



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

UF

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, Events, Videos | New user training | 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 | Blocked Accounts



HELP

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



INTERFACES

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

Tools
Recent changes
Help

<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`

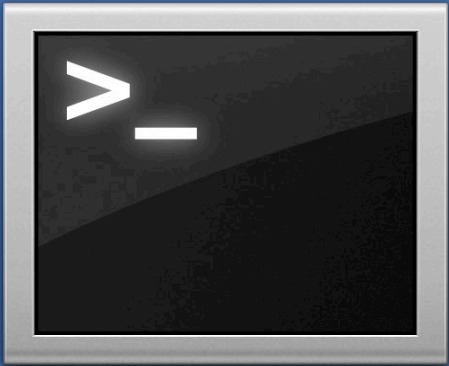


HiPerGator AI

UNIVERSITY OF FLORIDA

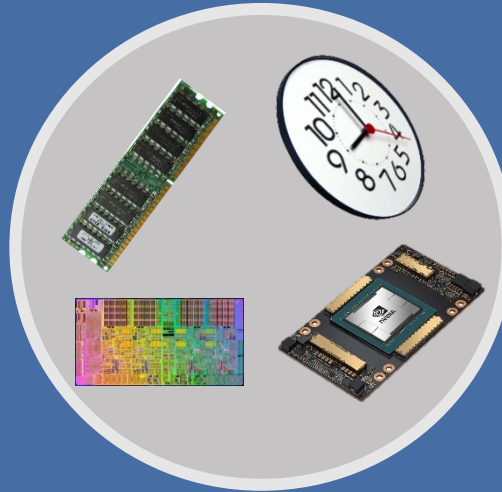
Cluster overview

User
interaction



Login node
(Head node)

SLURM
Scheduler



Tell SLURM what
you want to do

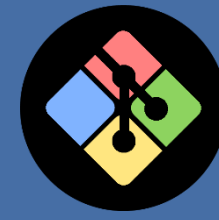
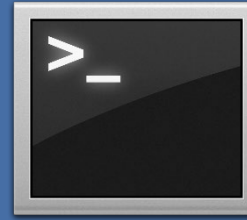
Compute
resources



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

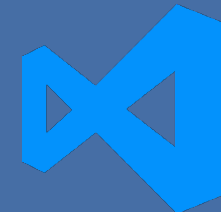
SFTP client to move files to/from
your computer
hpg.rc.ufl.edu



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

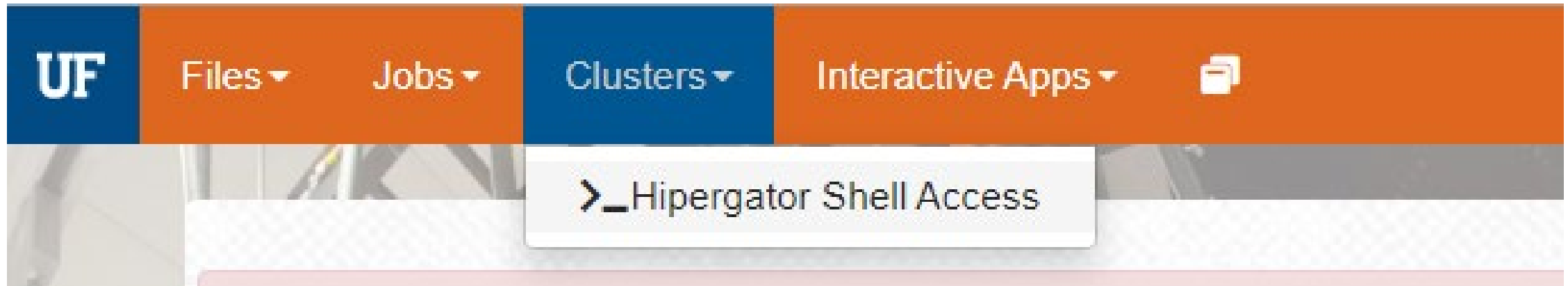
☒ gssapi-keyex authentication

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

Initial method: keyboard-interactive



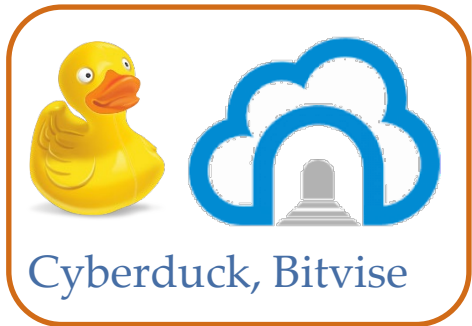
ood.rc.ufl.edu



Need to be on UF network (VPN if off campus)

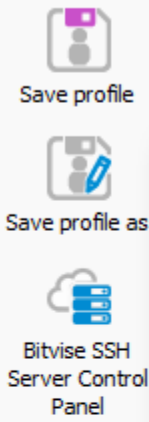


SFTP Client



hpg.tlp - magitz@hpg.rc.ufl.edu:22 - Bitwise 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 - Bitwise 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	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



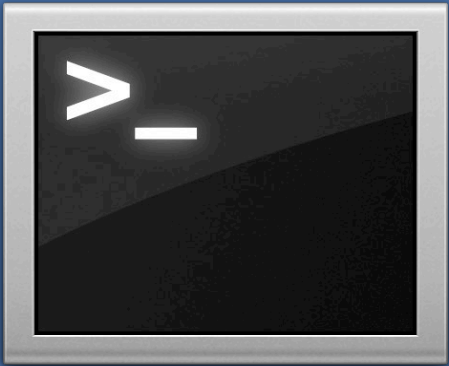
Storage on HiPerGator



- **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

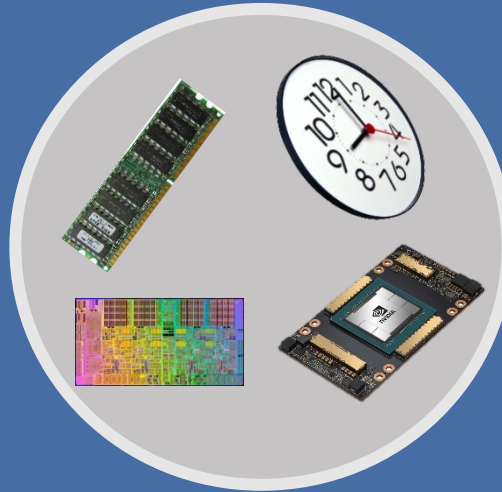
Cluster overview

User
interaction



Login node
(Head node)

SLURM
Scheduler



Tell SLURM what
you want to do

Compute
resources

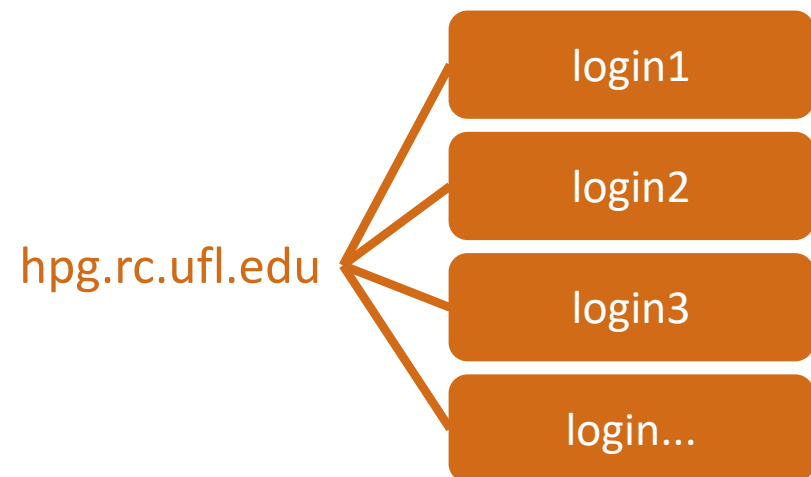


Your job runs
on the cluster





HiPerGator
The University of Florida Supercomputer for Research



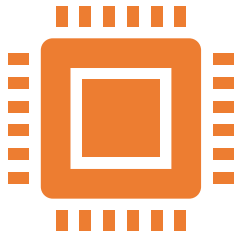

slurm
workload manager

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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

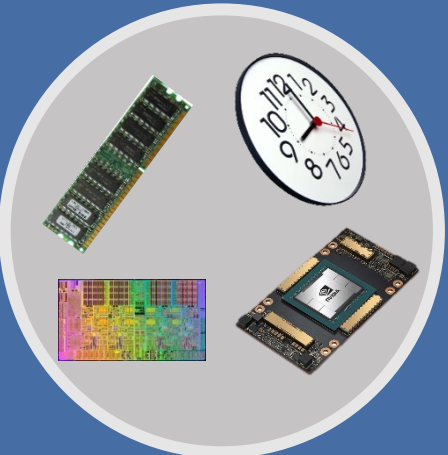


10 minutes



Resources

SLURM Scheduler




Tell SLURM what you want to do

Development servers



GPU Servers



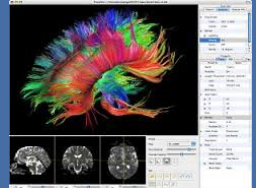
Galaxy



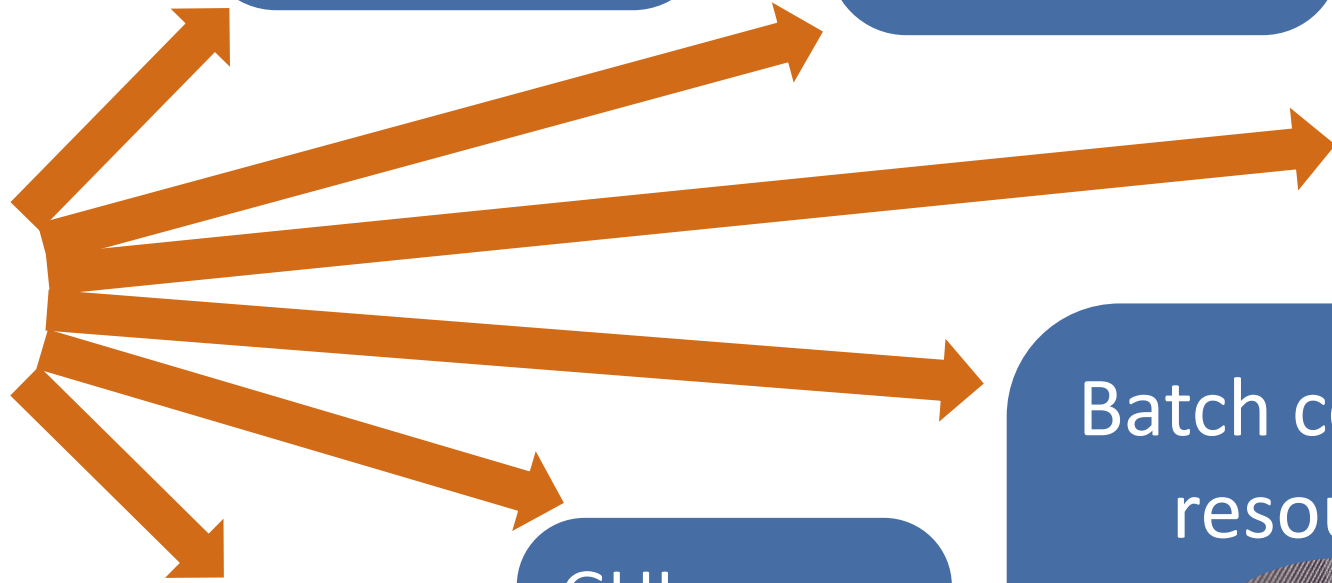
Jupyter servers



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
```



VPN required if
off campus



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:

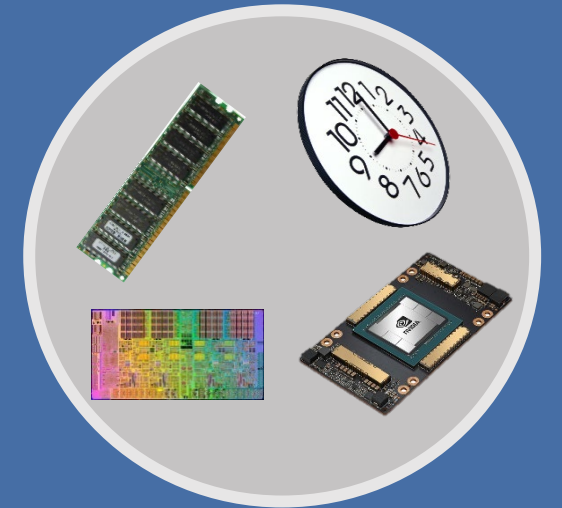
```
#!/usr/bin/env python
```




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
```

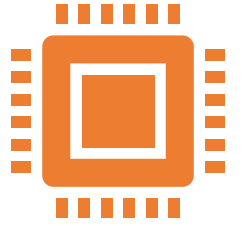
```
echo "Running plot script on a single CPU core"
```

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

```
date # Print ending time
```



SLURM CPU Requests

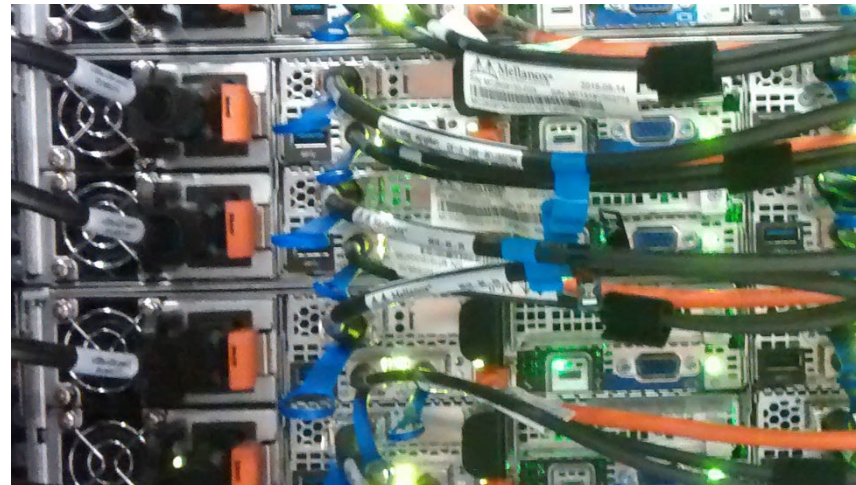
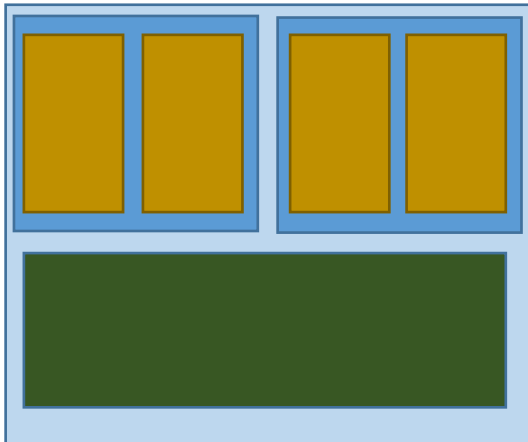


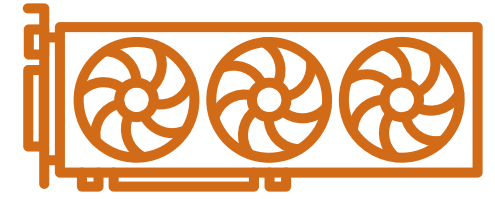
- For threaded applications (single node):

#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)

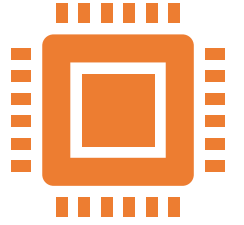
Generic Resource Request (--gres).

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

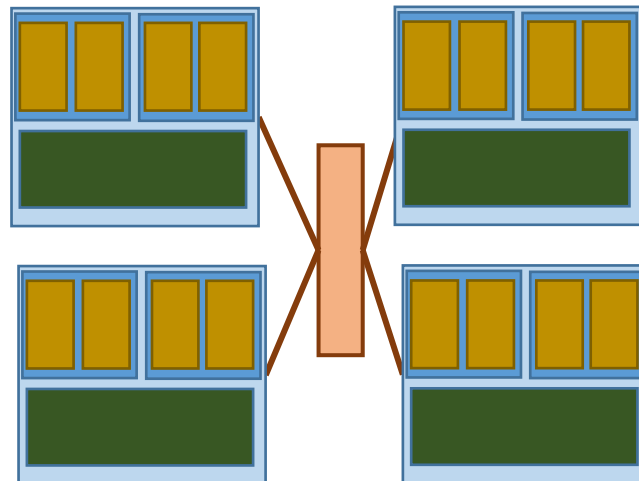
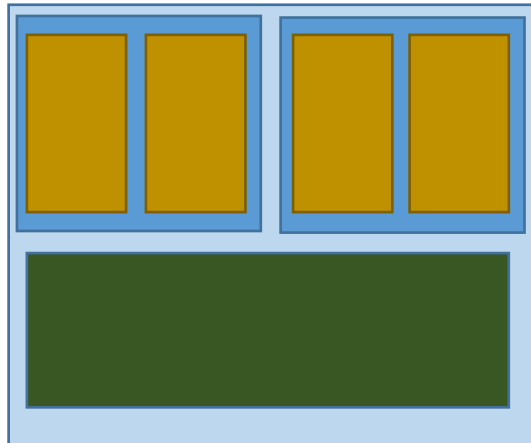
--gres: gpu:a100:1



SLURM CPU Requests

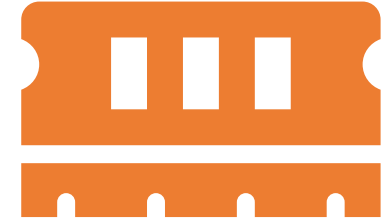


- Parallel applications
 - OpenMP, Threaded, Pthreads
 - All cores on one sever, shared memory
- MPI—**M**essage **P**assing **I**nterface
 - Can use multiple servers
 - See: [help.rc.ufl.edu/doc/Sample SLURM Scripts](http://help.rc.ufl.edu/doc/Sample_SLURM_Scripts)





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

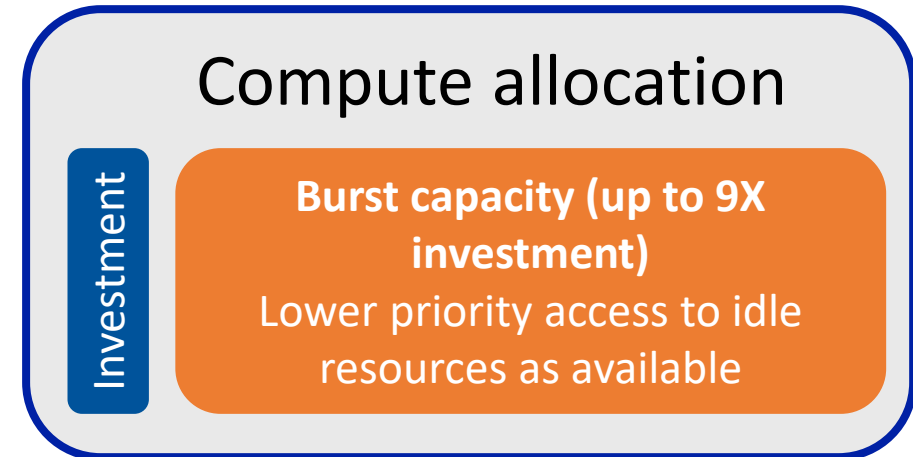


- Time: `--time` or `-t`
 - 120 (minutes)
 - 2:00:00 (hh:mm:ss)
 - 7-0 (days-hours)
 - 7-00:00 (days-hh:mm)
 - 7-00:00:00 (days-hh:mm:ss)



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]$
```



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

Tools

Recent changes

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Main page

Discussion

Read

Edit

View history



More ▾

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UFRC Help and Documentation

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HELP

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



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 HPG and more SLURM info.

[SLURM Commands](#) | [Account/QOS Limits Under SLURM](#) | [Big Memory Partition](#) | [Available Node Features](#) | [SLURM Job Script Examples](#) | [SLURM Job Arrays](#) | [GPU Access](#)



SOFTWARE AND REFERENCE DATA

View installed programs and tools, how to utilize them, and reference data that they can run.

[Installed Applications](#) | [HiPerGator ufrc Tools](#) | [Environment Modules System](#) | [Reference Data](#) | [AI Reference Datasets](#)



TRANSFER DATA

How to move different sizes of data to and from HPG



SPECIFIC RESEARCH AREAS

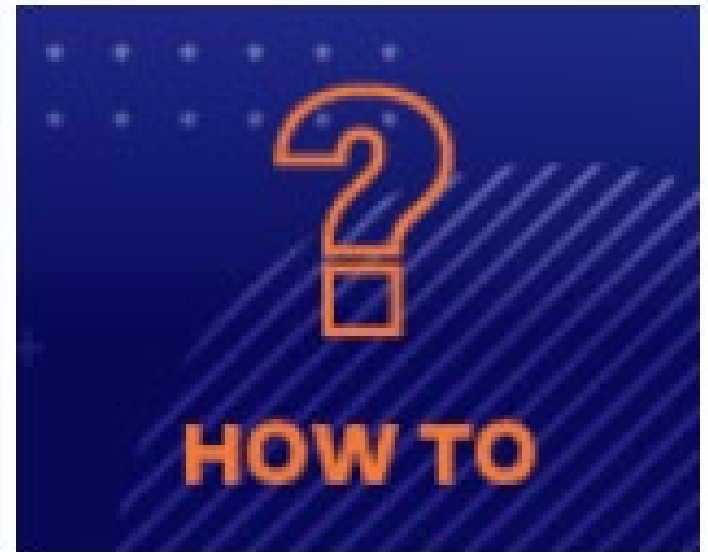
Highlighted areas of specialization commonly seen with HPG

help.rc.ufl.edu

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Training



help.rc.ufl.edu/doc/Training