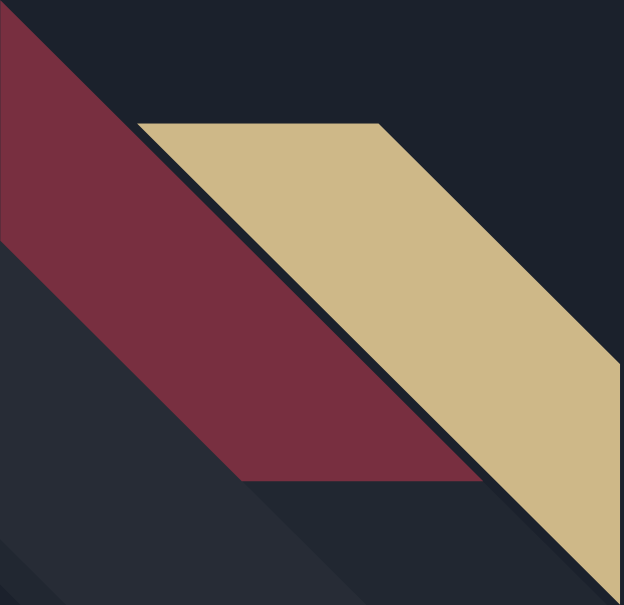




Introduction to High Performance Computing (HPC)

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Research Computing Center
September 9 2025



Agenda

- What is High Performance Computing (HPC)
 - HPC Definitions
- Accessing the HPC
 - Exercises
- Support from RCC Team



What is High Performance Computing?

Specialized Hardware

- Contains more processors than the average home computer
- Has several generations of both AMD and Intel Processors
- Can house custom machines (via a research grant) with specialized hardware like special CPUs, DSPs, SSDs, GPUs and otherwise.

Offload Your Work

- Takes pressure off your regularly used desktop, laptop or other devices
- Scales computational processes not possible on home machines
 - parallel processes
- Runs tasks that need to be repeated many times over a long period of time



RCC System Metrics

649
Nodes

Beowulf Cluster
AlmaLinux 8.6

114
GPUs

NVIDIA:
- H100 (2)
- A4000
- A4500 Ada Gen
- GTX 1080 Ti

20,144
Processors

AMD, Intel

958.64
TeraFLOPS

Very Fast
Maximum
Speeds

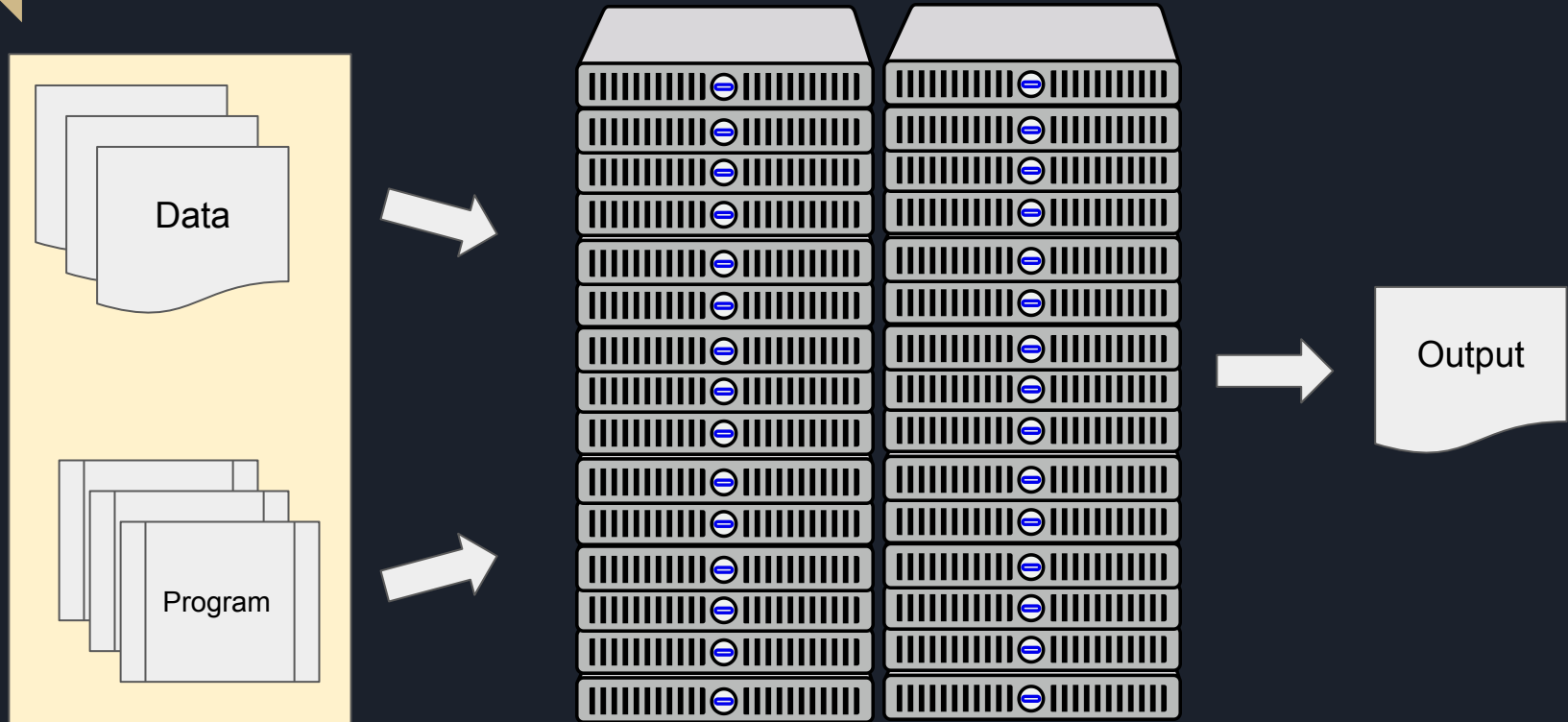
29,170,841
jobs

Since 2008

HPC Definitions



HPC Job



How HPC Works

FSU's HPC is a shared resource for all FSU researchers

Job Scheduler: SLURM

- Directs jobs so they can be processed quickly and effectively
- Allocates resources to jobs so the cluster does not freeze up

User Accounts

- Logins and Home Directories

Slurm Accounts

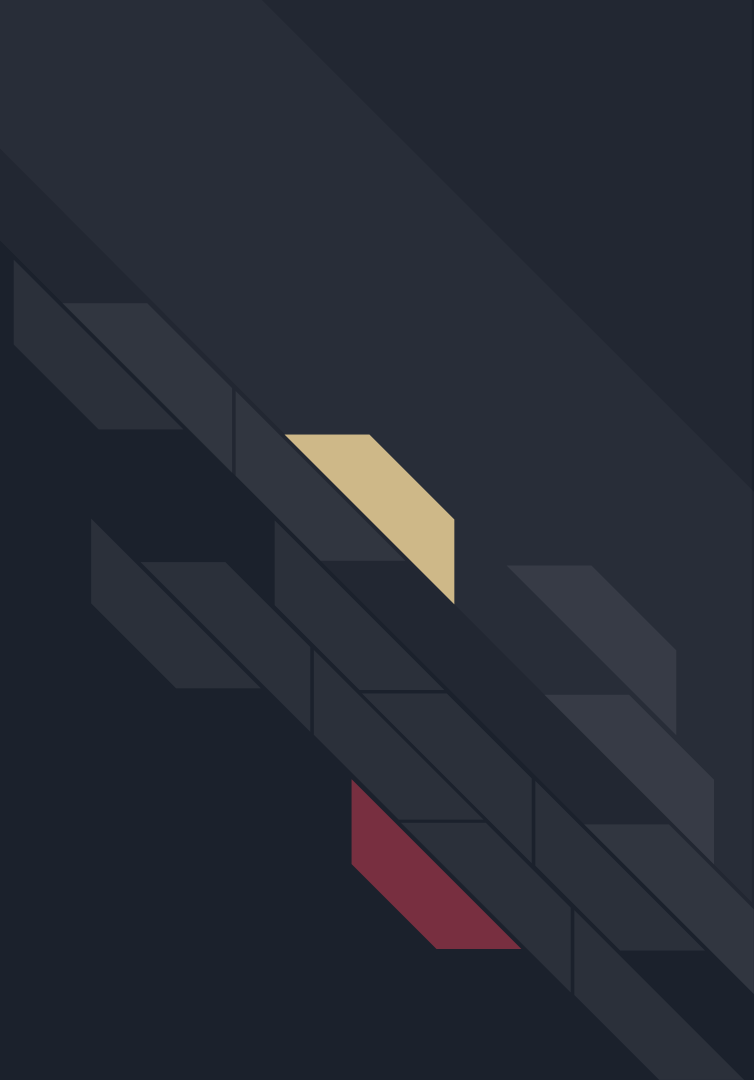
- Queues / Partitions



Job Scheduler: SLURM



How to Access the HPC



Ways to Use HPC

Command-Line Interface

- Any SSH-Supporting CLI Terminal
 - Windows PowerShell
 - Cygwin Emulator
 - MobaXTerm Emulator
 - PuTTY
 - Linux Terminal
 - Mac Terminal

Graphical Interface

- Open OnDemand

```
Warning: Permanently added 'hpc-login.rcc.fsu.edu,144.174.41.26' (ECDSA) to the list of known hosts.
Welcome to the RCC

-----
NOTICE: The HPC will be offline for planned maintenance Dec 3 - 7
Details: https://fla.st/UULW5953

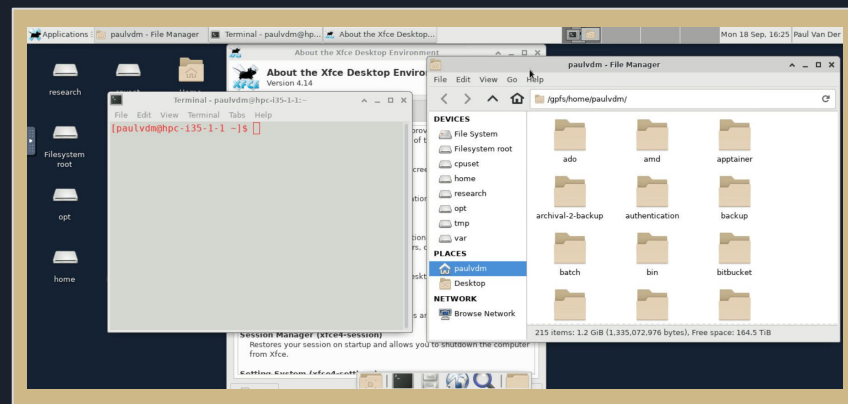
-----
RCC/HPC Documentation can be found here:
https://rcc.fsu.edu/docs
-----
Last login: Mon Sep 18 09:27:42 2023 from 10.146.38.184

** Disk usage (GPFS) quota report: 115.8G used of 150G available
For a disk quota report, run: gpfs_quota

WARNING: Files in the /gpfs/research/eoas volume will be deleted after 90 days

[mn13gh22-login-26 ~]$ ls
8
agisof2-2021-12-28-13.47.lic      FPLD                                lifeexpectancycountries.csv
agisof2Metashape_testing        Gau-1727753.inp                    LK_LineError
agisof2 trial 2022-01-06-16-26.lic GPU_rawtest                        log_lammps
bigdiff                          gromacs                            LWP_xalt_test_temp.py
bozanicgroup                    GULP                               marcelina
calceinch.txt                  hello                              Marcelina-RPM-GPG-KEY
cb_enu_script.env              hello.a                             meshroom-2021.1.0.def
citations                       hello.c                             meshroom-2021.1.0.sif
cli_productivity               hello.py                            mln13 browser.p12
CMA32_user_manual.doc           hello-world-1.1.x86_64.rpm         mycode.R
commands.ref                    I16 S1 M1 W Freq LS.com           mycode.Rout
Cu3FeS4 009 Example'           input_tmp.in                       n2.mw
Desktop                         Jb RCC metashape-log.txt          namelist.input
deviceQuery.cu                  kaji_repos                         ntk_data
fast5struct                     lammps                              rumpy-1.22.3-mkl-cp310-cp310-win32.whl
fort.7                           libxc                               mchew

[mn13gh22-login-26 ~]$
```



Command Line Interface

- RCC uses Linux on all of our compute nodes and login nodes
 - RCC offers an Intro to Linux Workshop
- Connect using SSH (Secure Shell)

```
Warning: Permanently added 'hpc-login.rcc.fsu.edu,144.174.41.26' (ECDSA) to the list of known hosts.
Welcome to the RCC
-----
NOTICE: The HPC will be offline for planned maintenance Dec 3 - 7
Details: https://fla.st/UULW59S3
-----
RCC/HPC Documentation can be found here:
https://rcc.fsu.edu/docs
-----
Last login: Mon Sep 18 09:27:42 2023 from 10.146.38.184

** Disk usage (GPFS) quota report: 115.8G used of 150G available
For a disk quota report, run: gpfs_quota

WARNING: Files in the /gpfs/research/eoas volume will be deleted after 90 days

[mln13@h22-login-26 ~]$ ls
6
agisoft-2021-12-20-13.47.lic      FPL0
AgisoftMetashape_testing        Gau-1727753.inp
agisoft_trial_2022-01-06-16-26.lic Gau-4171429.inp
bigdft                          GPU_rawtest
bozanicgroup                    gromacs
calcbench.txt                   GULP
cb_env_script.env               hello
citations                       hello3
cli_productivity                hello.c
COAST User Manual.doc           hello.py
commands.ref                    hello-world-1-1.x86_64.rpm
'Cu3FeS4 G99 Example'           I16_S1_M1_W_Freq_LS.com
Desktop                          input_tmp.in
deviceQuery.cu                  jb_rcc_metashape-log.txt
fastStruct                       koji_repos
fort.7                           lammps
                                  libxc
                                  lifeexpectancycountries.csv
                                  LK_libError
                                  log.lammps
                                  LWP
                                  LWP_xalt_test_temp.py
                                  marcelina
                                  Marcelina-RPM-GPG-KEY
                                  meshroom-2021.1.0.def
                                  meshroom-2021.1.0.sif
                                  mln13_browser.pl2
                                  mycode.R
                                  mycode.Rout
                                  n2.nw
                                  namelist.input
                                  nltk_data
                                  numpy-1.22.3+mk1-cp310-cp310-win32.whl
                                  nwchem
```

Open OnDemand Applications

GUI Applications

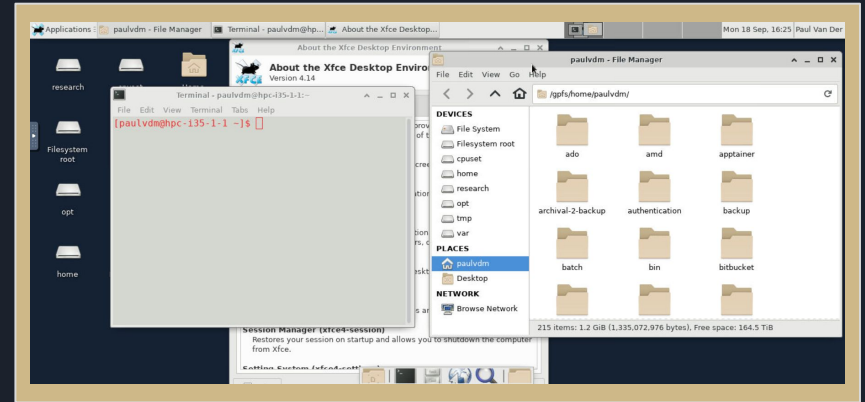
- Desktop
- MATLAB
- STATA
- VisIt

Servers

- Jupyter Notebooks
- RStudio Server

Visualizations

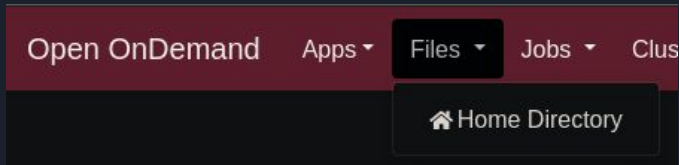
- PyMOL
- VMD



ood.rcc.fsu.edu

<https://rcc.fsu.edu/docs/ood>

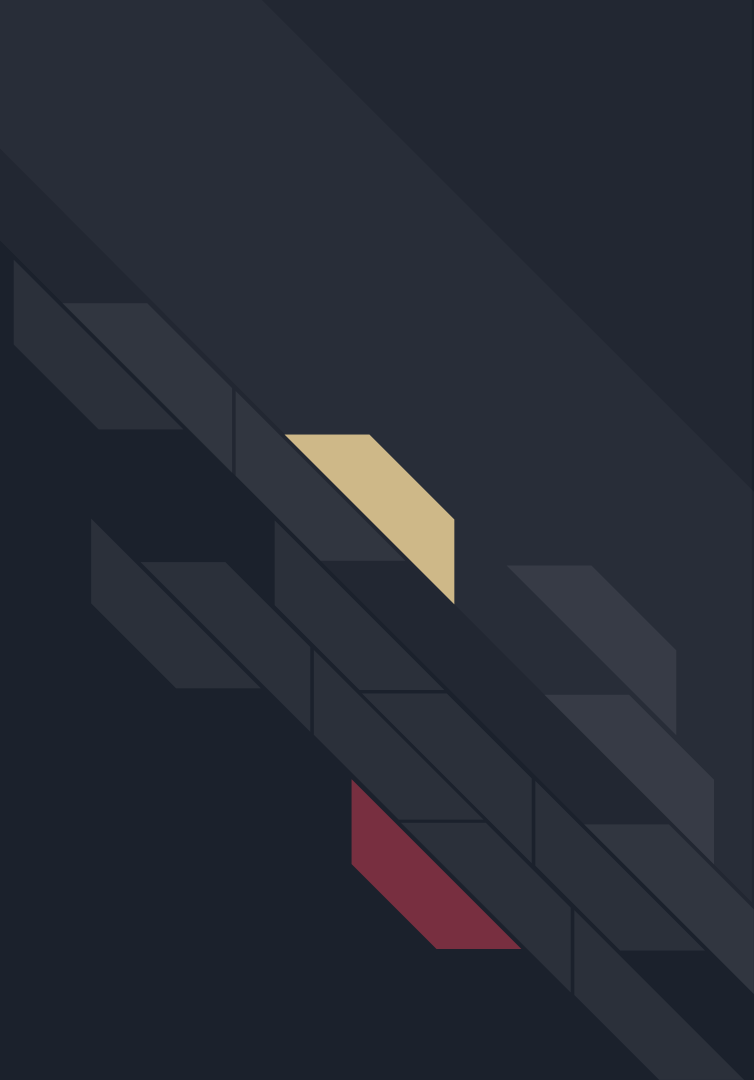
Open OnDemand File Manager



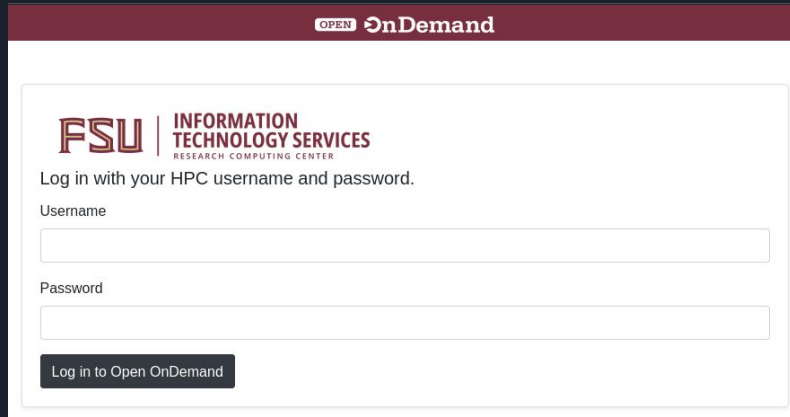
A screenshot of the Open OnDemand File Manager interface. The top navigation bar is dark red and contains links for 'Open OnDemand', 'Apps', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'My Interactive Sessions', and 'All Apps'. On the right side of the bar are links for 'Develop', 'Help', 'Logged in as sat10c', and 'Log Out'. Below the navigation bar, there is a toolbar with buttons for 'Open in Terminal', 'Refresh', 'New File', 'New Directory', 'Upload', 'Download', 'Copy/Move', and 'Delete'. The main content area shows the 'Home Directory' with a breadcrumb path '/ gdfs / home / sat10c /' and a 'Change directory' button. Below the path, there are checkboxes for 'Show Owner/Mode' and 'Show Dotted Files', and a 'Filter' input field. A table displays a list of files and directories. The table has columns for 'Type', 'Name', 'Size', and 'Modified at'. The files listed are: '00-sat10c_staffdir', 'ado', 'cryosparc_test', 'cryosparc_tutorial', 'Desktop', 'Dissertation', 'Documents', 'Downloads', and 'jupyterenv'. Each file has a checkbox in the 'Type' column and a dropdown arrow in the 'Name' column. The 'Size' column shows '-' for all files, and the 'Modified at' column shows the last modified date and time for each file. At the bottom of the table, it says 'Showing 51 of 114 rows - 0 rows selected'.

- Browse files on the HPC
- Upload small files (code or small datasets < 10 GB)
- Download small files (code or small datasets < 10 GB)
- Open and look at files.
- Edit files.
- Delete and move files.

Submitting Jobs to the HPC System



Open OnDemand Interactive Jobs



OPEN OnDemand

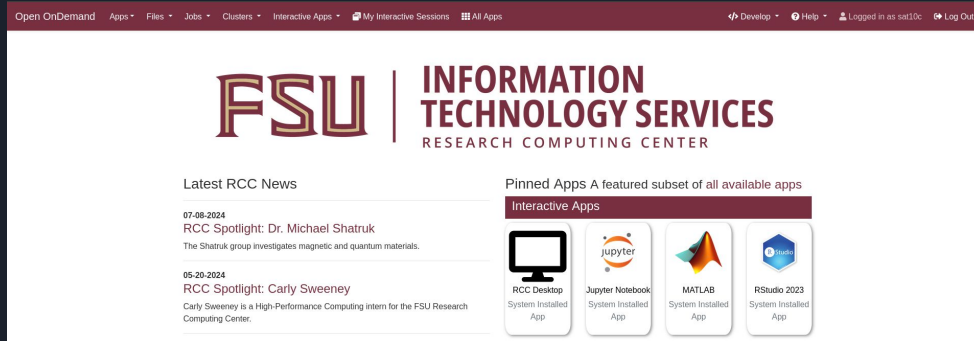
FSU | **INFORMATION TECHNOLOGY SERVICES**
RESEARCH COMPUTING CENTER

Log in with your HPC username and password.

Username

Password

Log in to Open OnDemand



Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions All Apps

Develop Help Logged in as sat10c Log Out

FSU | **INFORMATION TECHNOLOGY SERVICES**
RESEARCH COMPUTING CENTER

Latest RCC News

07-08-2024
RCC Spotlight: Dr. Michael Shatruk
The Shatruk group investigates magnetic and quantum materials.

05-20-2024
RCC Spotlight: Carly Sweeney
Carly Sweeney is a High-Performance Computing intern for the FSU Research Computing Center.

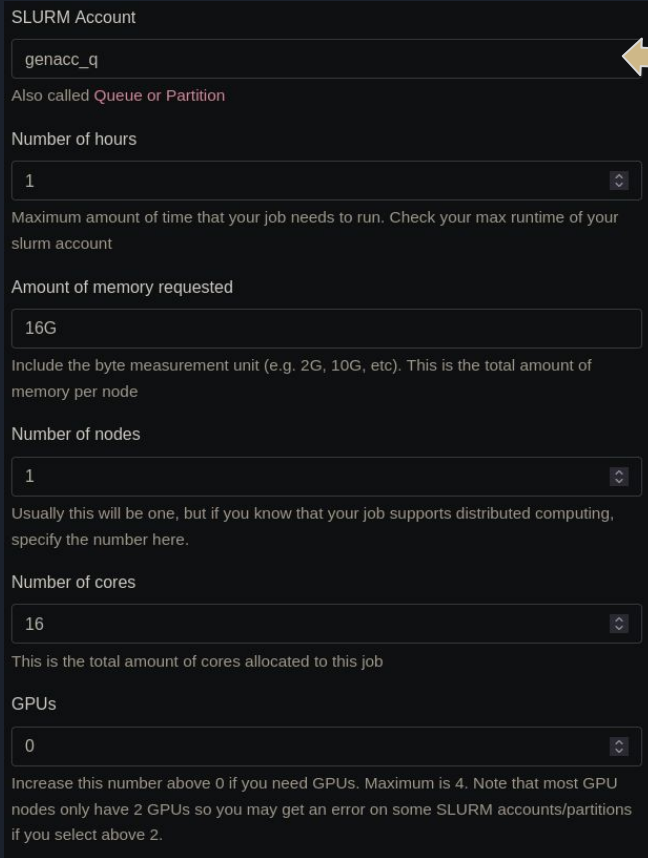
Pinned Apps A featured subset of all available apps

Interactive Apps

- RCC Desktop System Installed App
- Jupyter Notebook System Installed App
- MATLAB System Installed App
- RStudio 2023 System Installed App

- ood.rcc.fsu.edu
- Login credentials
 - *Your RCC Account details*
- Open OnDemand landing page.
- Interactive Apps
- Job Creator
- Terminal Access
- File Browser

Resource Allocation (OOD)



SLURM Account

genacc_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

16G

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

1

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

16

This is the total amount of cores allocated to this job

GPUs

0

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

Queue/SLURM Account

- The set of computers you want to use
- If you leave this blank, it will default to the **genacc_q** SLURM Account.

Resource Allocation (OOD)

SLURM Account

genacc_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

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16

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GPUs

0

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

Number of Hours

- *Maximum amount of time you expect to need for your work*

Resource Allocation (OOD)

SLURM Account

genacc_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

16G

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

1

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

16

This is the total amount of cores allocated to this job

GPUs

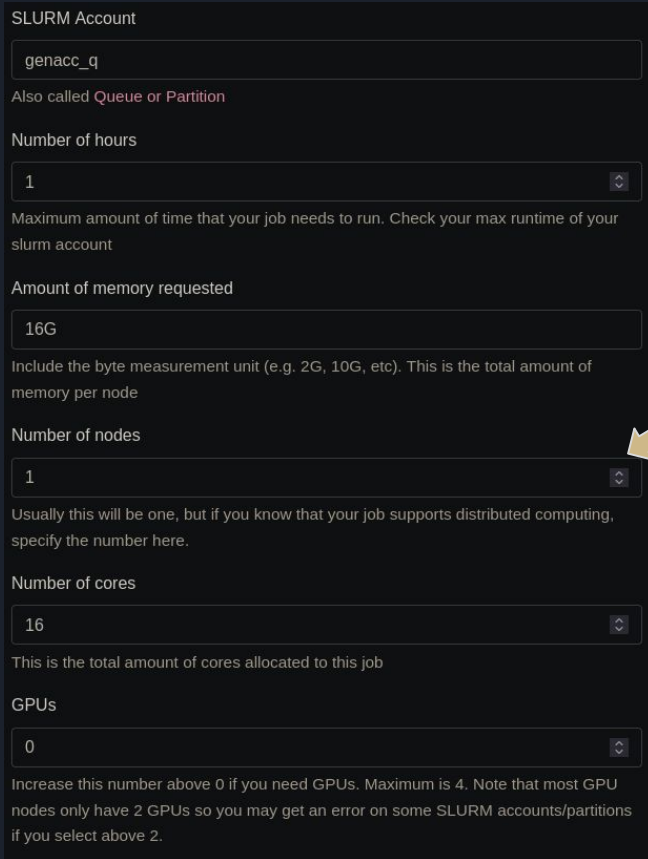
0

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

Amount of Memory Requested

- *The total amount of memory you expect to need per node for your job.*

Resource Allocation (OOD)



SLURM Account

genacc_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

16G

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

1

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

16

This is the total amount of cores allocated to this job

GPUs

0

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

Number of Nodes

- *The number of individual computer machines you want to use. (Not all OOD apps will have this option available!)*

Resource Allocation (OOD)

SLURM Account

genacc_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

16G

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

1

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

16

This is the total amount of cores allocated to this job

GPUs

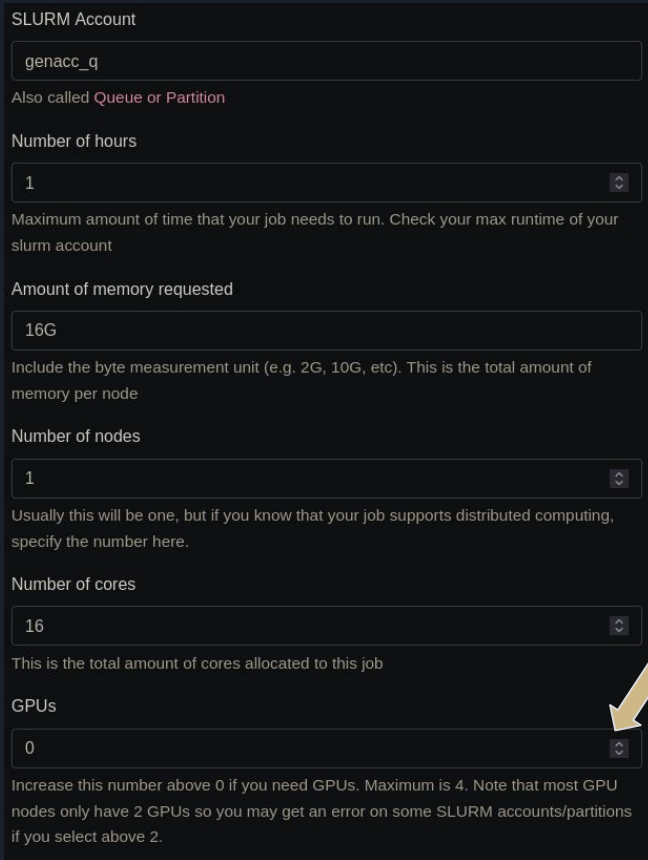
0

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

Number of Cores

- *The total number of cores you want to use for your job.*

Resource Allocation (OOD)



SLURM Account

genacc_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

16G

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

1

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

16

This is the total amount of cores allocated to this job

GPUs

0

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

A yellow arrow points from the text 'GPUs' on the right towards the 'GPUs' field in the form.

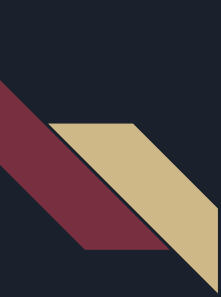
GPUs

- The number of GPU cards you want to use for your job (can leave at 0 if none needed).



Exercise

1. Navigate to <https://ondemand.rcc.fsu.edu>
2. Log in with your RCC workshop Credentials
3. Navigate to the RCC Desktop
4. Set up a RCC Desktop job with the following resources:
 - a. *4 Hours*
 - b. *Using the **workshop** SLURM Account*
 - c. *4 Cores*
 - d. *16 GB of Memory*
 - e. *No GPUs*
 - f. *Leave everything else default*
5. Launch the job
6. Open the RCC Desktop window in OOD and look around a bit!



Exercise

1. Navigate to <https://ondemand.rcc.fsu.edu>
2. Log in with your RCC Credentials
3. Navigate to the MATLAB Interactive App
4. Set up a MATLAB Job with the following resources:
 - a. 4 Hours
 - b. Using the **workshop** SLURM Account
 - c. 4 Cores
 - d. 16 GB of Memory
 - e. No GPUs
 - f. MATLAB 2022b Version
 - g. Leave everything else default
5. Launch the job
6. Open the MATLAB window in OOD and look around a bit!

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Job Name

- *The job name parameter is simply an identifier for your job. This can be helpful for keeping track of what each job is doing.*

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Queue/SLURM Account

- *If this is not specified, it will default to the **genacc_q** SLURM Account.*

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Number of Hours

- Time requests are more flexible in batch jobs. SLURM's time allocation format is:
- **Days-Hours:Minutes:Seconds**
- Example: 14-00:00:00 = 14 Days
- Example: 34:25:16 = 34 Hours, 25 Minutes and 16 Seconds.
- If this is not specified, it will default to the listed **Default Wall Time** [listed in the documentation.](#)

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill2
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Amount of Memory Requested

- *If you don't specify this, you'll be automatically allocated:*
 - *Number of Cores * Default Memory per Core ([see the documentation](#)) as this number depends on the SLURM Account)*

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Number of Cores

- *This is the number of physical CPU processors you want to use.*
- *Most of the benefits of HPC come from parallel processing.*
- *Check your software's documentation to see if it supports this!*

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Number of Nodes

- This is the number of full computers (think desktop/workstation towers for reference) that you want to use.
- This is for programs that support Distributed Computing.
- If this parameter is left out the job scheduler will decide this on its own.

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

GPUs

- *If you don't want GPUs, you can omit the entire #SBATCH --gres=gpu: line.*

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Environment Modules

- *Open OnDemand Apps will often do this for you. These load software and applications into your terminal environment for you.*

Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu/openmpi
srun example.x
```

Command to Run your Program

- *In non-interactive jobs, you have to tell the computer what you want it to do in your job ahead of time.*



Command-Line Batch Jobs

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

Translating the Job Script

- *Run it in the backfill2 SLURM Account*
- *Give me at most 4 hours to run my job*
- *I need 16 GB of memory per node for this.*
- *I also need 16 cores for this.*
- *I also need all 16 cores to be localized onto 1 physical computer node (don't spread the cores over multiple nodes).*
- *I also need 1 GPU card of any type.*
- *My program needs the OpenMPI built with the default GNU compilers.*
- *Please run my code called example.x*

Exercise: MPI Trapezoid Example Program

Using Files already on your system, run these commands

```
module load gnu openmpi  
srun --export=ALL trap.x  
sbatch submit-trap.sh
```

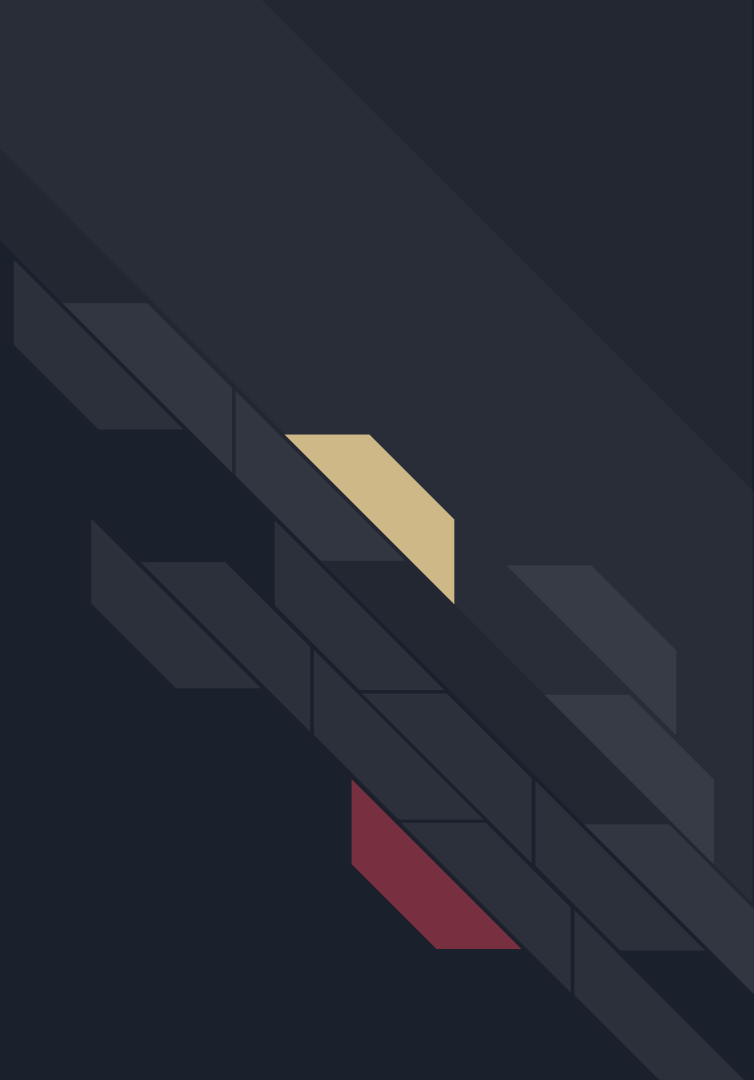
This will return a job ID number (number will change each job)

```
Submitted batch job 123456
```

When the job is complete, a new file will be present called:

- ***Slurm-123456.out*** (again, the number will change from job to job)
- *The results from your job will be in there.*

Support from RCC Team



What is the FSU Research Computing Center (RCC)

- A unit of the FSU Information Technology Services department
- Originally a division of Scientific Computing back before 2013
- The team that hosts and administers the main supercomputing resource at FSU: the High Performance Computing system (HPC)



Register For an Account

Faculty Requirements

- FSU ID and password

Student Requirements

- FSU ID and password
- Faculty Sponsor

Guest (non-FSU)

- Guest FSU ID
- Faculty Sponsor



The screenshot shows the FSU Research Computing Center (RCC) login and registration page. The header includes the Florida State University logo and the text "FSU RESEARCH COMPUTING CENTER" and "INFORMATION TECHNOLOGY SERVICES". The page has a navigation bar with "HOME" and "MANAGE" links. On the left, there is a "Manage" section with links for "Account", "Groups", and "HPC Partitions". The main content area is divided into two columns. The left column contains the "FSUID Login" section, which includes a text input for the FSUID, a password input, and a "Login" button. Below the login section is a link to "Reset system account password." The right column contains the "Don't have an FSUID?" section, which explains that a FSUID is required to sign up for a RCC account and provides a "Signup as Guest" button. A small note at the bottom of the login section states: "(this is the same account you use to login to Canvas or my.fsu.edu)".

www.rcc.fsu.edu/manage

Infrastructure

Physical Location

- Cluster held in the Sliger Data Center in Innovation Park.
Tours available!

Standard RCC accounts

- 1 Home directory per user
- 150GB of Parallel Storage
- Temporary Scratch Space (Space Limit is variable)
- Access to the General Access and Backfill Queues
- Accessible via Open On Demand and CLI



Infrastructure

Additional Features for Paid RCC Accounts

- Access to highly scalable Parallel and Archival storage systems
- Priority access to dedicated computing resources in your own queue
- Custom and specialized hardware and infrastructure (as available)

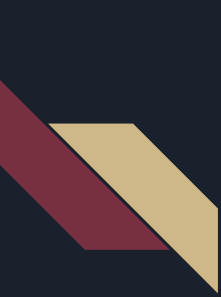




General Access Slurm Accounts

https://acct.rcc.fsu.edu/manage/hpc_partitions

Slurm Account	Default Runtime	Max Runtime	Max CPU Cores/Job	Max Jobs/User	Max Running Jobs/User
genacc_q	14 days	14 days	400	100	100
backfill	4 hours	4 hours	512	100	100
backfill2	4 hours	4 hours	512	100	100
condor	14 days	90 days	8	100	100
quicktest	10 minutes	10 minutes	8	2	1



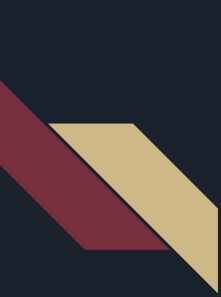
Support Services

Basic Software Support

- Basic Software installation, configuration, and maintenance
- Technical support for installed applications and software
- Workflow process support and improvement assistance
- Assistance with HPC commands and utilities

Basic Hardware Support

- Data Center Colocation



Support Services

Additional Paid Support ([more Information](#))

- Software Development Consulting
- Complex or Highly Customized Software Installations
- In-depth HPC and software focused consulting for research projects

Software

Scientific

Armadillo (C++)
BOOST
FFTW
OpenCV

Data Science

NiftyReg
HDF5
Apache Spark
R

Chemistry

ABINIT
NWChem
GROMACS
Wannier90

Bioinformatics

Trimmomatic
MIGRATE
MAUVE
MAFFT

Parallel

OpenMPI
MVAPICH2
CUDA
TotalView

<https://rcc.fsu.edu/software>



RCC Service Metrics

2 Million

Average Jobs per
Year

600

Research
Software Tools
Managed and
Supported

2,200

Support Cases
Serviced since
2022



Software Team Services

Email us at support@rcc.fsu.edu
for any questions or concerns

- Regular Office Hours 8AM - 5PM Monday through Friday
 - We work a hybrid schedule and are available by Zoom or email
 - Dirac Science Library 151
- [HPC Drivers Ed](#) - Introductory HPC materials
- docs.rcc.fsu.edu - RCC Official Documentation

Questions?



Survey

https://fsu.qualtrics.com/jfe/form/SV_3arW54ZInjjRg1g?Q_CHL=qr

