripting with Bash

Application and Package Management



Lmod



Spack



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





```
1  spack:
2    config:
3      install_missing_compilers: true
4    view: true
5    definitions:
6      - compilers: [gcc@10.3.0, gcc@11.2.0]
7      - packages: [openblas threads=openmp, python@3.8.12, py-numpy+blas+lapack]
8      - targets: [target=broadwell, target=zen2, target=x86_64_v3]
9    specs:
10      - matrix:
11          - [%compilers]
12          - [%packages]
13          - [%targets]
```

Readings and Assignments



Readings

- Introduction to Writing Module Files
- Spack Basic Usage



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