Lecture 5 - Introduction to ISAAC

DSE 512

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2022-02-08

From Last Time

- No announcements
- Questions about Docker? EC2?
- Questions about anything else?
- *What scientists must know about hardware to write fast code*
  https://biojulia.net/post/hardware/

Using ISAAC

What is ISAAC

- **I**nfrastructure for **S**cientific **A**pplications and **A**dvanced **C**omputing
- Campus cluster
- Heterogeneous
- System overview https://oit.utk.edu/hpsc/isaac-open-enclave-new-kpb/system-overview-cluster-at-kpb/

Where to get help

- Read the documentation! https://oit.utk.edu/hpsc/isaac-open-enclave-new-kpb/
- Ask question in class
- ISAAC Office Hours TRF 11:00am-11:59am https://oit.utk.edu/hpsc/
- Email and/or schedule office hours with instructor

ISAAC vs EC2

Similarities

- Hardware is entirely managed
- "Someone else's computer"

Differences

- Software environment is *largely managed*
- No administrative privileges
- No Docker

Logging in with ssh

- ~~ISAAC acf-login.acf.tennessee.edu~~
- ISAAC-NG login.isaac.tennessee.edu
- Credentialing:
  - Username is netid
  - Enter netid password when asked
  - Use 2-factor method specified

Logging in with ssh

```
$ ssh username@login.isaac.tennessee.edu
```

```
$ ssh mschmid3@login.isaac.tennessee.edu
```

ssh config

Add a similar line to `~/.ssh/config`

```
Host isaac
HostName login.isaac.tennessee.edu
User mschmid3
ServerAliveInterval 30
Port 22
```

```
$ ssh isaac
```

Node Tiering

- Login nodes
  - Where you land after logging in
  - *Not where jobs should run*
  - Shared resource
  - file editing, code compilation, job submission
- Compute nodes
  - You have to go out of your way to get here
  - *Where jobs should run*
  - Semi-isolated resource

Basic Slurm

Task	Command	Example
Submit job	`sbatch`	`sbatch myjob.slurm`
Run interactive job	`srun`	`srun ... --pty bash -i`
Show jobs	`squeue`	`squeue`
Show my jobs	`squeue`	`squeue --me`
Cancel job	`scancenl`	`scancel 123456`

- Course account
  - ACF-UTK0188
  - `/lustre/isaac/proj/UTK0188`
- Opportunistic account
  - ACF-UTK0011

Software

- No root
  - no `sudo apt install ...`
  - no Docker
- Instead
  - modules
  - building from source
  - pip/conda/...
  - singularity

Modules

Task	Command
Show available modules	`module avail`
Load module	`module load ${MODULE}`
Unload module	`module unload ${MODULE}`
Show loaded modules	`module list`
Module description	`module whatis ${MODULE}`
Search modules for string	`module apropos ${MY_STRING}`
Get help	`module help`

- Load with `module load Python`
- `pip`
- `conda` (`module load anaconda3`)

R on ISAAC

- /sw/isaac/applications/r_studio/4.0.4/singularity_r_studio/R.4.0.4.simg

```
RIMGPATH="/sw/isaac/applications/r_studio/4.0.4/singularity_r_studio/R.4.0.4.simg"
alias R="singularity exec ${RIMGPATH} R --no-save --quiet"
alias Rscript="singularity exec ${RIMGPATH} Rscript"

$ Rscript -e "1+1"
[1] 2
```

Job Files

```bash
#!/bin/bash
#SBATCH --account UTK0188
#SBATCH --partition=campus
#SBATCH --job-name=R_hello_world
#SBATCH --nodes=1
#SBATCH --time=00:00:30

RIMGPATH="/sw/isaac/applications/r_studio/4.0.4/singularity_r_studio/R.4.0.4.simg"
singularity exec ${RIMGPATH} Rscript -e "print('hello world')"
```

```
sbatch myjob.slurm
```

Next Time

- Multi-node jobs
- Singularity
- Homework?

Live Demo