INTRO TO HIGH SECURITY HPC (RIO)

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High Performance Computing (HPC) at UVA

HPC computing systems tailored to data sensitivity

- Rivanna/Afton (Standard Security)
  - To process and store public data, internal use data, or sensitive data.
  - Highly Sensitive Data is not permissible
  - More information on the SSZ HPC can be found in our [Intro to HPC slides](#).

- Rio (High Security)
  - To process and store Highly Sensitive Data such as HIPAA, FERPA, dbGAP, etc.
  - **Not** CUI certified yet, use Ivy VM

For more information please see [RC Systems Data Sensitivity](#)

Highly Sensitive Data

Data that require restrictions on access under the law or that may be protected from release in accordance with applicable law or regulation.

Examples:

- Personally identifiable information (PII) is any information that can be used to identify a person. Examples include social security number, passport number, driver's license number, military identification number, or biometric records

- Health information that reveals an individual's health condition and/or medical history, including information defined by the Health Insurance Portability and Accountability Act (HIPAA)

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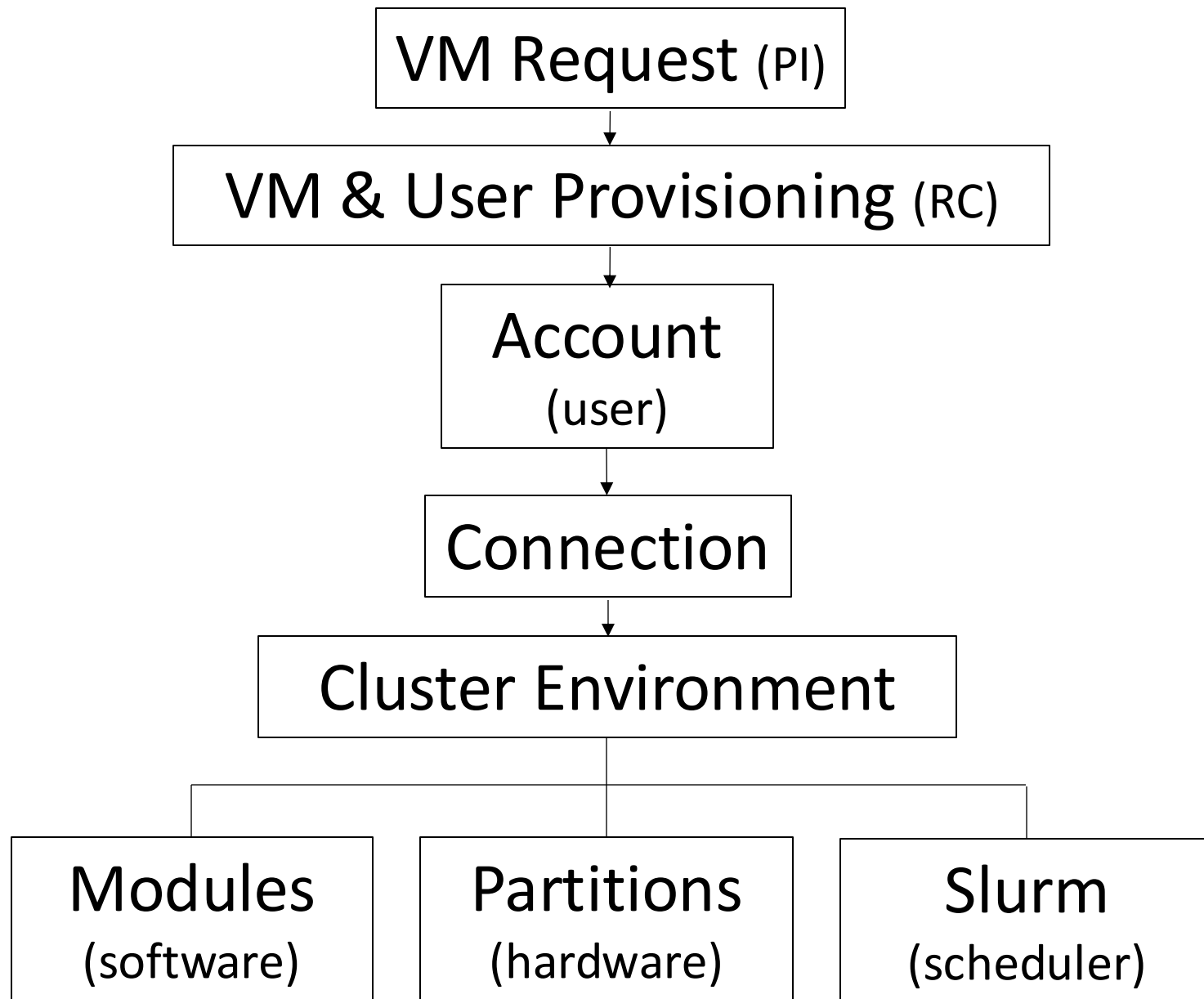
Ivy and Rio (Overview)

Ivy

- Secure computing environment, offering Virtual Machines (VM) with both Linux and Windows operating systems.

- Ivy VM is designed for interactive and small-scale analysis of highly sensitive data including HIPAA, FERPA, and CUI.

- Access to Ivy platform is project based. Each project gets a VM.

- Project-specific storage volumes are mounted to the VM and available on the HPC system enabling a seamless transition between tasks on VM and HPC environment.

- Ivy Linux VMs can serve as a frontend for accessing the Rio HPC system (available upon request).

Rio

- For large scale analysis of HIPAA, FERPA, and dbGaP data

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Terminology

- Node
  - Nodes are a type of computer called a server
  - They generally have more power than a typical computer.
  - They may have specialty hardware like graphical processing units
  - Two types of Nodes:
    - **Login node** - a server used for logging in and submitting jobs.
    - **Compute node** - a server that carries out the computational work.
- Core
  - An individual processor on a computer
- Memory
  - The random-access memory on a node
- Storage
  - Disk storage visible from a node

VM Request (PI)

VM & User Provisioning (RC)

Account
(user)

Connection

Cluster Environment

Modules
(software)

Partitions
(hardware)

Slurm
(scheduler)

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Requesting Access to HSZ HPC (Rio)

- Principal Investigators (PIs) can request access by submitting an Ivy Linux VM request through the [services app](#)

  - Research staff may apply for an exception.
  - Students must be sponsored by a faculty or research staff.
  - In addition to being a login node to Rio, a Linux VM can be used for preliminary computations as well
  - VMs comes in different sizes. Request a VM sized appropriately for your workflow. For larger groups or projects with computationally intensive tasks, choose a larger VM. We recommend Small and above.
  - VMs exist in a private, secure network and cannot reach outside resources on the Internet. Most inbound and outbound data transfer is managed through the Data Transfer Node (DTN).
  - More information on requesting a VM can be found [here](#) on our website.

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VM Provisioning

After access is requested, the Research Computing (RC) team will handle the provisioning of the Virtual Machine (VM).

The following steps are carried out by the RC team

- RC will create a Grouper group for Rio access

- RC will request access to the High Security VPN (HSVPN) on your group's behalf and provision 1 TB of High Security Research Standard storage for your project. This storage volume will also be available when using Rio HPC for your project.

- The PI and researchers will be notified upon the completion of the VM provisioning, and the associated IP address and group name will be provided to them.
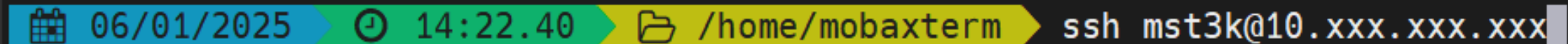
User Provisioning

- Any users of the VM must be added to the project in the <u>services app</u> by the PI

- Once a project is approved, a PI and her/his researchers must sign a RUDA (one for every researcher on each project).
  - Each researcher must also complete the <u>High Security Awareness Training (HSAT)</u>
  - This must be completed to permit each researcher access to the HSVPN filter

- More information on security training and HSVPN access can be found <u>here</u> on our website

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Connecting to the System

- Before connecting to your VM, you must install the following on your personal machine/device.
  - Install the Cisco AnyConnect Secure Mobility Client.
  - Install Opswat.
  - Install Duo MFA on personal smartphone.
  - See [here](#) for details.
- There are two ways to connect to your Linux VM:
  - Accessing the VM from a browser window
  - Using SSH (Secure Shell)
    - Use a terminal window with Mac/Linux
    - Windows users will need to install an SSH client application. We recommend [MobaXTerm](#).
  - In either case, you need the IP address of your VM along with your Netbadge credentials to connect to the VM.

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Accessing from SSH

- Start the HSVPN

- Open your SSH client and type: ssh mst3k@10.xxx.xxx.xxx, where mst3k is replaced with your user ID and the x's are replaced with your VM's IP address (given in the Services app).

```
📅 06/01/2025  🕐 14:22.40  📂 /home/mobaxterm  ssh mst3k@10.xxx.xxx.xxx
```

- When prompted for a password, use your EServices password.

This login method provides only command line access to the VM. No graphical user interfaces (GUIs) are usable.

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SSH Clients

- SSH clients mostly use instructions typed at the command prompt.

- You will need to become familiar with Linux/Unix commands.

  - See learning.rc.virginia.edu/tutorials/unix-tutorial/ to learn more

- Some useful Unix/Linux commands:

```
$ ls
$ pwd
$ cd folder_name
$ cp file_1 file_2
$ rm file_1
$ cd ..
```

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Accessing from a Browser

- Start the HSVPN

- Open a web browser and enter the IP address for your VM (e.g., https://10.xxx.xxx.xxx)
  - If you get a warning message, you may need to click on Advanced Settings and/or a Connect Anyway option, depending on your web browser.

- Upon login, you will see a selection of different graphical applications that you can use.
 - Jupyterhub
  - RStudio
  - FastX Desktop
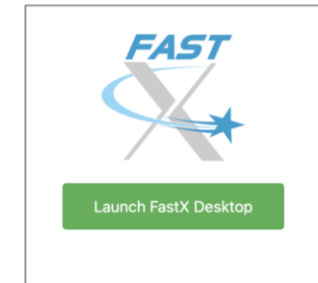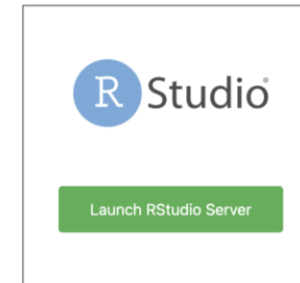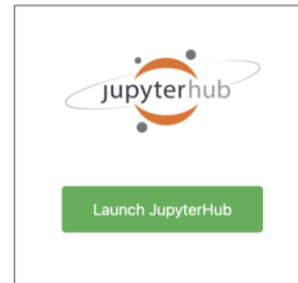
  - These applications run on the VM itself and do not use HPC resources.

Working with Files Using FastX

- FastX Desktop is a great tool for managing files and launching applications with a graphical user interface.

- Once signed-in, you can select either a "MATE" (GUI Linux Desktop) or "Terminal" session

- MATE sessions provide a terminal (black box in menu bar) and a file browser (white box) in menu bar. The CAJA file browser can help with management and navigation of the filesystem.

- More information on using FastX can be found on [our website](#) and in our [Intro to HPC slides](#).
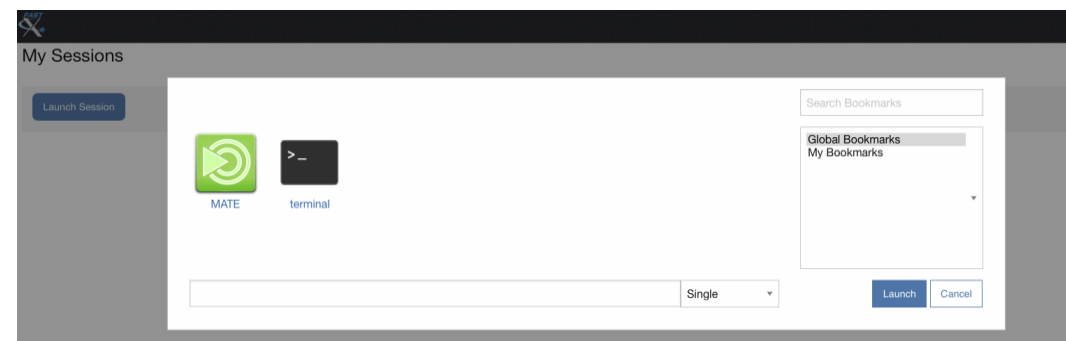
FastX Dashboard

MATE Desktop with CAJA file browser open (white box on menu bar)
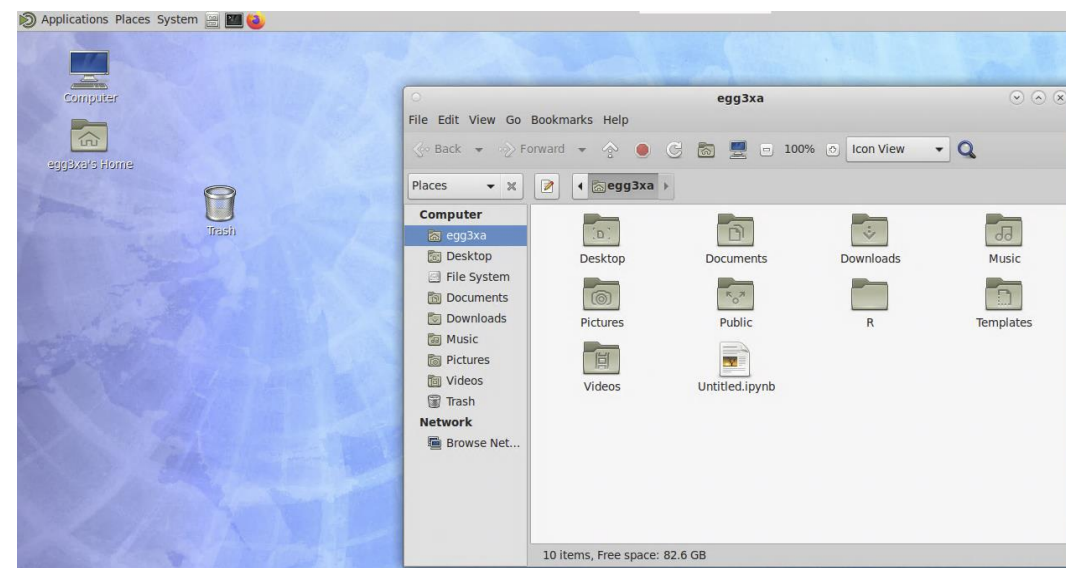
How to edit a file in Linux VM

Editors you can use:

- When in a Terminal Window, use vi/emacs/pluma.

    - vi/emacs uses all keyboard shortcuts and may take a while to learn.
    - pluma is a very basic editor. To launch, type: pluma myfile.txt

- In Desktop, you can use Pluma Text Editor.

Storing Data

- VMs do not come with any significant disk storage of their own.
- A PI specifies the storage space they would like to have when requesting access to Ivy.

  - Default of 1TB of Research Standard Storage
  - Mounted under *data/ivy-hip-name* where "ivy-hip-name" is replaced by the name of your ivy project's Grouper group name
  - Storage can be resized upon request. Submit your request [here](#)

- JupyterLab, RStudio, Rio, and FastX can all save data into the shared storage at *data/ivy-hip-name*.

Transferring Data

- Globus is the only permitted data-transfer protocol for highly sensitive data.
- **UVA IVY-DTN** is the the official collection for moving files into High-Security Research Standard Storage.

    - To transfer data to High-Security Research Standard Storage, please see the special instructions [here](#) on our website.
    - Ensure that you are **NOT** connected to the HSVPN. Data transfer will not work if you are connected to the HSVPN.

- Additional instructions and information on using Globus can be found [here](#) on our learning site.

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Preinstalled Software

- Every VM comes with a base installation of software by default. See here for a list of preinstalled software and how to request new software installations.

  - Additional software packages are pre-approved and available for installation upon request.
  - Software not already approved will need to undergo a security evaluation to determine if it is suitable for a High Security environment.
  - Python and R packages are available to users through the normal pip, conda, and CRAN library installation methods.

- Access to installed software is done using the **lmod** Module System.

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Modules

- Any application software that you want to use will need to be loaded with the **`module load`** command.

- For example:
    - module load apptainer/1.3.1

- You will need to load the module any time that you create a new shell
    - Every time that you log out and back in
    - Every time that you run a batch job on a compute node

Modules Basics

Some basic commands to use lmod:

- `module avail` – lists every module avaiable to load

- `module key <keyword>` - searches for modules in a category specified
    - Example: `module key bio`

- `module spider <module-name>` - prints information about the software including different offered versions

- `module load <module-name>` - load the desired software
    - Use `module load <module-name/ver-number>` to load a specific version

- `module unload <module-name>` – unloads the desired software

- `module list` – prints all currently loaded modules

- `module purge` – unloads all modules

Partitions (Queues)

- Rio has several partitions (or queues) for job submissions.

  - You will need to specify a partition when you submit a job.

  - To see the partitions that are available to you, type `qlist` at the command-line prompt.

```
Queue           Total   Free    Jobs    Jobs    Time
(partition)     Cores   Cores   Running Pending Limit
==================================================================
neo             960     836     0       0       7-00:00:00
neo-gpu         104     104     0       0       7-00:00:00
standard        1520    1200    0       0       7-00:00:00
gpu             96      96      0       0       3-00:00:00
```

  - The neo partitions are exclusive to a specific group and are not for general users of Rio.

Slurm

- Slurm manages the hardware resources on the cluster (e.g. compute nodes/cpu cores, compute memory, etc.).

- Slurm allows you to request resources within the cluster to run your code.
  - It is used for submitting jobs to compute nodes from an access point (Ivy VM).
  - Frontends are intended for editing, compiling, and very short test runs.
  - Production jobs go to the compute nodes through the resources manager.

- Slurm documentation:
  - https://www.rc.virginia.edu/userinfo/hpc/slurm/
  - https://slurm.schedmd.com/

Slurm Script Example

- A Slurm script is a bash script with Slurm directives (#SBATCH) and command-line instructions for running your program.

```
#!/bin/bash
#SBATCH --nodes=1                  #total number of nodes for the job
#SBATCH --ntasks-per-node=1        #how many copies of code to run
#SBATCH --time=1-12:00:00          #amount of time for the whole job
#SBATCH --partition=standard       #the queue/partition to run on
#SBATCH --account=myGroupName      #the account/allocation to use


module purge
module load goolf R    #load modules that my job needs
Rscript myProg.R                   #command-line execution of my job
```

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Submitting a Slurm Job

- To submit the Slurm command file to the queue, use the `sbatch` command at the command line prompt.
  - /home only exists on VM. Compute nodes do not have access to /home.
  - Job submission needs to be done from /standard/storage/
  - Recommended to include the complete file paths in the script
- For example, if the script on the previous slide is in a file named job_script.slurm, we can submit it as follows:

```
[jus2yw@ivy-tst-rc-1 ivy-tst-rc]$ sbatch job_script.slurm
Submitted batch job 18316
```

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Submitting an Interactive Slurm Job

- To submit an interactive SLURM job to the queue, use the **`ijob`** command at the command line prompt.

- For example, if you want to run an interactive application on a compute node in the standard queue using one cpu, we can submit it as follows:

```
-bash-4.1$ ijob -c 1 -p standard -A MyGroupName -t 06:00:00
salloc: Pending job allocation 21640112
salloc: job 21640112 queued and waiting for resources
salloc: job 21640112 has been allocated resources
salloc: Granted job allocation 21640112
srun: Step created for job 21640112
udc-aw34-21c0-teh1m$
```

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Checking Job Status

- To display the status of only your *active* jobs, type: `squeue -u <your_user_id>`

- The squeue command will show pending jobs and running jobs, but not failed, canceled or completed job.

```
-bash-4.2$ squeue -u mst3k

JOBID     PARTITION     NAME      USER    ST    TIME    NODES   NODELIST(REASON)
18316     standard      job_sci   mst3k   R     1:45    1       udc-aw38-34-l
```

- A job's status is indicated by:
  - PD – pending, R – running, CG – exiting

Checking Job Status

- To display the status of all jobs, type: `sacct –S <start_date>`

```
[jus2yw@ivy-tst-rc-1 ivy-tst-rc]$ sacct –S 2025-01-01
JobID              JobName       Partition     Account        AllocCPUS     State        ExitCode
-----------        ---------     ---------     ---------      ---------    ---------     --------
3104009            RAxML_NoC+    standard      hpc_build         20        COMPLETED        0:0
3104009.bat+        batch                      hpc_build         20        COMPLETED        0:0
3104009.0          raxmlHPC-+                  hpc_build         20        COMPLETED        0:0
3108537            sys/dashb+         gpu      hpc_build          1        CANCELLED+       0:0
3108537.bat+        batch                      hpc_build          1        CANCELLED       0:15
3108562            sys/dashb+         gpu      hpc_build          1          TIMEOUT        0:0
3108562.bat+        batch                      hpc_build          1        CANCELLED       0:15
3109392            sys/dashb+         gpu      hpc_build          1          TIMEOUT        0:0
3109392.bat+        batch                      hpc_build          1        CANCELLED       0:15
3112064             srun              gpu      hpc_build          1          FAILED         1:0
3112064.0           bash                       hpc_build          1          FAILED         1:0
```

- The sacct command lists all jobs (pending, running, completed, canceled, failed, etc.) since the specified date.

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Canceling a Job

- To delete a job from the queue, use the **scancel** command with the job ID number at the command line prompt:

```
-bash-4.2$ scancel 18316
```

- To cancel all your jobs, run this command:

```
-bash-4.2$ scancel -u $USER
```

- We use scontrol to print information of a running job
  - scontrol show job <jobid>

More Commands

- `sacct` will return accounting information about your job. See [Slurm's docuementation](#) for a full list of options.
  - Use the option `-j <jobid>` to inspect a particular job
- `seff` will return information about the utilization (called the "efficiency") of core and memory.

NEED HELP?

Research Computing Zoom Office Hours

Tuesdays: 3 pm – 5 pm
Thursdays: 10 am – noon

To connect to the Zoom sessions, go to https://www.rc.virginia.edu/support/#office-hours and click on the "Join us via Zoom" button

Or, contact us through the forms at:
https://www.rc.virginia.edu/support/

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