Summary of the tutorial

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Dalla (NYU Abu Dhabi) Group

- Transferri ng data to/from the clusters
- Transferri ng data to/from the clusters using Globus
- Submitting jobs with slbatch
- Building software on the HPC Cluster
- Available software
- Licensed software
- Available software

- Programming for Biologists
- Tutorials
- FAQs
- Cleanup Program

Scratch Areas
# Running jobs on the Prince Cluster

## Accessing the Prince Cluster

- From Windows workstation
- From Mac workstation

## Software and Environment Module

## Job script and resource request

- Introduction to job scheduling
- Submitting jobs with `sbatch`
- Requesting resources
Using computing nodes interactively

Monitoring batch jobs

Monitoring batch jobs - squeue

What is running and where? slurmtop

Canceling your jobs

Compiling your own software

Putting all pieces together

An Amber example

A R example

Summary

- You can compile, edit scripts and view results on the login nodes, but **computational work should be run on the compute nodes**
- You can access compute nodes with `srun`
  - Either via a job script, or interactively
  - Compute nodes are allocated to jobs by the scheduler, so your job might not start immediately
  - Jobs must request resources, but mostly need not specify a queue.
  - Requesting just slightly more than when you expect to need is generally the best practice
- **Short jobs get higher priority, and short or small jobs are easier to schedule quickly**
- You can monitor your job's progress with `squeue`, `sstat`, `sacct`, `scontrol` or `slurmtop`
- Software is managed by Environment Modules
  - Use `module avail` to find software packages
  - And `module load` to load them into your environment
    - including within job scripts!
  - Use `module purge` to return to a clean environment before loading a new set of modules
  - Other useful commands are 'module list' and 'module show'