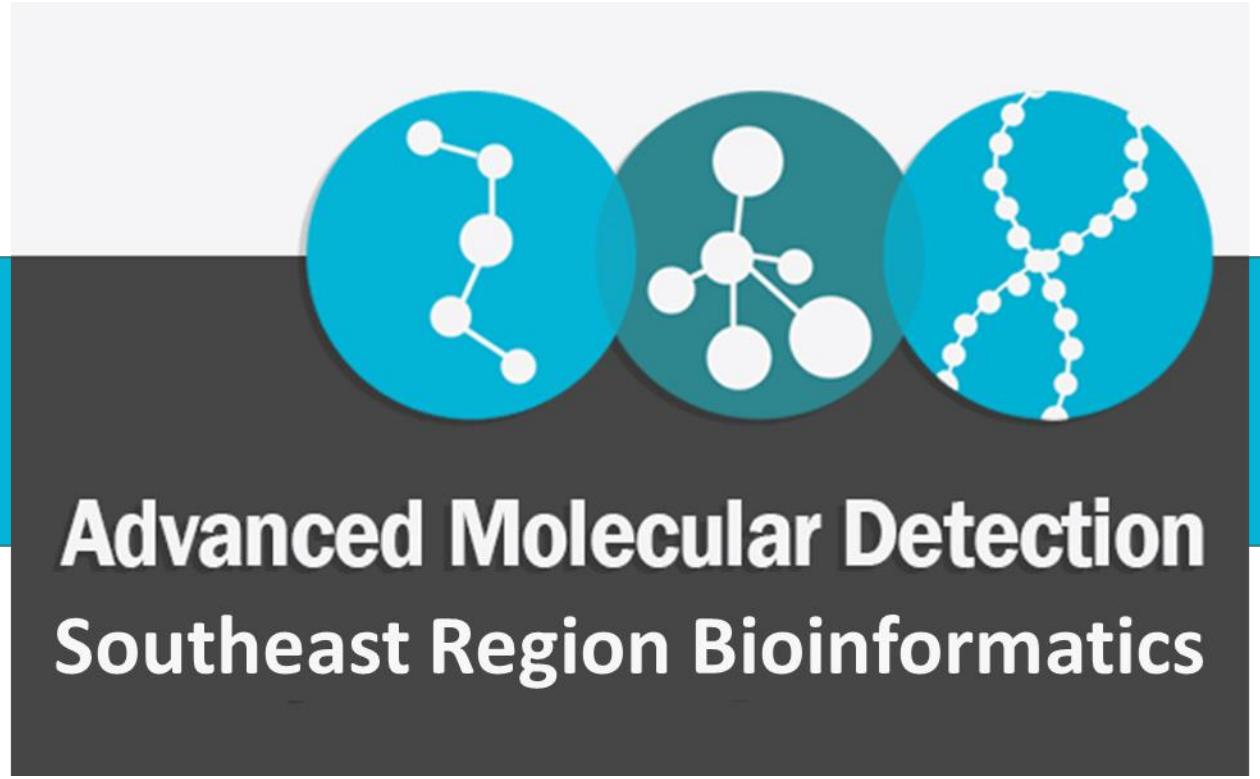


**High Performance Computing & HiPerGator**

12/8/2022

# Outline

High Performance Computing

HPC Architecture

HiPerGator Storage

Job scheduling via Slurm

# Introduction – High Performance Computing (HPC)

- Technology that harnesses the power of **supercomputers** or computer clusters to solve complex problems requiring massive computation.
- Also, the practice of aggregating computing power in a way that delivers much **higher horsepower** than traditional computers and servers.
- HPC lets users process large amounts of **data** quicker than a standard computer.
- Solutions delivered by HPC can be one million times more **powerful** than the fastest laptop.
- HPC allows enterprises to run large **analytical computations**, that includes millions of scenarios that use up to terabytes of data.

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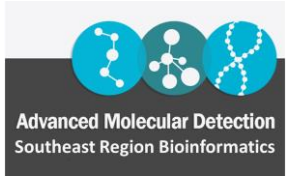
# Applications of HPC

- HPC helps in digitizing more complex processes like **genome sequencing** & **drug testing**.
- Human brain mapping, **3D mapping** of the brain including brain slices images through a modern microscope and allows analysis of compact cell patterns.
- Used in simulation of **chemical reactions**, in order to understand the disorders and to propose precise treatments.
- Used in simulation of **weather forecasting**, climate changes and earth resource evolution.
- Drug discovery and **protein docking**.
- For **driverless cars**, to analyze their position, road conditions, passenger safety and vehicle conditions.



# How does HPC work?

- HPC mostly is performed on **supercomputers** and they require processors to perform jobs at a faster pace compared to standard computer and run processors in parallel to obtain solutions in a shorter duration.
- HPC  jobs require **fast disks** and **high-speed memory** for executing jobs.
- HPCs are servers networked together and managed with a **scheduler**.
- Compared to standard computers, HPCs can perform **multiple jobs** at once within less time.
- Time required for the job execution depends on the **resources available** and the **design** used.
- **Job queue** is formed if there are more jobs than the processors.

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- HPC systems scaled

  vertically – for computing with powerful CPUs

  horizontally – by clusters
- Clusters consist of networked computers, which include scheduler, compute and storage capabilities.
- Clusters can accommodate multiple applications and resources for a user group.
- Clusters work in binding computational power of computer nodes to offer increased computational power.
- **1 HPC cluster – as large as 100 thousand or more compute cores.**
- HPC clusters offer parallel computing by providing a solution to a problem with more processing power.

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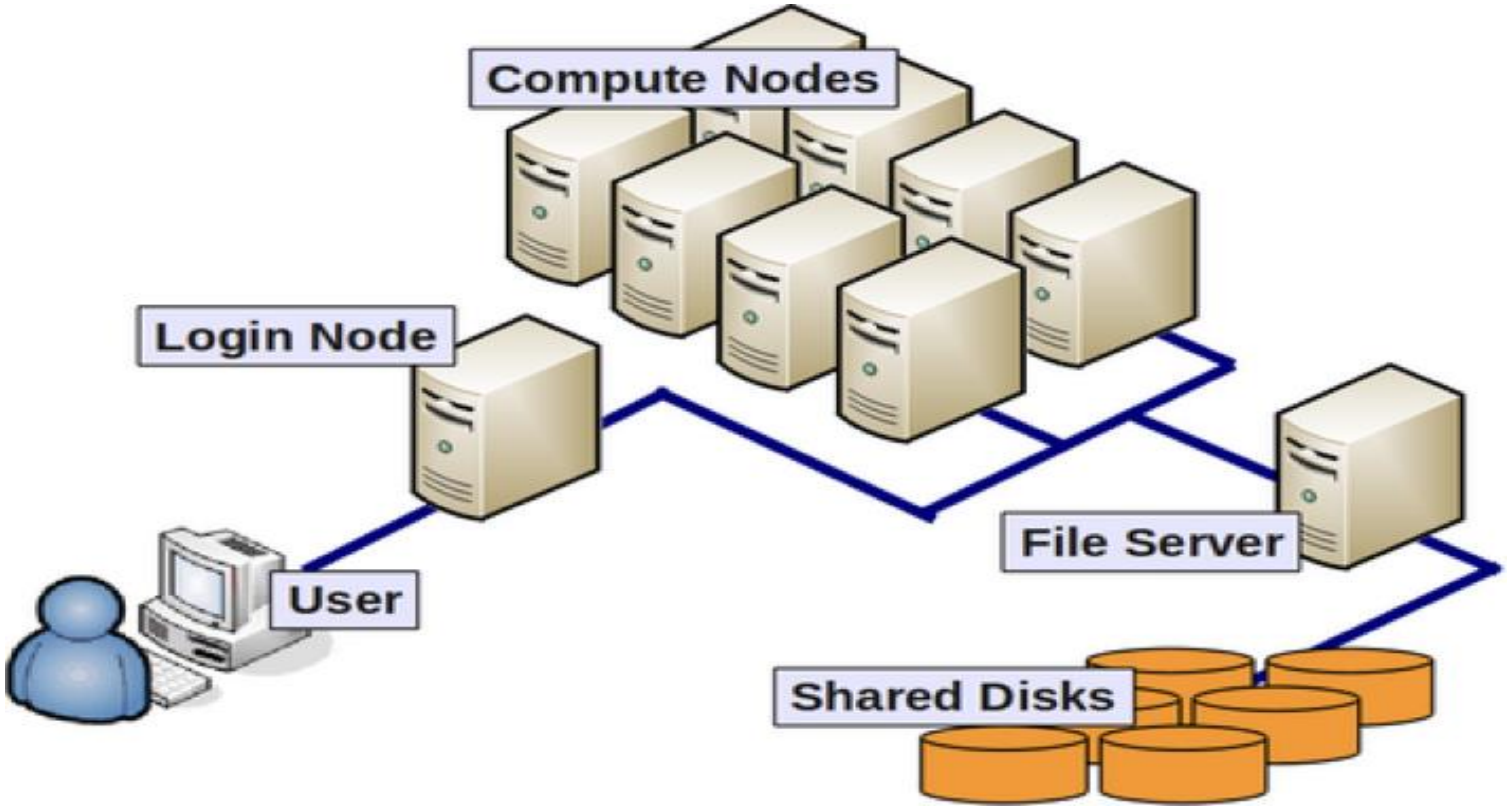
# HPC architecture




high performance computing nodes - Bing images

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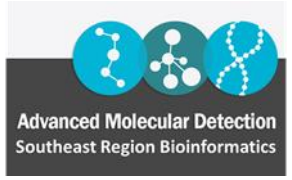
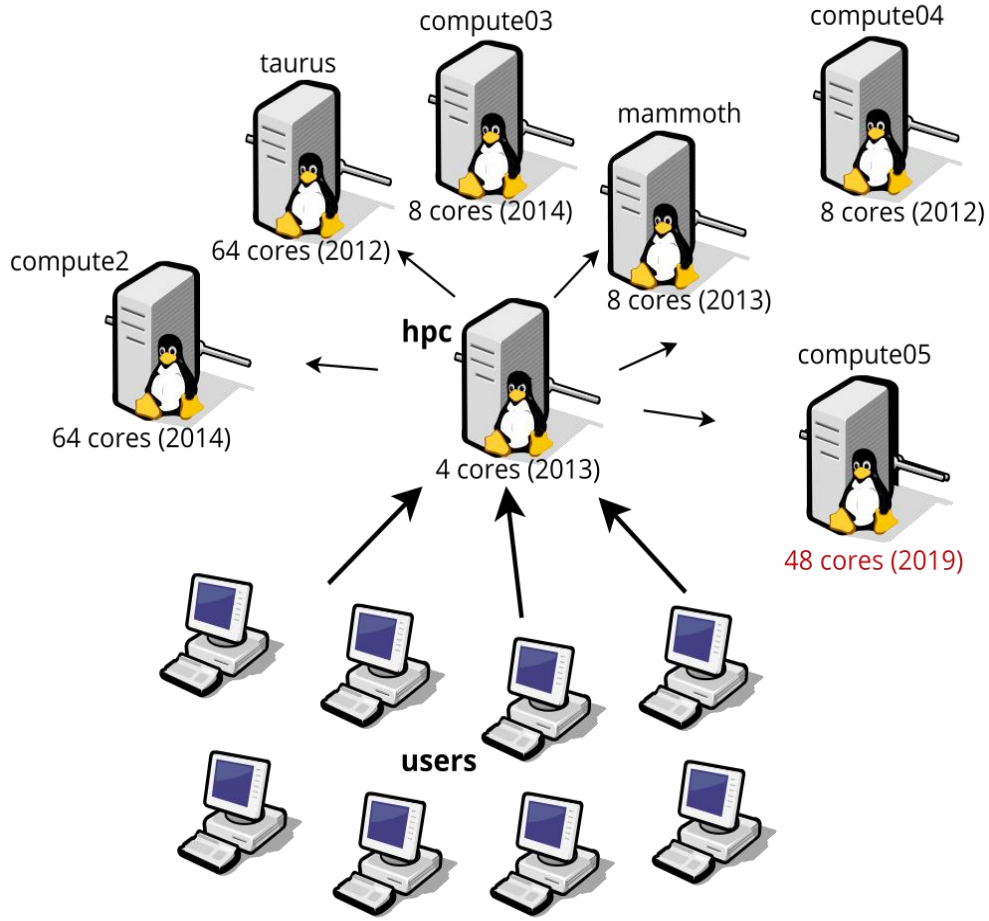
# HPC Cluster Architecture

- **Cluster** – group of computers networked together.
- **Nodes** – individual computers in HPC system, each node has certain memory and access to the storage.
- HPC clusters has small servers that are connected to network switches, it has head node and many computational nodes.
- **Login node** – where you connect to cluster and submit jobs.
- **Head node** – holds responsibility of serving files to client nodes, in small clusters they have storages attached to them.
- **Administrative nodes** – manage the cluster scheduling and other admin tasks, users do not login to these.
- **Compute nodes** – computational tasks are carried out.



# HPC System Designs

- **Parallel computing**: involves hundreds of processors, with each processor running calculation payloads simultaneously.
- **Cluster computing**: type of parallel HPC system which consists collection of computers working together as an integrated resource, also includes scheduler, compute and storage capabilities.
- **Grid & Distributed computing**: helps connect the processing power of multiple computers within a network.



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# What is a job?

- A successful request sent via **srun** or **sbatch** to the scheduler creates a job, then this job is appended to the queue.
- Job is executed once the resources become available, followed by job transferring to the resources.
- Accessing HPC cluster resources requires requesting them from a scheduler, our scheduler is **slurm**, it might be different for different institutions.

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# What is a Slurm?

- **Slurm** – powerful job scheduler that enables optimal use of an HPC cluster of any size.
- Slurm works by taking certain information about the resource requirements of a calculations and send that calculation to run on a compute node that satisfy the criteria.
- Slurm ensures HPC cluster is used fairly among all users.
- 2 basic components of Slurm cluster are

  **master node** – provides a shared filesystem on which the Slurm software runs

  **execute node** – hosts that mount the shared filesystem and execute the jobs submitted.

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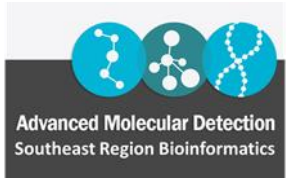
# HiPerGator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# HiPerGator

hipergator - Bing images

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- **HiPerGator** – State's most powerful supercomputer, unveiled by **University of Florida** on May 7, 2013, helps researchers in finding life-saving drugs, make decades-long weather forecasts and to improve armor for troops.
- University of Florida is first in nation to fully implement the **Internet2Innovation Platform**, allowing UF researchers to easily share enormous amounts of data at ultrahigh speeds in collaborations with scientists worldwide.
- **Internet2Innovation Platform** provides high-speed, friction free computing environment and requires participating universities to commit to three changes in research computing architecture:
  - 100 Gbps connection to Internet2
  - a science DMZ
  - use of software defined networking(SDN)

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# HiPerGator Evolution

| Phase | Year | Cores | RAM/core |
|---|---|---|---|
| HiPerGator 1.0 | 2013<br>Retired 2021 | 16,000 AMD Opteron 6378 Abu Dhabi<br>2.4 GHz Cores | 4GB |
| HiPerGator 2.0 | 2015 | 30,000 Intel Xeon E5-2698 v3 Haswell<br>3.2 GHz Cores | 4GB |
| HiPerGator 3.0 | Jan 2021 | 30,720 AMD EPYC 7702 Rome<br>2.0 GHz Cores | 8GB |
| HiPerGator 3.0 | Q2 2021 | 9,600 AMD EPYC 75F3 Milan<br>2.95 GHz Cores | 8GB |

HiPerGator 3.0 – Research Computing (ufl.edu)

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- **HiPerGator 3.0** has been growing nearly for a year with addition of GPUs, storage and new processors. As of 2021:
  - total of **66,000** cores
  - **544** NVIDIA GeForce RTX 2080TI GPUs
  - **48** NVIDIA Quadro RTX 6000 GPUs
- **HiPerGator 3.0 CPUs** – the system has number of machines with 4TB of memory for large jobs.
- **HiPerGator 3.0 GPUs** – As of 2019, it has 608 new GPUs in production which are installed in nodes from Exxact with 32 Intel xeon Gold 6242, 2.80 GHZ CPU cores and 192GB of ram in each node.
- **HiPerGator 3.0 storage** - blue storage is mainly used and the size is 4 PB

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# Storage on HiPerGator

- **Home storage**: /home/<user>
  - 40 GB limit
  - scripts, code, compiled applications
- **Blue storage**: /blue/<group>/<user>;
- **Orange storage**: /orange/<group>/; long term storage
- To check your storage, you can navigate to the command line and enter
  blue_quota
  orange_quota
- Orange and Blue storage quotas are at the group level and based on investment.
- Also, if you are having data that you are not actively using on HiPerGator, make sure you move the data to orange storage or to separate storage off HiPerGator.
- As every lab is different, make sure your laboratory has a long-term data storage plans like **cloud**, **server or hard drive backups** that follow your lab's data retention policies.

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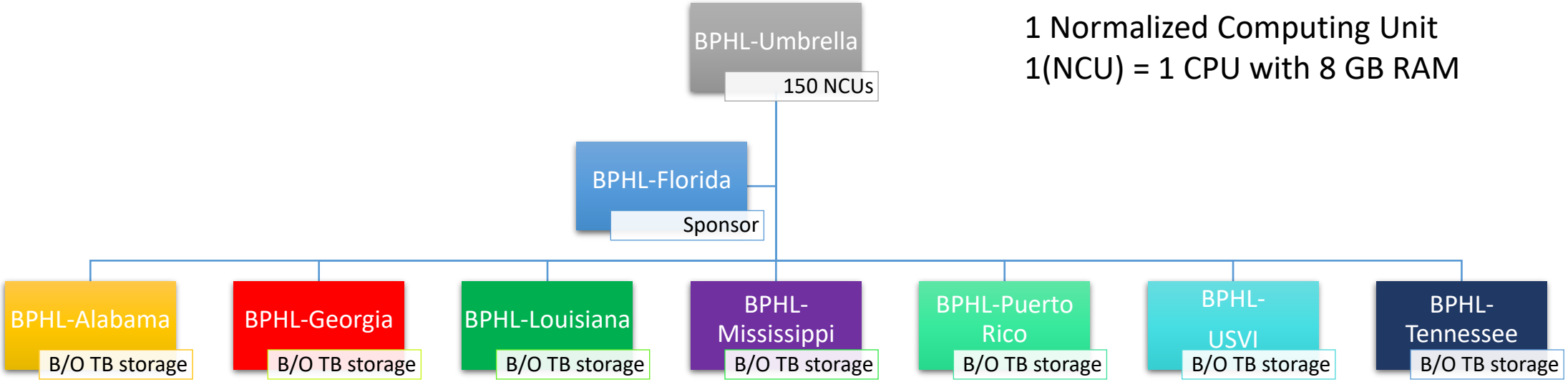
# HiPerGator State Groups




1 Normalized Computing Unit
1(NCU) = 1 CPU with 8 GB RAM

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# HiPerGator for Research Computing

- Introduced in the year **2011** for **research computing**.
- HiPerGator 3.0 is less expensive, **high-capacity** storage.
- Added 600+ GPUs
- Added  AMD EPYC Rome cores(30,720 cores) and Milan cores(9,600).
- Compute capacity is sold in **NCUs** which is **1 CPU core** and **7.8GB RAM**.
- **Storage**: Blue for high performance file system and orange for low performance file system; can be purchased in terabyte quantities.
- 1 GPU token will give access to any of the available GPUs.
- **Southeast Region jurisdictions receive computational resources for FREE (supported by BRR funding from CDC ELC)!!!**

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# How to Login & use HiPerGator?

- Work on HiPerGator is submitted to scheduler to run in the batch system when resources are available.
- How to access HiPerGator?
    - through **Linux** command line via **ssh** clients
    - through jupyter notebooks – **python, R**
    - through **galaxy** – web based bioinformatics platform
    - through open on demand – **jupyter, R studio**
- Talk with your IT department about applications that are already installed and/or can be installed. (Our tutorials are done using Putty).

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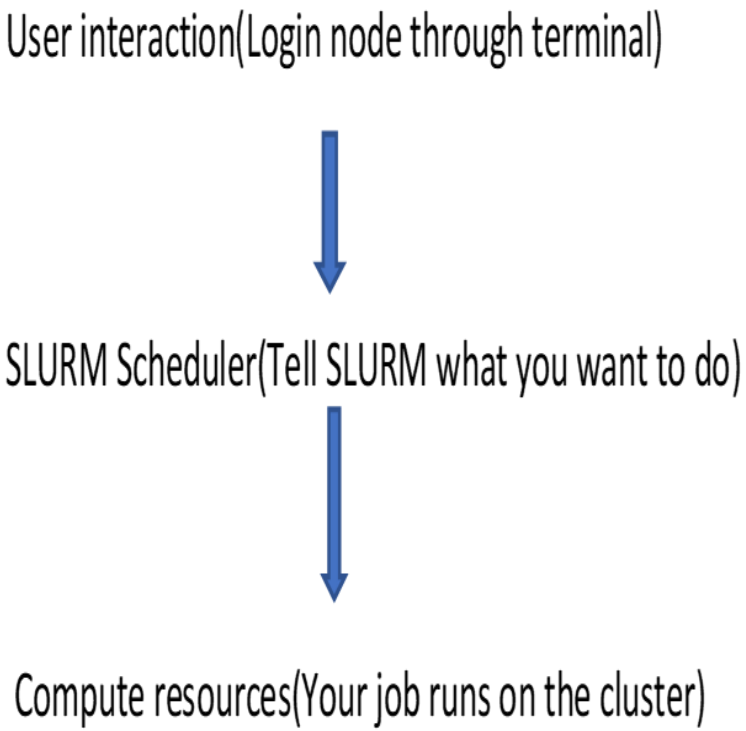
# Cluster Overview

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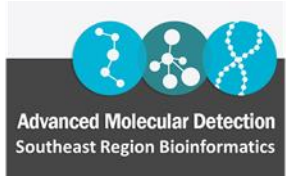
# Slurm Scheduler

- Software which manages all the different jobs making sure each job has the resources required for each group and each group having access to the resources.
- **Login nodes** are for file and job management, short-duration interactive testing and development.
- Limit your usage to no more than **16 cores**, **10 minutes**, **64GB** memory.
- If you need more time/cores/memory, then you need to use srun to start an interactive session on a compute node.



- SLURM scheduler – acts like a conveyer belt where

**all the jobs will run one by one**

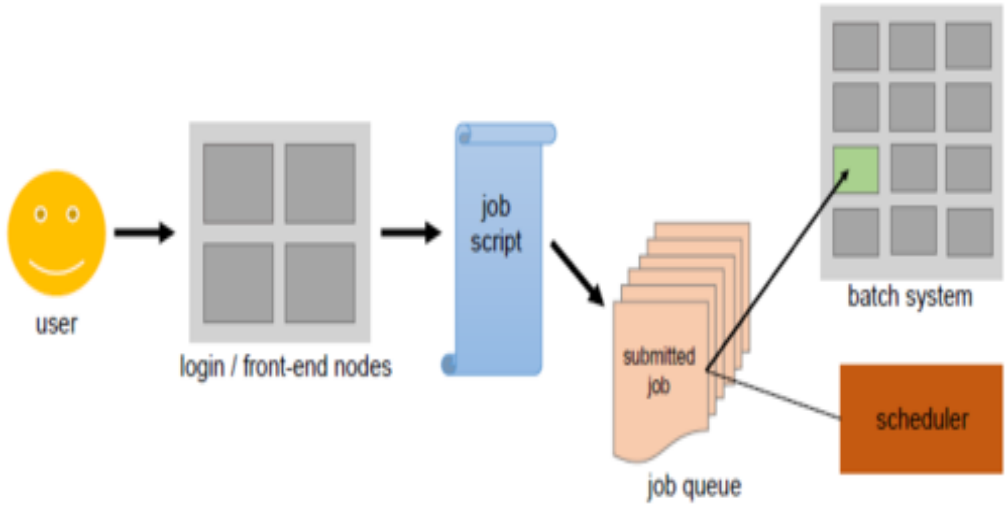
↓

**job will look for its bucket group once it takes it turn**

↓

**job will be finished**

- If there are many jobs related to a single group, then job will be **queued**.
- SLURM job script is a **bash script**.



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# Slurm requests

- **SLURM CPU requests**:

  # HiPerGator 2.0 compute servers : **32 cores – two 16 - core sockets**

  # HiPerGator 3.0 compute servers : **128 cores – two 64 – core sockets**

- **SLURM memory requests**:

  # --mem = **1GB**(total memory)

  # --mem – per – cpu =**1GB**(memory per core)

  - can use MB or GB

  - no decimal values: use 1500MB, not 1.5GB

  # HPG 2.0 = 120 GB RAM

  # HPG 3.0 = 1000 GB RAM

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# How to schedule a job?

- Resources needed for the job to run:
  - How many **CPU cores** you want and how you want them to be grouped?
  - How much **memory**(RAM) your job will use?
  - How **long** your job will run?
  - How many **GPUs**?
- Commands needed to run the job?
  - Account and qos group( i.e. **bphl-umbrella**)
  - Email notification for end of job or job failure
  - Job name and output log and error log names

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# HiPerGator

- For all the documentation and help regarding HiPerGator, go to UFRC (ufl.edu).
- For accessing new user training videos related to HiPerGator, storage and SLURM scheduler, go to Training Videos - UFRC (ufl.edu)
- If you are experiencing any problem with the HiPergator, please contact us. If we are not able to resolve the issue, we will ask you to submit a support request. This can be found here UFRC (ufl.edu). Go to help menu and click on “Submit Support Request”.
- HiPerGator login password needs to be reset every year and more information on this is located here Gatorlink Account Management - Forgot Password (ufl.edu) – Set a reminder in your calendar!

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# References


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2. How To Videos - UFRC (ufl.edu)
3. HiPerGator 3.0 – Research Computing (ufl.edu)
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6. What is HPC? Introduction to high-performance computing | IBM
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# Additional Reading

1. How Florida researchers are using UF's supercomputer - State University System of Florida (flbog.edu) about supercomputer
2. HiPerGator-RV - Research Computing - University of Florida (ufl.edu)
3. 07 Slurm Basics – Intro-to-HPC (thejacksonlaboratory.github.io) SLURM basics
4. UF offers powerful new NVIDIA supercomputer to students and researchers across State University System - News - University of Florida (ufl.edu) NVIDIA supercomputer

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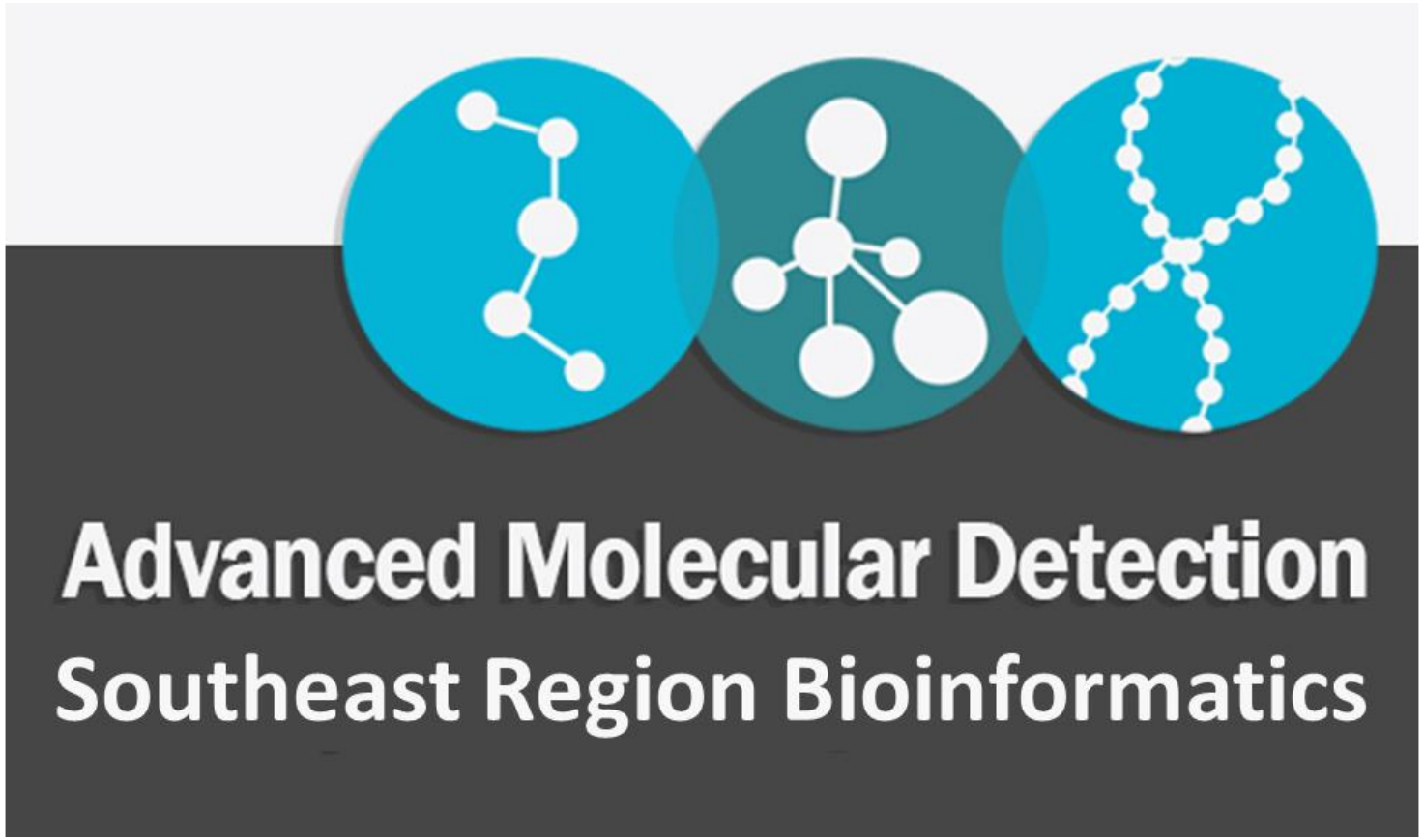


# Questions???

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