UNIVERSITY OF Nebraska.

HOLLAND COMPUTING CENTER

High Performance Computing Core

Learning Objectives

Session 1 – Wednesday, October 21st

- Introduction to high performance computing

- What is a supercomputing cluster?

- Who is HCC and what services do we provide

- Using the SLURM job scheduler

  - Interactive jobs

  - Submitting batch jobs

Session 2 – Thursday, October 22nd

- Data storage on Crane

- Transferring files to and from Crane

  - scp

  - Introduction to Globus

- Using Applications on Crane

  - module system

Running Applications

- All applications installed on HCC clusters are loaded in individual modules
- Modules dynamically change the user environment
  - $PATH
  - $LD_LIBRARY_PATH

- Hierarchical structure
  - If module A is dependent on module B, then module B must be loaded first to load module A

- Typically follows the naming convention <software>/<version>
  - Example: python/2.7

- Load using the `module` command

Lmod Commands

Command	What it does
`module avail`	Lists all modules available to be loaded
`module spider <name>`	Information about a specific module – can also be used to search
`module load <module_name>`	Load module(s) – can load a list of space delimitated modules
`module unload <module_name>`	Unload module(s) – can unload a list of space delimitated modules
`module purge`	Unloads all currently loaded modules
`module list`	Lists all currently loaded modules

For more information:

- `module --help`

- **Available software lists for each cluster:**
  - Crane: https://hcc.unl.edu/docs/applications/modules/available_software_for_crane/
  - Rhino: https://hcc.unl.edu/docs/applications/modules/available_software_for_rhino/

Exercises

1. Find a list of available modules.

2. Load one or more of the modules from the list you just found. Now unload them. Try doing it two different ways.

3. Lookup information about the QIIME2 module.

   - How many different versions are available? Load a specific version using `<module_name>/<version>`

4. Try loading the meme-suite/5.1 module. Did it work?

   - Now load these modules first

     - compiler/gcc/9.1   openmpi/4.0

   - Now try loading meme-suite/5.1 again. Does it work now? Why?

   - Unload all modules with only one command.

Once you have finished, please click "yes" in the Zoom participants panel.

If you have issues, please click "no" in the Zoom participants panel.

What if I want to use something else?

- Users are allowed (and encouraged) to install their own software by:

  - [Compiling from source](#)

  - [Creating Anaconda environments](#)

  - [Using and creating Docker and Singularity Images](#)

- Or we can install it for you:

  - https://hcc.unl.edu/software-installation-request

Exercises

1. Navigate into the matlab directory of the job-examples directory and locate the serial.slurm file

    - This submit file runs a MATLAB script which inverts a 10,000 x 10,000 randomly generated matrix and outputs the length of time it took to perform the inversion.

    - Look at the contents of serial.slurm - How many nodes this will run on? How many cores? How much memory and time is requested?

    - Submit the serial.slurm job. Check the output to see how long it took to invert the matrix.

2. Copy the serial.slurm file to a new file using the `cp` command.

    - Edit the serial.slurm file to use 4 cores.

        - If you need help, look at the parallel.submit file which is already configured to run on 4 cores

    - Submit the job again and compare the time to your initial run. How much faster or slower is it?

    - Compare times with your neighbor. Did you see the same amount of improvement?

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