



Research Computing Orientation for Courses

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UF | Information Technology







HiPerGator AI

UNIVERSITY OF FLORIDA



Course use of **HiPerGator**

The University of Florida Supercomputer for Research

- **Course is allocated 32 cores, 256GB RAM, 2TB Blue storage, GPUs as needed**
 - Design projects with this in mind
 - Time your work with this in mind
 - Use resources efficiently
- **Support requests should go through course TA**
 - If TA cannot solve the issue, the TA should open support requests
- **By using your account, you agree to the AUP**
 - <http://www.rc.ufl.edu/about/policies/>
 - No restricted data



HiPerGator Account Training

- Content and links at: help.rc.ufl.edu/doc/New_user_training
 - Page also has additional information for classes at the end

Main page Discussion Read Edit View history More Search UFRC Go

UFRC Help and Documentation

Welcome to the University of Florida Research Computing Help and Documentation site. General information, announcements, and purchase request forms are on our main web site. The information here is focused on particular applications, services, and usage examples. Provide Feedback.



FOR NEW USERS

Guides to get you started with HPG and best practices!

Getting Started | Training Videos | Trainings & Events | Interactive Development and Testing | Practical Storage Use



ACCESS

How to connect to HPG with Duo, authenticate multiple connections, or check account.

Multi-Factor Authentication | SSH Multiplexing | SSH Keys | Blocked Accounts | Federated Access and Login



HELP

Resources to ask questions, get support, or communicate directly.



INTERFACES

Guides for GUI/web interfaces you can run on HPG.

Jupyter (Python, R) | Galaxy Genomics

<https://help.rc.ufl.edu/>



For users with an account

- If you already have a Research Computing account for research:
 - Make a folder for yourself at
`/blue/pre1234/<gatorlink>`
 - When submitting jobs, add:
`--account=pre1234 --qos=pre1234`

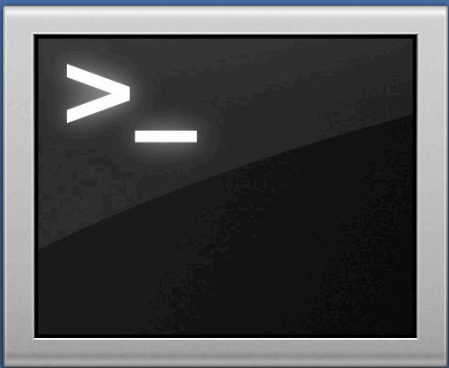


HiPerGator AI

UNIVERSITY OF FLORIDA

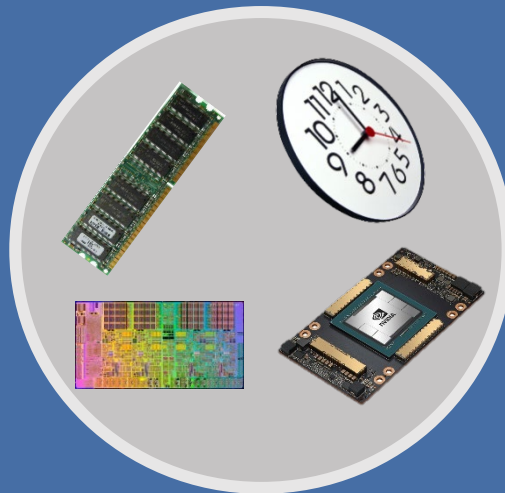
Cluster overview

User
interaction



Login node
(Head node)

SLURM
Scheduler



Tell SLURM what
you want to do

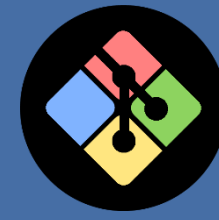
Compute
resources



Your job runs
on the cluster

Tools for working with HiPerGator

ssh client to connect to
hpg.rc.ufl.edu



e.g.: Terminal, Git Bash or Bitvise

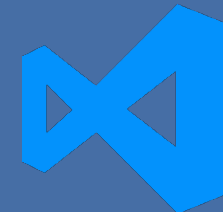
SFTP client to move files to/from
your computer
hpg.rc.ufl.edu



e.g.: Cyberduck, Bitvise, WinSCP

Text editor

Especially on Windows, be sure to convert DOS
line breaks to Unix, and *don't use Word*



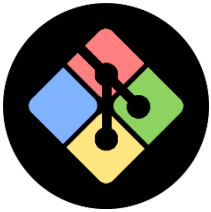
e.g.: VS Code



SSH Clients



Mac/Linux: Terminal



Windows: Git Bash,
MobaXterm, PuTTY, Bitvise

magitz@login1:~

```
$ ssh magitz@hpg.rc.ufl.edu
(magitz@hpg.rc.ufl.edu) Password:
(magitz@hpg.rc.ufl.edu) Duo two-factor login for magitz@ufl.edu
```

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-4066
2. Phone call to XXX-XXX-4066
3. Phone call to XXX-XXX-1960

Passcode or option (1-3): 1

Success. Logging you in...

Last login: Mon Nov 8 08:31:41 2021 from 10.138.154.11

Welcome to UF Research Computing

The user agrees to comply with Research Computing's policies.

<https://www.rc.ufl.edu/services/procedures/>

[Backup Policy](#)

`ssh user@hpg.rc.ufl.edu`

Bitvise



Profile: hpg.tlp

Save profile

Save profile as

Bitvise SSH Server Control Panel

New terminal console

Login Options Terminal RDP SFTP Services C2S S2C SSH Notes About

Server

Host hpg.rc.ufl.edu

Port 22 ☐ Enable obfuscation

Obfuscation keyword

Authentication

Username magitz

Initial method keyboard-interactive

Submethods bsdauth,pam,totp,pw,pk

Elevation Default

Kerberos

SPN

☐ GSS/Kerberos key exchange

☐ Request delegation

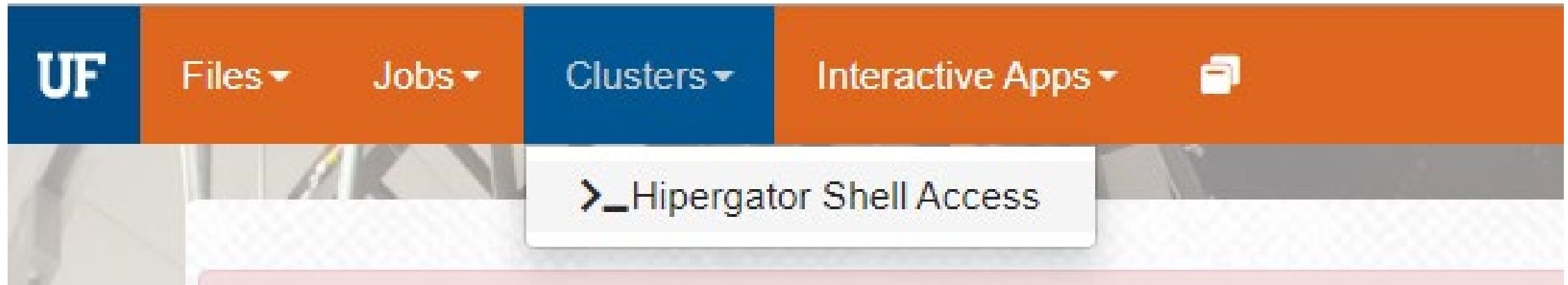
☒ gssapi-keyex authentication

[Proxy settings](#) [Host key manager](#) [Client key manager](#) [Help](#)

Initial method: keyboard-interactive

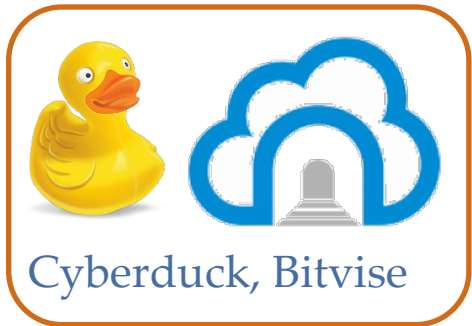


ood.rc.ufl.edu



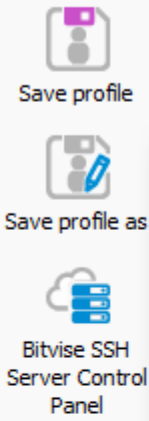


SFTP Client



hpg.tlp - magitz@hpg.rc.ufl.edu:22 - Bitrise SSH Client

Profile: hpg.tlp



Login Options Terminal RDP SFTP Services C2S S2C SSH Notes About

Server

Host hpg.rc.ufl.edu

Authentication

Username magitz

hpg.tlp - magitz@hpg.rc.ufl.edu:22 - Bitrise SFTP

Window Local Remote Upload queue Download queue Log

Browse Upload queue Download queue Log

Local files

Filter:

C:\Users\magitz\OneDrive - University

Name	Size	Type	Date Mod
.matplotlib	0	File folder	2/3/2021
Blackmagic Design	0	File folder	2/3/2021
cache	0	File folder	4/15/2021
CompToolsRes	0	File folder	2/3/2021
Custom Office Templates	0	File folder	2/3/2021
Downloads	0	File folder	2/3/2021
ml-training-site-master	0	File folder	2/3/2021
MobaXterm	0	File folder	2/3/2021
My Data Sources	0	File folder	2/3/2021
My Digital Editions	0	File folder	10/18/2021
OneNote Notebooks	0	File folder	2/3/2021
Outlook Files	0	File folder	2/3/2021
Personal	0	File folder	10/6/2021
R	0	File folder	2/3/2021
Downloads	0	File folder	2/3/2021

Remote files

Filter:

/home/magitz

Name	Size	Type	Date Mod
play	2,048	File folder	4/16/2021
playground	11,264	File folder	9/9/2021
playground.old	5,632	File folder	7/28/2021
python	512	File folder	4/6/2021
R	2,048	File folder	7/29/2021
ratfunc	1,536	File folder	7/3/2021
raxml-ng	6,144	File folder	9/25/2021
sasuser.v94	1,024	File folder	10/5/2021
scikit_learn_data	512	File folder	10/24/2021
scripts	4,608	File folder	4/19/2021
seaborn-data	0	File folder	5/11/2021
share	2,048	File folder	1/10/2021
SLURM	7,680	File folder	5/20/2021
small	4,608	File folder	7/3/2021
scikit_learn_data	1,024	File folder	2/6/2021

Upload Auto start Binary Ask if file exists Pause

Download Auto start Binary Ask if file exists Pause

Log out

Exit



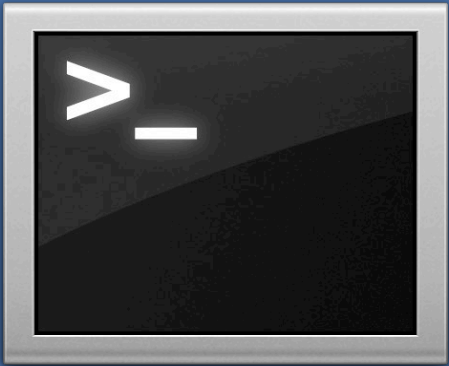
Storage on HiPerGator



- **Home storage:** `/home/<user>`
 - 40GB limit
 - Scripts, code, compiled applications
 - **Do NOT use for job input/output**
 - **Week of snapshots at `~/.snapshot/`**
 - **Blue storage:** `/blue/pre1234/<user>`
 - 2TB limit per class
 - **ALL input/output** from jobs should go here
- All storage systems are for research and coursework data only
 - Nothing is backed up
 - All course accounts are deleted at the end of the semester

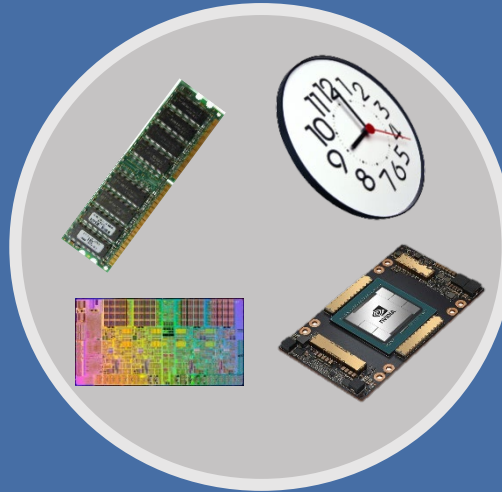
Cluster overview

User
interaction



Login node
(Head node)

SLURM
Scheduler



Tell SLURM what
you want to do

Compute
resources

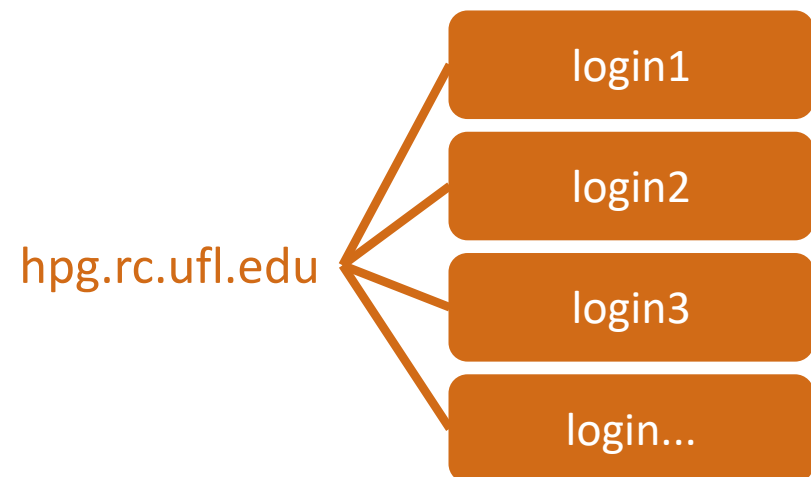


Your job runs
on the cluster





HiPerGator
The University of Florida Supercomputer for Research



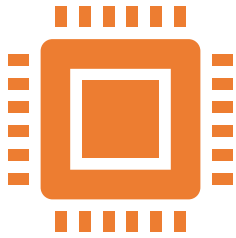

slurm
workload manager

UF | Information Technology

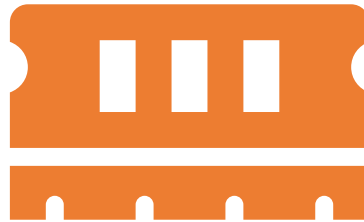


Appropriate use of login nodes

- Login nodes are for:
 - File and job management
 - Short-duration interactive testing and development
- Limit your use to **no more than:**



16 cores



64 GB memory

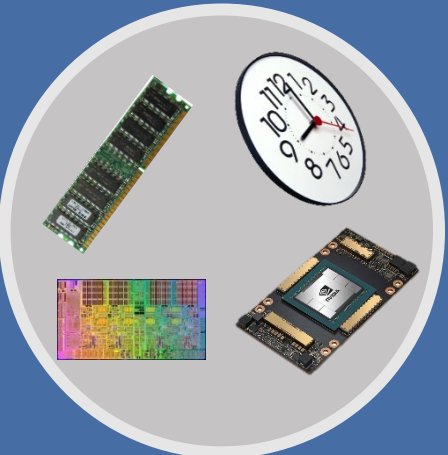


10 minutes




Resources

SLURM Scheduler




Tell SLURM what you want to do

Development servers



GPU Servers



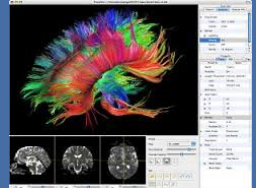
Galaxy



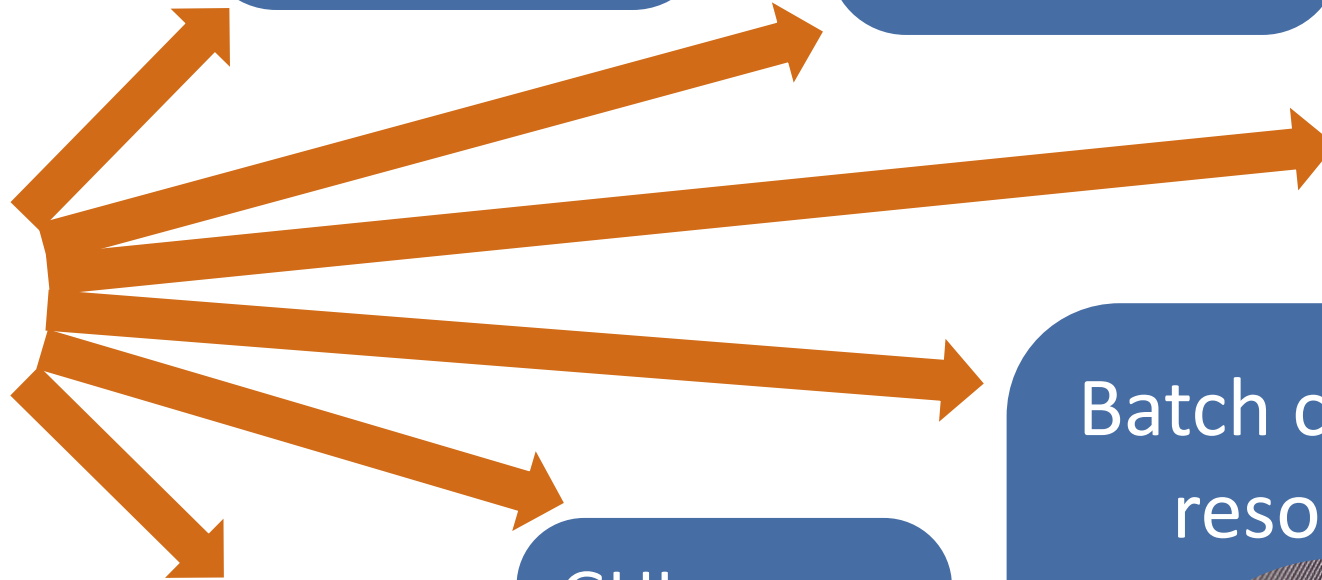
Jupyter servers



GUI servers



Batch compute resources





Jupyter Hub and on Demand

jhub.rc.ufl.edu

ood.rc.ufl.edu



To setup link to the class blue directory, open a Terminal (File> New > Terminal) and run (e.g. for class **ast4930**):

```
ln -s /blue/ast4930 blue_ast4930
```




Jupyter and conda environments

Be careful with `pip install`

- Can lead to conflicting versions of packages
- `pip` installs packages in
`~/.local/lib/python3.x/site-packages`

Use conda/mamba

- Create isolated environments
- To use in Jupyter, create custom kernel folder. See [help page](#).
- To use in script:

```
module purge; module load conda
conda activate my_env
python my_script.py
```

Script should start with:

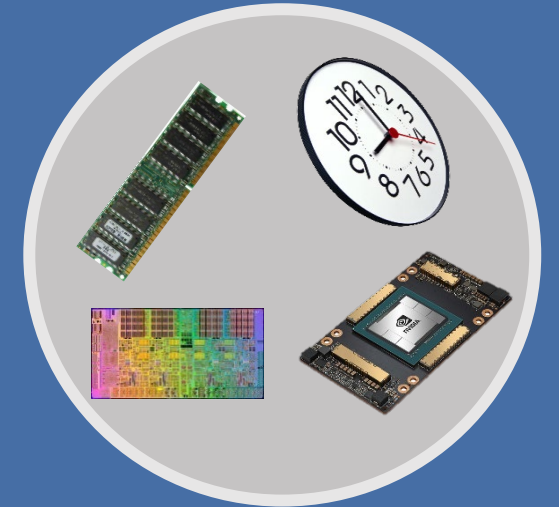
```
#!/usr/bin/env python
```



Scheduling a job

- What resources does your job need?
 - **How many CPUs** you want and how you want them grouped?
 - **How much RAM** your job will use?
 - **How long** your job will run?
 - **How many GPUs?**
- Also need the commands that will be run to do your work

SLURM Scheduler



Tell SLURM what you want to do

Basic SLURM job script



```
#!/bin/sh
```

```
#SBATCH --cpus-per-task=1
```

```
# Run on a single CPU
```

```
#SBATCH --mem=1gb
```

```
# Memory limit
```

```
#SBATCH --time=00:05:00
```

```
# Time: hr:min:sec
```

```
#SBATCH --job-name=job_test
```

```
# Job name
```

```
#SBATCH --mail-type=ALL
```

```
# Mail events
```

```
#SBATCH --mail-user=email_address
```

```
# Where to send mail
```

```
#SBATCH --output=serial_%j.out
```

```
# Output and error log
```

```
pwd; hostname; date # Print some information
```

```
module load python # Load needed modules
```

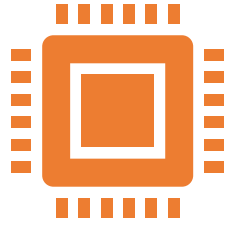
```
echo "Running plot script on a single CPU core"
```

```
python /data/training/SLURM/plot_template.py
```

```
date # Print ending time
```



SLURM CPU Requests

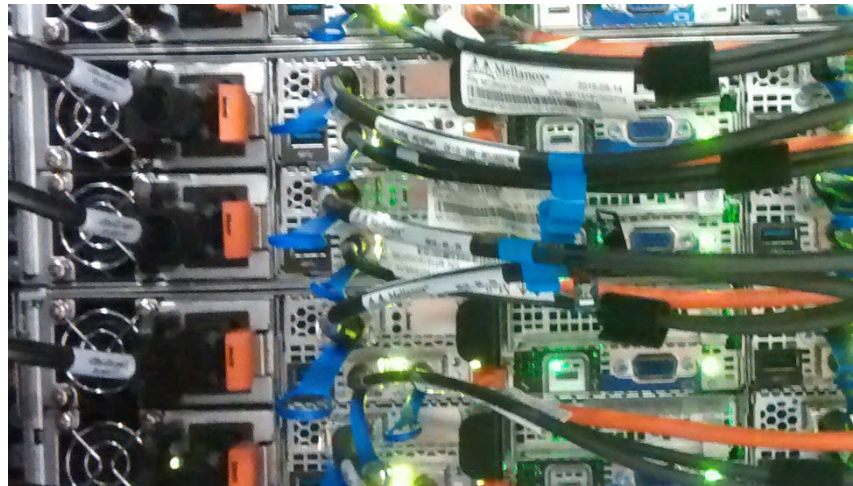
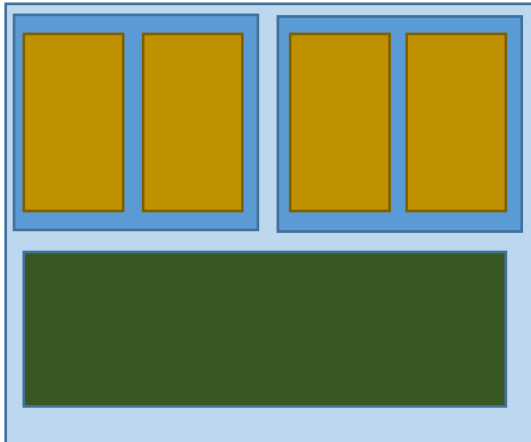


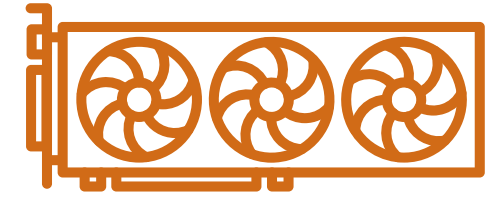
- For threaded applications (single node):

#SBATCH --nodes=1 # Physical servers

#SBATCH --ntasks=1 # MPI ranks or processes

#SBATCH --cpus-per-task=8





SLURM GPU Requests

#SBATCH --partition=gpu # required for GPUs

#SBATCH --gpus=1

#SBATCH --gpus=a100:1 #Specify type

- See: https://help.rc.ufl.edu/doc/GPU_Access

Cluster partition (--partition, -p)

Select a specific cluster partition for job. (default = first available compute partition)

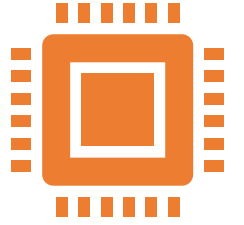
Generic Resource Request (--gres).

This is the Generic resource request string to request GPU resources. See also https://help.rc.ufl.edu/doc/GPU_Access

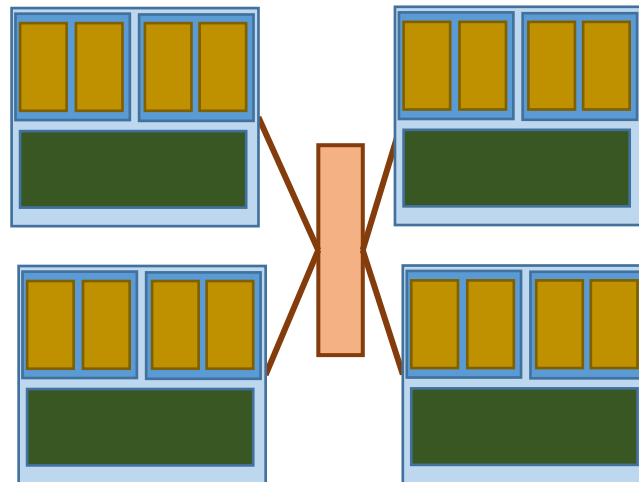
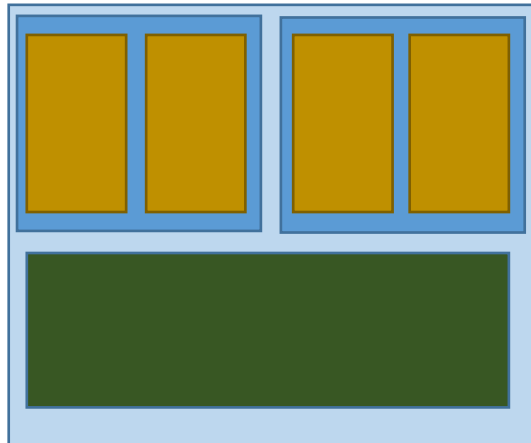
--gres: gpu:a100:1



SLURM CPU Requests

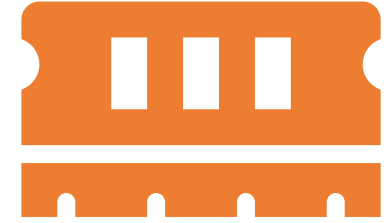


- Parallel applications
 - OpenMP, Threaded, Pthreads
 - All cores on one sever, shared memory
- MPI—**M**essage **P**assing **I**nterface
 - Can use multiple servers
 - See: [help.rc.ufl.edu/doc/Sample SLURM Scripts](http://help.rc.ufl.edu/doc/Sample_SLURM_Scripts)





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



SLURM Time Request

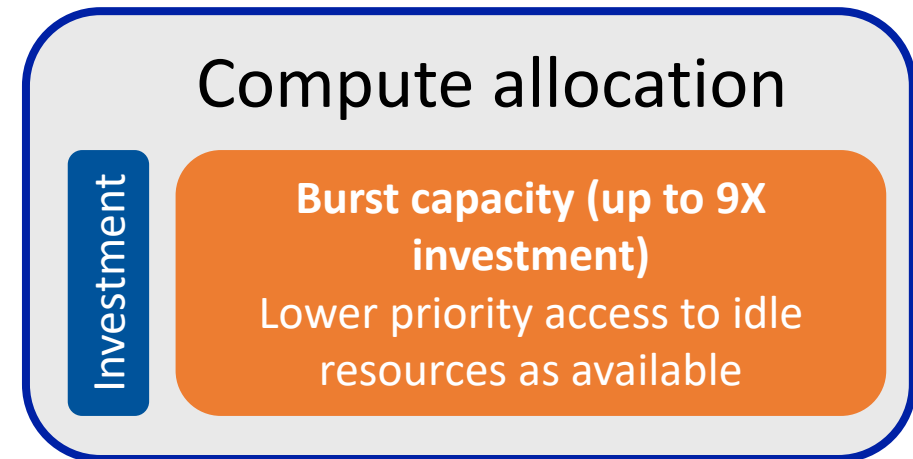


- Time: `--time` or `-t`
 - 120 (minutes)
 - 2:00:00 (hh:mm:ss)
 - 7-0 (days-hours)
 - 7-00:00 (days-hh:mm)
 - 7-00:00:00 (days-hh:mm:ss)



Quality of Service (--qos)

- Each group has two QOS options
 - Investment QOS: **--qos=group**
 - Burst QOS:
 - The burst capacity, available when idle resources are available on the cluster
 - **--qos=group-b**
- Users can choose higher priority, or larger pool of resources





SLURM

- Note that multi-letter directives are double-dash:
 - `--mail-type` `sbatch: error: distribution type 'ail-type=ALL' is not recognized`
 - `--ntasks`
 - `--mem-per-cpu`
- Use either, ***but not both***, space or =
 - `--mail-user=magitz@ufl.edu` ✓
 - `--mail-user magitz@ufl.edu` ✓
 - not: `--mail-user= magitz@ufl.edu`



Submit your job

```
[magitz@login3 SLURM_examples]$ sbatch single_job.sh
```

```
Submitted batch job 30592170
```

```
[magitz@login3 SLURM_examples]$ squeue --me
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST (REASON)
30592170	hpg2-comp	serial_j	magitz	R	0:30	1	c24b-s15

```
[magitz@login3 SLURM_examples]$
```



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- Help
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- Scheduler
- Services

Tools

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UFRC Help and Documentation

Welcome to the [University of Florida](#) Research Computing Help and Documentation site. General information, announcements, and purchase request forms are on our [main web site](#). The information here is focused on particular applications, services, and usage examples. [Provide Feedback](#).



FOR NEW USERS

Guides to get you started with HPG, and best practices!

[Getting Started](#) | [Training Videos](#) | [Trainings & Events](#) | [Interactive Development and Testing](#) | [Practical Storage Use](#)



ACCESS

How to connect to HPG with Duo, authenticate multiple connections, or check account.

[Multi-Factor Authentication](#) | [SSH Multiplexing](#) | [SSH Keys](#) | [Blocked Accounts](#) | [Federated Access and Login](#)



HELP

Resources to ask questions, get support, or communicate directly.

[How To Get Help](#) | [AI Help](#) | [FAQ](#) | [Submit a Support Request](#) | [HiPerGator Metrics](#)



INTERFACES

Guides for GUI/web interfaces you can run on HPG.

[Jupyter \(Python, R\)](#) | [Galaxy Genomics Framework](#) | [OnDemand \(Matlab, RStudio,...\)](#) | [Conda and Jupyter Kernels](#) | [Running GUI Apps](#)



SCHEDULER

How to schedule and manage jobs and resources on



SOFTWARE AND REFERENCE DATA

help.rc.ufl.edu



Training



- Applications
- Essentials
- Help
- Infrastructure
- Scheduler
- Services

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Page Discussion

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Training Videos

Quick How Tos [\[edit\]](#)

The following videos are designed to provide quick help for users on various topics, most are only a few minutes long.

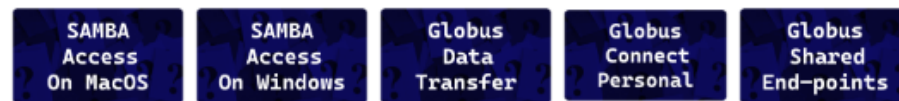
Please let us know if there are additional topics that you feel would be useful for a quick help video.

In addition to the pre-recorded content, we also provide in-person training sessions. Visit the main training page for additional training information.

Connecting to HPG [\[edit\]](#)



Data Transfer [\[edit\]](#)



Other How Tos [\[edit\]](#)



Recorded Trainings [\[edit\]](#)

HIPerGator Account Training [\[edit\]](#)

All new HIPerGator users are required to take the HIPerGator Account training: [Link and overview on this page](#).

Introduction to Research Computing and HIPerGator [\[edit\]](#)

Intended for new users, this training provides a general overview of the UF Research Computing facilities and basic usage of HIPerGator.

This training is available in three parts:

- Part 1: Intro to UF Research Computing and HIPerGator [\[video\]](#)
- Part 2: Getting logged in, storage and using HIPerGator [\[video\]](#)
- Part 3: Working with the SLURM Scheduler to run Jobs [\[video\]](#)

Or as a recording of the most recent Zoom session: [\[video\]](#)

You can download a copy of the slides used from [here](#).

Introduction to the Linux Command Line [\[edit\]](#)

This session will lead participants through some exercises that go over basic Linux commands such as moving around the file system, making directories, moving and copying files, etc. We will also go over some of the applications you can use on your computer to connect to and move files to and from HIPerGator. This session is largely aimed at users who are new to the Command Line.

This session is available as a pre-recorded video or zoom recording: [\[video\]](#) [\[zoom\]](#)

The handout and files for the session are now located in a git repository here:

https://github.com/UFRResearchComputing/Linux_training

The handout can be downloaded as a PDF file [\[pdf\]](#).

The molecules folder used in the training is at `/data/training/LinuxCLI/molecules`.

For those wishing to use this training outside of HIPerGator, the molecules folder is in the repository in the `idata` folder. There are also directions for non-HIPerGator use in the non-HIPerGator.md file or as a PDF [\[pdf\]](#). The repository can be downloaded to your own computer

HIPerGator: SLURM Submission Scripts for MPI Jobs [\[edit\]](#)

This session will go into depth on the details of scheduling MPI jobs on HIPerGator. Efficiently running MPI applications requires an understanding of both how to specify the needed resources as well as the layout and properties of the available hardware. This session will provide examples from several commonly used applications and provide guidelines for users to optimize their own runs.

This video is approximately 25 minutes and includes a demonstration. [\[video\]](#)

The files used in this video are on the [Sample_SLURM_Scripts](#) page and on the cluster in `/data/training/SLURM/`.

[\[video\]](#) Recording of the October 6th, 2022 session [\[note\]](#) Note due to Hurricane Ian, this session includes both the non-MPI and the MPI content.

Running Graphical Applications on HIPerGator [\[edit\]](#)

Users can run applications with graphical user interfaces (GUI) on HIPerGator either using Open on Demand or using the `gui` module and submitting jobs from the command line.

This video provides an overview of Open on Demand, which offers many GUI applications:

[\[video\]](#) [5 min, 11 sec]

This video reviews launching additional GUI applications using the `gui` module to submit jobs from the command line: [\[video\]](#) [5 min, 16 sec]

A recording of the most recent Zoom session, covering both Open on Demand and `gui` module is also available: [\[video\]](#)

The [GUI Programs](#) page has additional information.

Running MATLAB on HIPerGator [\[edit\]](#)

Users walk through a hands-on examples using MATLAB at Research Computing. Participants will work with the MATLAB GUI, compiling code and submitting MATLAB jobs to the scheduler to run on the cluster.

This video is approximately 24 minutes and includes a demonstration. [\[video\]](#)

Users should also review the [MATLAB](#) page for additional information.