HPC Documentation

Release 2.0.0

Research Computing, Northeastern University

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WELCOME

A dedicated platform for researchers, scholars, and students to access, learn, and leverage our state-of-the-art HPC resources.

Open OnDemand (OOD) OOD provides a various available software interactively through your favorite browser.

Learn more »

Classroom Integration Request a reservation devoted for the classroom, whether an entire curriculum or specific assignments and lessons.

Learn more »

Best Practices Learn to optimize your projects by following some best practices.

Learn more »

Note: Access to the HPC Cluster is subject to university policy and guidelines. Please ensure that you read and understand these guidelines before using the facility. If you require assistance or have any questions, please do not hesitate to contact our dedicated support team.

The Northeastern University HPC Cluster is a high-powered, multi-node, parallel computing system designed to meet the computational and data-intensive needs of various academic and industry-oriented research projects. The cluster incorporates cutting-edge computing technologies and robust storage solutions, providing an efficient and scalable environment for large-scale simulations, complex calculations, artificial intelligence, machine learning, big data analytics, bioinformatics, and more.

Whether you are a seasoned user or just beginning your journey into high-performance computing, our portal offers comprehensive resources, including in-depth guides, tutorials, best practices, and troubleshooting tips. Furthermore, the platform provides a streamlined interface to monitor, submit, and manage your computational jobs on the HPC cluster.

We invite you to explore the resources, tools, and services available through the portal. Join us as we endeavor to harness the power of high-performance computing, enabling breakthroughs in research and fostering innovation at Northeastern University.

CHAPTER

ONE

WELCOME

Welcome to the official online help system for Northeastern University's Research Computing team! This documentation will assist you in using Northeastern's HPC cluster system. It contains the most up-to-date information and instructions on obtaining an account, connecting to the system, loading modules, running jobs, and storing data. If you are unfamiliar with high-performance computing, we recommend taking our training courses before using the system. For information on training and services, visit our Research Computing team website.

This help system is frequently updated to reflect the latest discovery information and add new topics to assist you with your research. Check back often for updates.

We value your feedback! If you have any comments or suggestions for topics you want to be covered in this documentation, please submit a Research Computing Documentation request.

1.1 What is Discovery

Discovery is a high-performance computing (HPC) resource for the Northeastern University research community. The Discovery cluster is in the Massachusetts Green HPC Center (MGHPC) in Holyoke, MA. The MGHPC is a 90,000-square-foot, 15-megawatt research computing, and data center facility that houses computing resources for five institutions: Northeastern, BU, Harvard, MIT, and UMass.

CHAPTER

TWO

GETTING HELP

If you need help, you can contact the Research Computing (RC) team via email, ServiceNow ticket, or by scheduling an appointment through our Bookings page.

2.1 Email

To contact the RC team, email us at rchelp@northeastern.edu. This will generate a ticket in ServiceNow. Be sure to include details about your question or issue, including any commands or scripts you use, so that we can direct you to the right person.

2.2 Submit a ticket

To submit a ticket in ServiceNow, select from the RC ServiceNow catalog. You may need to sign in with your Northeastern username and password to view the catalog.

RC users can request services using our ticket system. Please select the appropriate category below to access the online ticket.

Get Assistance with RC Request | RC Access Form | Software Request Form | Documentation | Partition Access Request | Storage Request | Storage Extension Request | Data Transfer Consultation | Classroom Request Form | Unsubscribe

2.3 Scheduling consultations

We encourage you to schedule a consultation with one of our staff members to receive personal, one-on-one assistance for your research computing and data storage needs. Consultations are available to any Northeastern student, faculty, or staff member. We can assist you with starting Discovery, optimizing your code, benchmarking, installing and using software packages, detailing data storage options, and more.

We offer consultations by appointment most weekdays during regular business hours (9 AM to 5 PM). Please note that we follow the Northeastern University holiday schedule, so no consultations are available on holidays or during breaks. All consultations are conducted online through the Teams app.

Use our Bookings page to view our availability and schedule an appointment. You must sign in using your **@northeastern.edu** email address (for example, **a.student@northeastern.edu**).

2.4 Update Ticket

To check for updates on a submitted ticket, please follow these steps:

1. Log in to your ServiceNow account.
2. Select “My Tickets” to access a list of all your active tickets.
3. In the ticket list, you will be able to view the latest updates made to each ticket.

In addition, you will receive an email notification from ServiceNow mentioning your incident number, you can directly access the ServiceNow portal to view the updates on your ticket by following these steps:

1. Open the email and locate the incident number mentioned in the message.
2. Select the incident number; this will redirect you to the ServiceNow portal.
3. In the ServiceNow portal, you can see the updates made to your ticket.

By following these steps, you can easily track the progress and stay informed about any updates related to your submitted tickets.

2.5 Status Page

We use the ITS Systems Status page to post important information, such as power outages and maintenance windows. You can subscribe to this page to receive email updates on the status of ITS systems.

CHAPTER

THREE

GETTING ACCESS

3.1 Request an account

To access Discovery, you must first have an account. You can request an account through ServiceNow but need a Northeastern username and password. If you are new to the university or a visiting researcher, you should work with your sponsor to obtain a Northeastern username and password.

Important: If you previously had access to Discovery but are now working with a different PI, you should submit a ServiceNow RC Access Request form and enter the name of your current PI in the Sponsor field. This will link your account to your current PI and expedite updating your account with any of your current PI's resources on Discovery, such as shared storage or a private partition.

Valid NU Credentials

Access to the cluster is limited to Northeastern affiliates with a valid NU username and password. Research Computing cannot create or renew Northeastern accounts. You must work with your sponsor to obtain or update your credentials.

To request an account, follow these steps:

1. Visit the ServiceNow RC Access Request form.
2. Complete the form, check the acknowledgment box, and submit it.

Your request may take up to 24 hours after your sponsor approves it (see Sponsor Approval Process below). You will receive an email confirmation when your access has been granted. Once you have access, if you are unfamiliar with Discovery, high-performance computing, or Linux, you may want to take one of our training courses. Visit the Research Computing website for more information about our training and services.

PI and instructor access

If you are a PI, professor, or instructor at Northeastern and need access to the cluster, use the access form in the above procedure and enter your name in the `Sponsor Name` field.

3.1.1 Sponsor Approval Process

HPC users need a sponsor, usually a NU PI or professor, to approve their request. PIs, professors, and instructors can sponsor themselves. Students (undergraduate or graduate), visiting researchers, or staff members must have a sponsor approve their request. When you fill out the ServiceNow form, an email is sent to the specified sponsor upon submitting the request. Sponsors will receive email reminders until they approve the request through the link in the email to ServiceNow. We recommend letting your sponsor know to look for the email with the approval link before submitting an access request.

CHAPTER

FOUR

CONNECTING MAC

You connect to Discovery using a secure shell program to initiate an SSH session to sign in to Discovery. If you usually launch software from the command line that uses a graphical user interface (GUI), see *Using X11* for tips and troubleshooting information.

4.1 Mac

Mac computers come with a Secure Shell (SSH) program called Terminal that you use to connect to the HPC using SSH. If you need to use software that uses a GUI, such as Matlab or Maestro, make sure to use the -Y option in the second step below (see *Using X11* for more tips and troubleshooting information).

Note: If you use Mac OS X version 10.8 or higher, and you have XQuartz running in the background to do X11 forwarding, you should execute the following command in Terminal once before connecting:

```
defaults write org.macosforge.xquartz.X11 enable_iglx -bool true
```

You should keep XQuartz running in the background. If you close and restart XQuartz, you will need to execute the above command again after restarting. Do not use the Terminal application from within XQuartz to sign in to Discovery. Use the default Terminal program that comes with your Mac (see Step 1 in the procedure below).

To connect to Discovery on a Mac:

1. Go to Finder > Applications > Utilities, and then double click Terminal.
2. At the prompt, type `ssh <username>@login.discovery.neu.edu`, where `<username>` is your Northeastern username. If you need to use X11 forwarding, type `ssh -Y <username>@login.discovery.neu.edu`.
3. Type your Northeastern password and press `Enter`.

You are now connected to Discovery at a login node.

Watch this video of how to connect to Discovery on a Mac. If you do not see any controls on the video, right-click on the video to see viewing options.

4.2 Using X11

When you launch a software application that uses a graphical user interface (GUI) from the command line, this is completed through X11 forwarding. If you use MobaXterm on Windows, X11 forwarding is turned on by default. If you use the Terminal program on Mac, you'll need to log in using the -Y option (`ssh -Y <yourusername>@login.discovery.neu.edu`).

Tip: If you used the -Y option to enable X11 forwarding on your Mac, you can test to see if it is working by typing `xeyes`. This will run a small program that makes a pair of eyes appear to follow your cursor.

4.2.1 Passwordless ssh

You need to set up passwordless ssh to ensure that GUI-based applications will launch without any issues. You also need to make sure that your keys are added to the authorized.key file. This needs to be done anytime you regenerate your keys. If you're having an issue with opening an application that need X11 forwarding, such as MATLAB or Schrodinger, and you recently regenerated your keys, make sure to add your keys to the authorized.key file.

Note: Errors that you can see on both Mac and Windows when launching a GUI-based program include the following:

```
Error:  unable to open display localhost:19.0

Launch failed:  non-zero return code
```

If you are getting these types of errors, follow the steps below to set up passwordless ssh.

Setting up passwordless ssh:

Note: Make sure you're on your local computer for steps 1 through 4. If you are connected to the cluster, type `exit` to return to your local computer.

---

1. On a Mac, open Terminal and type `cd ~/.ssh`. This moves you to the ssh folder on your local computer.
2. Type `ssh-keygen -t rsa` to generate two files, `id_rsa` and `id_rsa.pub`.
3. Press `Enter` to all the prompts (do not generate a passphrase).
4. Type `ssh-copy-id -i ~/.ssh/id_rsa.pub <yourusername>@login.discovery.neu.edu` to copy `id_rsa.pub` to your `/home/.ssh` folder on Discovery. Enter your NU password if prompted. This copies the token from `id_rsa.pub` file to the `authorized_keys` file which will either be generated or appended if it already exists.
5. Connect to Discovery via `ssh <yourusername>@login.discovery.neu.edu`. You should now be connected without having to enter your password.

Note: If you are using a Windows machine using MobaXterm, sign in to the HPC as usual, then complete steps 6 through 9 to complete the passwordless ssh setup.

---

6. Type `cd ~/.ssh` to move to your ssh folder.
7. Type `ssh-keygen -t rsa` to generate your key files.
8. Press Enter to all the prompts (do not generate a passphrase). If prompted to overwrite a file, type `Y`.

9. Type `cat id_rsa.pub >> authorized_keys`. This adds the contents of your public key file to a new line in the `~/.ssh/authorized_keys` file.

Next Steps

After you are connected, you can run jobs either in interactive mode with `srun` or submit a script using `sbatch`. See *Using srun* and *Using sbatch* for more information.

To load and run software, see *Software Overview*.

To find out more about the hardware and partitions on Discovery, see *Hardware Overview* and *Partitions*.

For our introductory training video, go to Northeastern's LinkedIn Learning page.

CHAPTER

FIVE

CONNECTING WINDOWS

You connect to Discovery using a secure shell program to initiate an SSH session to sign in to Discovery. This topic is about how to connect using Windows. See *connect mac* for information about connecting with a Mac.

Before you can connect to Discovery on a Windows computer, you'll need to download a terminal program, such as MobaXterm or PuTTY. We recommend MobaXterm, as you can also use it for file transfer, whereas with other SSH programs, you would need a separate file transfer program.

To connect to Discovery with MobaXterm:

1. Open MobaXterm.
2. Click **Session**, then click **SSH** as the connection type.
3. In **Remote Host**, type `login.discovery.neu.edu`, make sure **Port** is set to 22, and click **OK**. (OPTIONAL: You can type your Northeastern username and password on MobaXterm, and it will save that information every time you sign in. If you opt to do this, you will be connected to Discovery after you click OK.)
4. At the prompt, type your Northeastern username and press Enter.
5. Type your Northeastern password and press Enter. Note that the cursor does not move as you type your password. This is expected behavior.

You are now connected to the cluster's login node.

Watch this video to see how to connect to the cluster with MobaXterm. If you do not see any controls on the video, right click on the video to see viewing options.

5.1 Passwordless ssh on Windows

You need to setup passwordless ssh to ensure that GUI-based applications will launch without any issues. You also need to make sure that your keys are added to the authorized.key file. This needs to be done anytime you regenerate your keys. If you're having an issue with opening an application that need X11 forwarding, such as MATLAB or Schrodinger, and you recently regenerated your keys, make sure to add your keys to the authorized.key file.

Note: Errors that you can see on Windows when launching a GUI-based program include the following:

```
Error:  unable to open display localhost:19.0
```

```
Launch failed:  non-zero return code
```

If you are getting these types of errors, follow the steps below to set up passwordless ssh.

To set up passwordless ssh:

1. Sign in to the cluster using MobaXterm.

2. Type `cd ~/.ssh` to move to your ssh folder.
3. Type `ssh-keygen -t rsa` to generate your key files.
4. Press `Enter` to all the prompts (do not generate a passphrase). If prompted to overwrite a file, type `Y`.
5. Type `cat id_rsa.pub >> authorized_keys`. This adds the contents of your public key file to a new line in the `~/.ssh/authorized_keys`.

Next Steps

After you are connected, you can run jobs either in interactive mode with `srun` or submit a script using `sbatch`. See *Using srun* and *Using sbatch* for more information.

To load and run software, see *Software Overview*.

To find out more about the hardware and partitions on Discovery, see *Hardware Overview* and *Partitions*.

For our introductory training video, go to Northeastern's LinkedIn Learning page.

CHAPTER

SIX

ACCESSING OPEN ONDEMAND

Open OnDemand (OOD) is a web portal to the Discovery cluster.

This topic is for connecting to the Discovery cluster through the browser application, Open OnDemand. If you are looking to access Discovery directly on your system rather than through a browser, please see *Connecting Mac* for connecting with a Mac and *Connecting Windows* for connecting with Windows.

A Discovery account is necessary for you to access OOD. If you need an account, see *Getting Access*. After you have created a Discovery account, proceed with the following steps in order to access Discovery.

To Access Discovery through Open OnDemand (OOD), do the following

1. In a web browser, go to http://ood.discovery.neu.edu.
2. At the prompt, enter your Northeastern username and password. Note that your username is the first part of your email without the @northeastern, such as **j.smith**.
3. Press **Enter** or click **Sign in**.

Watch the following video for a short tutorial. If you do not see any controls on the video, right-click on the video to see viewing options.

6.1 OOD: next steps

After you are connected, you use the interactive apps in OOD. See *OOD Interactive Apps* for more information.

CHAPTER

SEVEN

SHELL ENVIRONMENT ON THE CLUSTER

7.1 The Discovery Shell environment and .bashrc

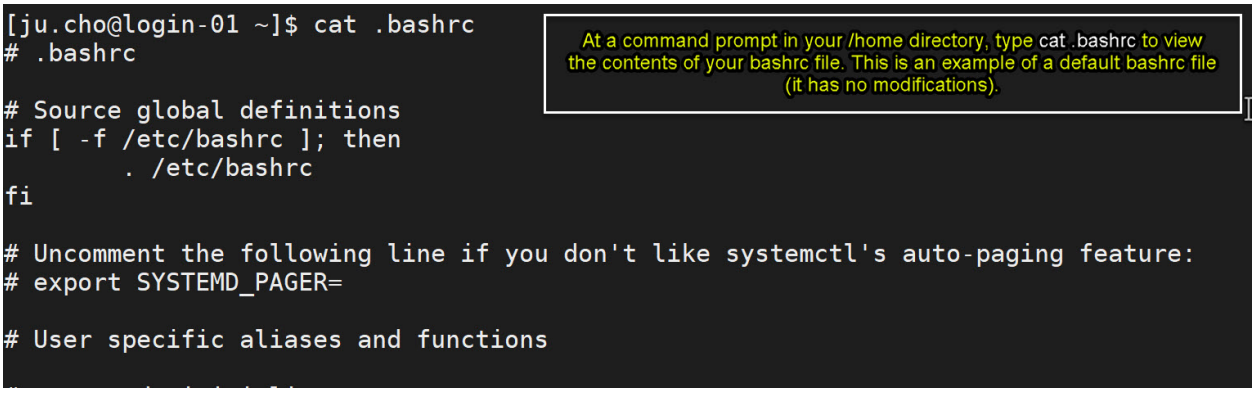
Discovery uses a Linux-based Operating System (CentOS), where the Shell program is used to interface with the user. Bash (Bourne Again SHell) is one of the most popular Shell implementations which is the default Shell on Discovery.

The Shell script `.bashrc` is used by Bash to initialize your Shell environment. For example, it is typically used to define aliases, functions and load modules. Note that environment variables settings (such as `PATH`) generally go in the `.bash_profile` or `.profile` files. Your `.bashrc`, `.bash_profile` and `.profile` files live in your `$HOME` directory. You can make changes to your .bashrc with a text editor like nano.

> **Caution:** Making edits to your `.bashrc` file can result in many issues. Some changes may prevent you from launching apps or executing commands. Modifying your `PATH` variable may result in the inability to use basic Shell commands (such as `cd` or `ls`) if not done correctly.
>
> Before making changes to your `.bashrc` file, make a backup of the default `.bashrc` file, so you can restore it if necessary. If you need help with editing `.bashrc`, reach out to mailto:rchelp@northeastern.edu or schedule a consultation with a staff member who can help suggest edits and troubleshoot any issues you might be having.

7.2 About your .bashrc file

You have a default `.bashrc` file in your home directory when your account is created. See the figure below for an example of a default `.bashrc` file.



Important: We recommend to keep .bashrc unchanged when using Discovery. You can source environment Shell scripts or load modules directly inside your job instead. This approach can prevent some runtime errors from load-

ing incompatible modules, setting environment variables incorrectly, or from mixing multiple software and Conda environments.

7.3 Conda and `.bashrc`

In addition to editing your `.bashrc` file as outlined in the example above, programs that you install can also modify your .bashrc file. For example, if you follow the procedure outlined in *Using Miniconda*, there may be a section added to your `.bashrc` file (if you didn't use the `-b` batch option) that automatically loads your conda environment every time you sign in to Discovery. See the figure below for an example of this:

```
# .bashrc

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi

# Uncomment the following line if you don't like systemctl's auto-paging feature:
# export SYSTEMD_PAGER=

# User specific aliases and functions

# >>> conda initialize >>>
# !! Contents within this block are managed by 'conda init' !!
__conda_setup="$('/home/ju.cho/miniconda3/bin/conda' 'shell.bash' 'hook' 2> /dev/null)"
if [ $? -eq 0 ]; then
    eval "$__conda_setup"
else
    if [ -f "/home/ju.cho/miniconda3/etc/profile.d/conda.sh" ]; then
        . "/home/ju.cho/miniconda3/etc/profile.d/conda.sh"
    else
        export PATH="/home/ju.cho/miniconda3/bin:$PATH"
    fi
fi
unset __conda_setup
# <<< conda initialize <<<
```

You should not modify this section in the `.bashrc` file directly. If it was changed, remove this section manually using a file editor.

Caution: We recommend removing the conda initialization section from your `.bashrc` as it may interfere with the correct startup environment when using Open OnDemand apps. You should always load your Conda environment after your job already started.

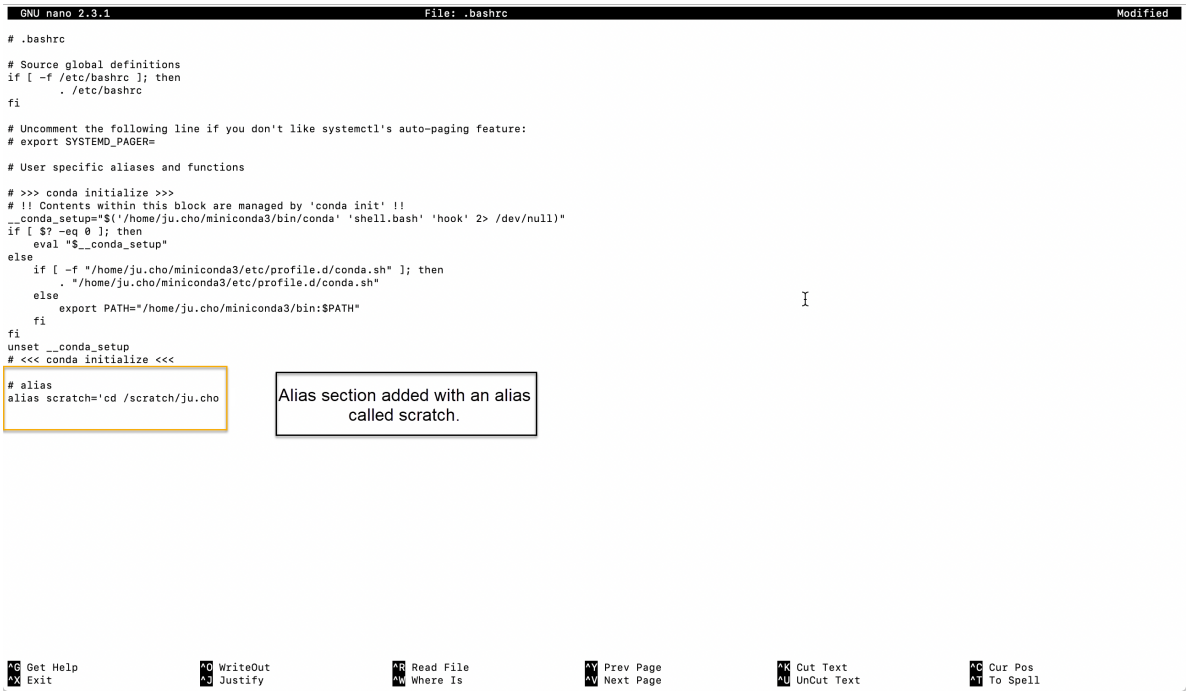
If you need help with your .bashrc file or would like it restored to its default, reach out to the RC team at mailto:rchelp@northeastern.edu, and we can provide you with a new, default `.bashrc` file and help troubleshoot issues with the file.

7.3.1 Editing your `.bashrc` file

The basic workflow for editing your `.bashrc` file is to sign in to Discovery, go to your `$HOME` directory, open the file in a text editor on the command line, make your edits, save the file, sign out of Discovery, then sign back in again. Your changes will take effect when you have signed back in again.

Example procedure for editing your `.bashrc` file:

1. Sign in to Discovery.
2. (Optional) Type `pwd` to make sure you are in your `/home` directory.
3. (Optional) Type `ls -a` to view the contents of your `/home` directory, including hidden files. Your .bashrc file is a hidden file (hidden files are preceded by a `.`). Using the `-a` option with `ls` displays hidden files.
4. (Recommended) Type `cp .bashrc .bashrc-default` to make a copy of your .bashrc file called `.bashrc-default`.
5. Type `nano .bashrc` to open your .bashrc file in the nano text editor.
6. Type the edits that you want to make to your file. In this example, an alias was added to create a shortcut to the user's `/scratch` space.



7. Save the file and exit the editor.
8. Sign out of Discovery and sign back in for the changes to take effect.

7.3.2 Sourcing a Shell script example

A safe alternative to using `.bashrc` is to source a Shell script inside your runtime job environment. Below is an example script to load an Anaconda module and source a Conda environment which will then be used inside the Slurm script.

Create a Shell script `myenv.bash`:

```
#!/bin/bash
module load anaconda3/2021.05
module load cuda/11.1
source activate pytorch_env_training
```

Then, source the Shell script inside your sbatch Slurm script (see *Using sbatch*):

```
#!/bin/bash
#SBATCH --partition=gpu
#SBATCH --nodes=1
#SBATCH --gres=gpu:1
#SBATCH --time=01:00:00
#SBATCH --job-name=gpu_run
#SBATCH --mem=4GB
#SBATCH --ntasks=1
#SBATCH --output=myjob.%j.out
#SBATCH --error=myjob.%j.err

source myenv.bash
python <myprogram>
```

CHAPTER

EIGHT

HARDWARE OVERVIEW

The Discovery computing cluster provides you with access to over 1024 CPU nodes, 50,000 CPU cores, and over 200 GPUs and is connected to the university network over 10 Gbps Ethernet (GbE) for high-speed data transfer. Compute nodes are connected to each other with either 10 GbE or a high-performance HDR200 InfiniBand (IB) interconnect running at 200 Gbps (with some nodes running HDR100 IB, if HDR200 IB is not supported on those nodes).

8.1 CPU nodes

Table 1 below shows the feature names, number of nodes by partition type (public and private), and the RAM memory range per node. The feature name follows archspec microachitechture specification.

Feature Name	Number of Nodes - public, private	RAM memory per node
skylake	0, 170	186 - 3094 GB
zen2	40, 292	256 - 2000 GB
zen	40, 300	256 - 2000 GB
ivybridge	64, 130	31 - 1031 GB
sandybridge	8, 0	384 GB
haswell	230, 62	109 - 1031 GB
broadwell	756, 226	128 - 515 GB
cascadelake	260, 88	186 - 3094 GB

If you are looking for information about GPUs, see *Working with GPUs*.

If you are interested in more information about the different partitions on Discovery, including the number of nodes per partition, running time limits, job submission limits, and RAM limits, see *Partitions*.

8.2 Using the `--constraint` flag

When using `srun` or `sbatch`, you can specify hardware features as part of your job by using the `--constraint=` flag. This may be particularly useful when benchmarking, optimizing, or if you're using code that was compiled on a certain micro-architecture. Currently, you can use the `--constraint=` flag to restrict your job to a specific feature name (e.g., `haswell`, `ivybridge`) or you can use the flag: `ib` to only include nodes that are connected by InfiniBand (IB) with a job that needs to use multiple nodes.

A few examples using `srun`:

```
srun --constraint=haswell --pty /bin/bash
srun --constraint=ivybridge --pty /bin/bash
```

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```
    srun --constraint=ib --pty /bin/bash
    srun --constraint="[ivybridge|zen2]" --pty /bin/bash #this uses the OR operator |␣
↪to select either an ivybridge or zen2 node.
```

You can add these same flags as an additional line in your `sbatch` script via (`#SBATCH --constraint=haswell`)

Note: Using the –constraint flag can mean that you will wait longer for your job to start, as the scheduler (Slurm) will need to find and allocate the appropriate hardware that you have specified for your job. For more information about running jobs, see *Using Slurm*. Finally, at this time only the OR operator `|` is supported when using `--constraint`.

CHAPTER

NINE

PARTITIONS

9.1 Introduction

Partitions are logical collections of nodes that comprise different hardware resources and limits to help meet the wide variety of jobs that get scheduled on Discovery. Occasionally, the Research Computing team might need to make updates to the partitions based on monitoring job submissions to help reduce job wait times. As our cluster grows, changes to the partitions also help to ensure the fair, efficient distribution of resources for all jobs being submitted to the cluster.

On Discovery, there are several partitions:

- General access (`debug`, `express`, `short`, `gpu`)
- Application only (`long`, `large`, `multigpu`)
- PI owned (accessed only by members of the PIs' group)

The general access and application only partitions span the hardware on Discovery, with `gpu` and `multigpu` spanning the GPUs on Discovery and the other partitions spanning the CPUs. For example, if you use the `debug` partition you're using the same hardware as `short`, just with different time, job, and core limits. Refer to the tables below for detailed information on the current partitions. Note that PI-owned partitions only include the hardware that those PIs own and are only accessible to the members of the PI's group.

Note: In the following table, the Running Jobs Per User/Per Research Group. Core and RAM limits are set per user, across all running jobs (not pending).

Name	Requires approval?	Time limit (default/max)	Running jobs	Submitted jobs	Core limit (per user)	RAM limit	Use Case
debug	No	20 minutes/20 minutes	10/25	5000	128	256GB	Best for serial and parallel jobs that can run under 20 minutes. Good for testing code.
express	No	30 minutes/60 minutes	50/250	5000	2048	25TB	Best for serial and parallel jobs that can run under 60 minutes.
short	No	4 hours/24 Hours	50/500	5000	1024	25TB	Best for serial or small parallel jobs (`--nodes=2` max) that need to run for up to 24 hours.
long	**Yes**	1 day/5 Days	25/250	1000 per user/5000 per group	1024	25TB	Primarily for serial or parallel jobs that need to run for more than 24 hours. Need to prove that your code cannot be checkpointed to use this partition.
large	**Yes**	6 hours/6 Hours	100/100	1000 per user/5000 per group	N/A	N/A	Primarily for running parallel jobs that can efficiently use more than 2 nodes. Need to demonstrate that your code is optimized for running on more than 2 nodes.

Name	Requires approval?	Time limit (default/max)	Running jobs	Submitted jobs	GPU limit	GPU limit	Use Case
gpu	No	4 hours/8 Hours	25/250	50/100	1	8	For jobs that can run on a single GPU processor.
multigpu	**Yes**	4 hours/24 Hours	25/100	50/100	12	12	For jobs that require more than one GPU and take up to 24 hours to run.

9.2 Viewing partition information

Slurm commands allow you to view information about the partitions. Three commands that can show you partition information are `sinfo`, `sacct`, and `scontrol`. The following are common options to use with these commands:

```
sinfo -p <partition name> #displays the state of the nodes on a specific partition
sinfo -p <partition name> --Format=time,nodes,cpus,socketcorethread,memory,nodeai,
↪features #displays more detailed information using the Format option, including␣
↪features like the type of processors
sacct --partition <partition name> #displays the jobs that have been run on this␣
↪partition
scontrol show partition <partition name> #displays the Slurm configuration of the␣
↪partition
```

For more information about these commands, see the Slurm documentation site https://slurm.schedmd.com/.

9.3 Allocating partitions in your jobs

To specify a partition when running jobs, use the option `--partition=<partition name>` with either `srun` or `sbatch`. When using a partition with your job and specifying the options of `--nodes=` and `--ntasks=`, make sure that you are requesting options that best fit your job. **Requesting the maximum number of nodes or tasks will not make your job run faster or give you higher priority in the job queue.** It can actually have the opposite effect on jobs that are better suited to running with smaller requirements, as you have to wait for the extra resources that your job will not use. See *Using Slurm* for more information on using Slurm to run jobs.

Tip: You should always try to have job requests that will attempt to allocate the best resources for the job you want to run. For example, if you are running a job that is not parallelized, you only need to request one node (`--nodes=1`). For some parallel jobs, such as a small MPI job, you can also use one node (`--nodes=1`) with the `--ntasks=` option set to correspond to the number of MPI ranks (tasks) in your code. For example, for a job that has 12 MPI ranks, request 1 node and 12 tasks within that node (`--nodes=1 --ntasks=12`). If you request 12 nodes, Slurm is going to run code between those nodes, which could slow your job down significantly if it isn't optimized to run between nodes.

If your code is optimized to run on more than 2 nodes and needs less than one hour to run, you can use the express partition. If your code needs to run on more than 2 nodes for more than one hour, you should apply to use the large partition. See the section Partition Access Request below for more information.

9.4 Partition Access Request

If you need access to the large, long, or multigpu partition, you need to submit a ServiceNow ticket. Access is not automatically granted. You will need to provide details and test results that demonstrate your need for access for these partitions. If you need temporary access to multigpu to perform testing before applying for permanent access, you should also submit a ServiceNow ticket. All requests are evaluated by members of the RC team, and multigpu requests are also evaluated by two faculty members.

CHAPTER

TEN

SOFTWARE OVERVIEW

Discovery offers you many options for working with software. Two of the easiest and most convenient ways are using the `module` command on the command line and using the interactive apps on Open OnDemand (OOD), Discovery's web portal. If you need a specific software package, first check to see if it is already available through one of the preinstalled modules on Discovery. The Research Computing team adds new modules regularly, so use the `module avail` command to view the most up-to-date list. You can also try using Spack, a software package manager available on Discovery. Spack has over 5,000 packages that you can install.

Using Module For more information about working with module.

OOD Interactive Apps For more information about OOD.

Using Spack For more information about Spack.

You can also use Conda, Miniconda, and Anaconda to manage software packages. See *Using Conda* for more information.

10.1 Using Make

If you want to use `make` to add software locally to you path you must first download the software package from its source (such as a webpage or GitHub), and you need to unpack it or unzip it, if need be. Then, you must set the installation path to a directory where you have write access on Discovery, such as your home directory. You can use `./configure` to do this, such as `./configure --prefix=/home/<yourusername>/software` After you have set the installation path, you need to compile the code using `make` and then install the software using `make install`.

10.2 Requesting Software Installation Assistance

If the software that you need is not a module on Discovery, cannot be installed through Spack, or is not available through another way of self-installation (such as using `make`), you can submit a ServiceNow software request ticket. Be aware that there might be packages that cannot be installed on Discovery due to incompatibility with the hardware on Discovery.

CHAPTER

ELEVEN

USING MODULE

The module system on Discovery includes many commonly used scientific software packages that you can load in your path when you need it and unload it when you no longer need it.

Use the `module avail` command to show a list of the most currently available software on Discovery.

Note: Some modules might conflict with each other, resulting in the software not behaving as expected. Also, if there are multiple versions of software, and you load more than one version of the software, only the latest version will be used. Use `module list` to view the modules you currently have loaded in your path.

Tip: Use the `which` command to display which version of a software package you have in your path. For example, `which python` will display the version of python that you have in your path.

11.1 Module commands

The following are common module commands that are useful for interacting with software packages on Discovery.

Module Command	Function
`module avail`	View a list of all of the available software packages on Discovery that you can load
`module list`	Displays a list of the software packages currently loaded in your path
`module show <module name>`	View the details of a software package (see the section "Module Show" below for more information)
`module load <module name>`	Load a software package into your environment
`module unload <module name>`	Remove a single software package from your environment
`module purge`	Removes all of the loaded software packages from your environment.

Caution: Using `module purge` will purge all modules from your environment, including the default module `discovery/2019-02-21`. This module contains the http proxy needed for nodes to have internet access. If you accidentally purge this module, it will be automatically reloaded the next time you log out and log back in again. You can also load it manually if you have purged it by using the `module load` command.

11.2 Module show example

Before loading a module, type `module show <name of module>` to see if there are any dependencies or commands that you need to execute before loading the module. In some cases, a module might depend on having other modules loaded to work as expected. While modules are a convenient way of loading software to use on Discovery, scientific software can come with many packages and dependencies. In addition to module, you should review other ways of loading software on Discovery. See *Software Overview* for more information on different ways you can install software on Discovery. The figure below shows an example of `module show` with the software package called amber.

```
[ju.cho@login-01 ~]$ module show amber
-------------------------------------------------------------------
/shared/centos7/modulefiles/amber/18-mpi:

module-whatis    loads the modules environment for Amber 18 MPI parallel executible on CPU nodes.

Please load the following modules:
module load openmpi/3.1.2
module load amber/18-mpi
module load python/2.7.15

setenv           AMBER_HOME /shared/centos7/amber/amber18-cpu
prepend-path     PYTHONPATH /shared/centos7/amber/amber18-cpu/lib/python2.7/site-packages
prepend-path     PATH /shared/centos7/amber/amber18-cpu/bin
prepend-path     LD_LIBRARY_PATH /shared/centos7/amber/amber18-cpu/lib
prepend-path     C_INCLUDE_PATH /shared/centos7/amber/amber18-cpu/include
prepend-path     CPLUS_INCLUDE_PATH /shared/centos7/amber/amber18-cpu/include
-------------------------------------------------------------------
```

11.3 Module load and unload example

In the figure below, the software module stata/15 was loaded and then unloaded. After loading and unloading, module list was used to check that the STATA was loaded and unloaded.

```
[ju.cho@login-00 ~]$ module load stata/15
[ju.cho@login-00 ~]$ module list
Currently Loaded Modulefiles:
  1) discovery/2019-02-21   2) stata/15
[ju.cho@login-00 ~]$ module unload stata/15
[ju.cho@login-00 ~]$ module list
Currently Loaded Modulefiles:
  1) discovery/2019-02-21
```

11.4 Using software applications with X11 Forwarding

If you are attempting to open a GUI-based software application that uses X11 forwarding to display, such as MATLAB or Maestro, and you get an error such as `Error: unable to open display localhost:19.0`, this is most likely due to an issue with passwordless SSH. See *Using X11* for tips and troubleshooting information opening applications that use X11 forwarding.

CHAPTER

TWELVE

USING MATLAB

MATLAB is available as a module on Discovery (see *Using Module* for more information), and it is also an interactive app on Open onDemand (see *Introduction to OOD* for more information). You can also download MATLAB for use with your personal computer through the Northeastern portal on the MATLAB website. Note that the procedures detailed below are specific to using MATLAB on Discovery and not with using MATLAB on your personal computer.

12.1 Installing MATLAB toolboxes

Use the following procedure if you need to install a MATLAB toolbox:

1. Download the toolbox from its source website.
2. Connect to Discovery.
3. Create a directory in your /home directory. We recommend creating a directory called `matlab` by typing:

```
mkdir /home/<username>/matlab  #where <username> is your username
```

4. Go to the directory you just created by typing:

```
cd /home/<username>/matlab
```

5. Unzip the toolbox file by typing:

```
unzip <toolboxname>
```

6. Load MATLAB by typing:

```
module load matlab
```

7. Start MATLAB by typing:

```
matlab
```

8. Add the toolbox to your PATH by typing:

```
addpath('/home/<username>/matlab/<toolbox>') #where <toolbox> is the name of the␣
↪toolbox you just unzipped
```

9. If this is a toolbox you want to use more than once, you should save it to your path by typing:

```
savepath()
```

10. You can now use the toolbox within MATLAB. When you are done, type `quit`.

12.2 Using MATLAB Parallel Server

The Discovery cluster has MATLAB Parallel Server installed. This section details an example of how you can setup and use the MATLAB Parallel Computing Toolbox. This walkthrough uses MATLAB 2020a launched as an interactive app on the Open onDemand web portal. There are several parts to this walkthrough. We suggest that you read it through completely before starting. The parameters presented represent only one scenario.

This walkthrough will use Open onDemand, the web portal on Discovery, to launch MATLAB. You'll then create a cluster profile. This allows you to define cluster properties that will be applied to your jobs. Supported functions are *batch, parpool, and parcluster*. The Parallel Computing Toolbox comes with a cluster profile called *local*, which you will change in the walkthrough below.

Note: This walkthrough details submitting jobs through Discovery's Open onDemand web portal. Some parameters will vary if you are using MATLAB from the command line. This walkthrough does not apply to other versions of MATLAB.

Before starting, you should create a folder in your `/scratch/<yourusername>` directory. This folder is where you'll save your job data.

1. Go to your /scratch directory: `cd /scratch/<yourusername>` where `<yourusername>` is your NU username
2. Make a new folder. We suggest calling it *matlab-metadata*: `mkdir matlab-metadata`

To start MATLAB and add a Cluster Profile, do the following:

1. Go to http://ood.discovery.neu.edu. If prompted, sign in with your Discovery username and password.
2. Click **Interactive Apps**, and select **MATLAB**.
3. Select **MATLAB version 2020a**, and keep the default time of 1 hour and default memory of 2GB. Click **Launch**.
4. If necessary, adjust the **Compression** and **Image Quality**, and then click **Launch MATLAB**.
5. On the MATLAB Home tab, in the **Environment** section, select **Parallel**, then click **Create and Manage Clusters**. This opens the Cluster Profile Manager window.
6. On the Cluster Profile Manager window, select **Add Cluster Profile**, then click **Slurm**. If prompted, click **OK** to the notice about needing Parallel Server.
7. Double click the new profile name in the Cluster Profile column, and type a name such as **TestProfile**. Press **Enter** to save the change.
8. Select **Edit** in the **Manage Profile** section. This lets you edit the options on the **Properties** tab. For this walkthrough, make the following edits:
    1. In the **Folder where job data is stored on the client** option, type `/scratch/<yourusername>/matlab-metadata` (this is the directory that you created in the first procedure above).
    2. In the **Number of workers available to cluster** option, type a number between between 1 and 10. This field is the number of MPI processes you intend to run. This corresponds to the `--ntasks` Slurm option. The maximum is 128 per job; however, for this task, we recommend keeping it lower and use threading inside the nodes. The number you set here will be the default maximum for the job. You can set it for less than or equal to this number in the MATLAB Command Window when submitting your job.
    3. In the **Number of computational threads to use on each worker** option, type a number between 1 and 10. This field represents the number of threads that each worker will possess. This corresponds to `cpus-per-task` in Slurm. Do not exceed the number of available cores on the node.
9. When you have finished editing your properties, click **Done**.

10. (Optional) If you want to validate your setup, click the **Validation** tab (next to the Properties tab). Ensure all the stages are checked, then click the **Validate** button at the bottom of the page.

This will check the properties of your profile. You might need to wait a minute or two for this to complete.

> **Caution:** Do not click the green **Validate** button. This will attempt validation using the maximum number of workers, which can cause the validation to hang or fail. If you accidentally click the green Validate button, click **Stop** to end the validation process.

(OPTIONAL) In the **Cluster Profile** column, right-click on the TestProfile name and select **Set as Default**. This sets your profile to be the default.

Now that you have set up your profile, you can use the default cluster profile you just created (*TestProfile*) with the following commands:

```
#with parpool
parallel.defaultClusterProfile('TestProfile')
parpool

#with parcluster
c = parcluster('TestProfile')
```

12.2.1 Using parcluster example

This section will detail how to submit batch jobs to the cluster to perform scaling calculations for an integer factorization sample problem. It's a computationally intensive problem, where the complexity of the factorization increases with the magnitude of the number. We'll use the myParallelAlgorithmFcn.m MATLAB function. This section assumes you have configured a MATLAB Cluster Profile according to the procedure above.

On Discovery, there are benchmarking scripts and examples located in the `/shared/centos7/matlab/R2020a/examples/parallel/main` folder. To add the path to this folder to the list of available paths, do one of the following:

- On the MATLAB Home tab, in the **Environment** section, click **Set Path** and add the path to the script.
- Alternatively, provide the full path of the script in the MATLAB command line.

The contents of myParallelAlgorithmFcn are as follows:

```
function [numWorkers,time] = myParallelAlgorithmFcn ()

complexities =  [2^18 2^20 2^21 2^22];
numWorkers = [1 2 4 6 16 32 64];

time = zeros(numel(numWorkers),numel(complexities));

% To obtain predictable sequences of composite numbers, fix the seed
% of the random number generator.
rng(0,'twister');

for c = 1:numel(complexities)

   primeNumbers = primes(complexities(c));
   compositeNumbers =    primeNumbers.*primeNumbers(randperm(numel(primeNumbers)));
   factors = zeros(numel(primeNumbers),2);
```

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```
   for w = 1:numel(numWorkers)
       tic;
       parfor (idx = 1:numel(compositeNumbers), numWorkers(w))
          factors(idx,:) = factor(compositeNumbers(idx));
       end
       time(w,c) = toc;
   end
end
```

To submit myParallelAlgorithmFcn as a batch job, in the MATLAB Command Window, type:

```
totalNumberOfWorkers = 65;
cluster = parcluster('TestProfile');
job = batch(cluster,'myParallelAlgorithmFcn',2,'Pool',totalNumberOfWorkers-1,
↪'CurrentFolder','.');
```

This specifies the `totalNumberOfWorkers` as 65, where 64 workers will be issued to run *parfor* in parallel (so the pool is set as 64), and the additional worker will run the main process.

To monitor the job after you submit it, click **Parallel**, then **Monitor Jobs** to open the Job Monitor. You can view some job information, such as the state of the job (i.e. running, failed, finished etc.), as well as the ability to fetch outputs if you right-click on the job line.

You can close MATLAB after you submit the job the scheduler. The job monitor tool will keep track of the jobs.

If you want to block MATLAB until the jobs are finished, type `Wait(job)`.

When the jobs complete, you can transfer the outputs of the function using the `fetchOutputs` command:

```
outputs = fetchOutputs(job);
numWorkers = outputs{1};
time = outputs{2};
```

You can plot the performance (speedup) by typing:

```
figure
speedup = time(1,:)./time;
plot(numWorkers,speedup);
legend('Problem complexity 1','Problem complexity 2','Problem complexity 3','Problem␣
↪complexity 4','Location','northwest');
title('Speedup vs complexity');
xlabel('Number of workers');
xticks(numWorkers(2:end));
ylabel('Speedup');
```

CHAPTER

THIRTEEN

USING CONDA

Conda is an open source environment and package manager. Miniconda is a free installer for Conda, Python, and comes with a few other packages. Anaconda is also a package manager that has a much larger number of packages pre-installed.

A question that frequently comes up is "Should I use Anaconda or Miniconda?"

Note: It is not recommended to build your Miniconda and Conda virtual environments inside your /home directory due to its limited space quota (see *Storage Accessible on Discovery*). Use the /work file system instead. If your group needs access to /work, the group PI can request it using: New Storage Space request.

13.1 Creating an Environment

Using a locally installed Conda virtual environment is highly recommended so that you can install the specific packages that you need. You can also have more than one environment with different packages for different research projects or for testing purposes. This procedure uses the Anaconda module already available on Discovery.

If you are on a login node, move to a compute node by typing:

Listing 1: Requesting 1 node with 1 cpu core and load anaconda.

```
srun --partition=short --nodes=1 --cpus-per-task=1 --pty /bin/bash
module load anaconda3/2022.05
```

To create a new Conda environment where <environment-name> is the path and name. You can see a list of your existing environments with `conda env list`.

```
conda create --prefix=/<path>/<environment-name> python=3.11 anaconda
```

Follow the prompts to complete the Conda install, then activate the environment.

```
source activate /<path>/<environment-name>
```

Your command line prompt will then include the path and name of environment.

```
(/<path>/<environment-name>) [username@c2001 dirname]$
```

Tip: `conda config --set env_prompt '({name}) '` modifies your `.condarc` to only show the environments name as such:

```
(<environment-name>) [username@c2000 dirname]$
```

With your Conda environment activated you can install a specific package with

```
conda install [packagename]
```

To deactivate the current active Conda environment

```
conda deactivate
```

To delete a Conda environment and all of its related packages, run:

```
conda remove -n yourenvironmentname --all
```

13.2 Using Miniconda

This procedure assumes that you have not installed Miniconda. If you need to update Miniconda, do not follow the installation procedure. Use `conda update`. This procedure uses the Miniconda3 version with Python version 3.8 in step 2, although there are other versions you can install (e.g., 3.9 or 3.11).

13.2.1 Installing Miniconda

Attention: Make sure to log on to a compute node.

```
srun --partition=short --nodes=1 --cpus-per-task=1 --pty /bin/bash
```

Download Miniconda, check the hash key, and install as follows:

```
wget --quiet https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
sha256sum Miniconda3-latest-Linux-x86_64.sh
bash Miniconda3-latest-Linux-x86_64.sh -b -p <dir>
```

Where <dir> is the full path to your desired installation directory (e.g., `/work/mygroup/mydirectory/miniconda3`).

Activate the base Miniconda environment

```
source <dir>/bin/activate
```

You can now create a new environment with this command where we're using python version 3.8:

```
conda create --name my-py38env python=3.8
```

Type `y` if asked to proceed with the installation.

Now you can activate your new environment

```
conda activate my-py38env
```

To deactivate the environment, type `conda deactivate`. You can type this command again to deactivate the base Miniconda environment.

13.3 Conda Best Practices

See also:

Best practices for home storage: *Conda*.

1. Your `~/.conda` may get very large if you install multiple packages and create many virtual Conda environments. Make sure to clean the Conda cache and clean unused packages with: `conda clean --all`.
2. Clean unused Conda environments by first listing the environments with: `conda env list` , and then removing unused ones: `conda env remove --name <environment-name>`.
3. You can build Conda environments in different locations to save space on your home directory (see *Storage Accessible on Discovery*). You can use the `--prefix` flag when building your environment. For example: `conda create myenv --prefix=/work/<mygroup>/<mydirectory>`.
4. Another recommended step is to update your Conda version (possible only when using Miniconda): `conda update conda -y`

CHAPTER

FOURTEEN

USING SPACK

Research Computing recommends using Spack to conveniently install software packages locally to your path. Please refer to the Spack documentation for the latest information about the packages that Spack contains. To use Spack, you first need to copy it to your `/home` directory or a `/work` directory, then you need to add it to your local environment.

Note: Spack software installations are part of your research and should preferably be stored in your PI's `/work` directory.

14.1 Getting started with Spack

These instructions will demonstrate how to install Spack in your local `/home` directory (step 2) and then how to add Spack to your local environment while on a compute node, so you have access to the Spack commands (steps 4-5).

1. Connect to Discovery via ssh (*Connecting Mac* or *Connecting Windows*).
2. From the terminal, type `git clone -c feature.manyFiles=true https://github.com/spack/spack.git` to copy Spack to your `/home`.
3. Type `srun -p short --pty -N 1 -n 28 /bin/bash` to allocate an interactive job on a compute node. Spack will attempt to run `make` in parallel when Spack builds the software you choose to install, so this `srun` request is for 28 cores on one node (`-N 1 -n 28`). To use Spack, it needs to add it to your local environment on the compute node, which is why this is completed after step 3.
4. To use a newer version of python for compatibility with Spack, type: `module load python/3.8.1`.
5. To add Spack in your local environment so you can use the Spack commands, type `export SPACK_ROOT=/home/<yourusername>/spack`.
6. Next, type `. $SPACK_ROOT/share/spack/setup-env.sh`.
7. After you have the Spack commands in your environment, type `spack help` to ensure Spack is loaded in your environment and to see the commands you can use with Spack. You can also type `spack list` to see all the software that you can install with Spack, but note this command can take a few moments to populate the list.
8. To see information about a specific software package, including options and dependencies, type `spack info <software name>`. Make sure to note the options and/or dependencies that you want to add or not add before installing the software.
9. To install a software package plus any dependencies or options, type `spack install <software name> +<any dependencies or options>`; you can specify `-<any dependencies or options>`. You can also list + or - different options and dependencies within the same line. Do not put a space between each option/dependency that you list.

10. To view your installed software packages, type `spack find`. If you want to view information about a specific installed package, type `spack find <software package name>`.

When you have installed a software package, you can add it to the module system by typing: `. $SPACK_ROOT/share/spack/setup-env.sh`

Note: Spack can be installed in a `/work`, which enables members of the `/work` to use the programs that are installed with Spack in that directory.

14.2 Installing LAMMPS with Spack example

This section details how to install the LAMMPS application with the KOKKOS and User-reaxc packages using Spack. This example assumes that you do not have any previous versions of LAMMPS installed. If you have any previous versions of LAMMPS, you must uninstall them before using this procedure. To see if you have any previous versions of LAMMPS, type `spack find lammps`. If you do have a previous version, you will need to uninstall LAMMPS by typing `spack uninstall --dependents lammps`. Then, you can try the example procedure below. Note that the installation can take about two hours to complete. As part of the procedure, we recommend that you initiate a screen session so that you can have the installation running as a separate process if you need to do other work on Discovery. If you decide to use screen, make note of the compute node number (compute node numbers start with c or d with four numbers, such as c0123) to make it easier to check on the progress of the installation.

1. Install Spack by following steps 1 through 5 in the *Getting started with Spack* procedure above.
2. Type `exit` to exit from the compute node you requested in step 2 above.
3. Type the following to request a GPU node for 8 hours:

```
srun --partition=gpu --nodes=1 --ntasks=14 --pty --export=All --gres=gpu:1 --mem=0 -
↪-time=08:00:00 /bin/bash
```

4. (Optional) Initiate a `screen` session:
    1. Type `screen -S lammps-install` to create a screen session.
    2. Type `screen -ls` to check to see if the session was created (you'll see it listed if it was successfully created).
    3. Type `screen -rd lammps-install` to enter that screen session.
    4. Type `echo $STY` to check that you are in the screen session.
    5. Type `CTRL+A+D` to exit the screen.
5. Type:

```
spack install lammps +asphere +body +class2 +colloid +compress +coreshell +cuda \
cuda_arch=70 +cuda_mps +dipole +granular +kokkos +kspace +manybody +mc +misc +molecule \
+mpiio +peri +python +qeq +replica +rigid +shock +snap +spin +srd +user-reaxc +user-misc
```

1. Type `spack find LAMMPS` to view your installed software package.
2. Type `spack load lammps`.

CHAPTER

FIFTEEN

USING R

R is available as a module (see *Using Module* for more information) and it is also an interactive app on Open onDemand (see *Introduction to Open OnDemand (OOD)* for more information). You can also use R with Anaconda. See *Working with Conda/Miniconda/Anaconda* and the Anaconda documentation for more information

If you work with R packages, using a Packrat environment can be helpful. Use the procedure below to create a Packrat environment on Discovery.

15.1 Creating a Packrat Environment (for R)

Packrat is an application that helps you manage packages for R. After you create a new directory for your R project, you can then use Packrat to store your package dependencies inside it. For more information about Packrat, see the website: https://rstudio.github.io/packrat/.

1. Connect to Discovery.
2. Type `module load R/4.2.1`.
3. Create a new directory for your R project by typing, `mkdir /scratch/<username>/<directoryname>` where `<username>` is your username, and `<directoryname>` is the name of the directory you want to create for your R project. For example, `/scratch/j.smith/packrat_r`.
4. Create a new directory for your R project by typing, `mkdir /scratch/<yourusername>/<directoryname>` where `yourusername` is your user name, and `directoryname` is the name of the directory you want to create for your R project. For example, `/scratch/j.smith/r_testlab`
5. Open the R interface and install Packrat:

```
install.packages("packrat") # install in a local directory, as you cannot install as␣
↪root
```

5. Initialize the environment where R packages will be written to:

```
packrat::init("/scratch/<yourusername>/<directoryname>")
```

You can then install R packages that you need. For example, to install a package called `rtracklayer`, type the following:

```
if (!requireNamespace("BiocManager", quietly = TRUE))
install.packages("BiocManager")
BiocManager::install("rtracklayer")
```

When using RStudio in the OOD App:

The instructions below can be applied on any RStudio "flavor" available (i.e., RStudio, Geospatial, and Tidyverse). Once a packrat snapshot is created it can easily be transfered between flavors and even machines (e.g., personal laptop, Discovery).

1. Launch an RStudio instance on the OOD. Specify the flavor and other parameters as usual.
2. In the RStudio console type: `install.packages("packrat)`.

Note: This will install by default in `$HOME/R/x86_64-pc-linux-gnu-library/<version>/` as long as you don't have previous environments or those have been turned off (see below). For packrat installation, it is best to specify a "project folder" in your `$HOME`, `/scratch` or `/work` directory (if you do not have `/work` please see here for access). The location `/tmp/Rtmp8CbQCA/downloaded_packages` would not work because `/tmp` corresponds to the compute node that you were on while running the R session. Optimally, you would like to have the packrat location in a persistent place so that all packages and libraries are available to you at all times regardless of the compute node you are on.

---

3. Create a packrat project directory at the desired location by selecting "New Folder" in the "Files" tab in the lower right hand side of the RStudio screen. Alternatively, use `mkdir` in the terminal tab on the lower left-hand side of the RStudio screen. For example: `mkdir projectfolder`.
4. In the RStudio console, initialize the packrat. If your current directory is the project folder (i.e., `getwd() ==` "packrat project folder") you can omit the path here.

```
packrat::init("<path-to-project-folder>")
```

5. You can now record all the currently installed packages to your packrat with the snapshot command. This may take some time if you have installed a lot of packages.

```
packrat::snapshot()
```

6. And now you can check on the status of your packrat with:

```
packrat::status()
```

7. Now turn packrat on. Packrat will now stay on for all your RStudio sessions and across the RStudio flavors (RStudio, geospatial, and tidyverse).

```
packrat::on()
```

8. You can now install packages as normal. You should see the install location for your packrat project folder. E.g., "Installing package into '/work/groupname/username/packrat_R/'"

```
install.packages("viridis")
```

15.2 Packrat Tips

- At any time you can check the status of your packrat with `packrat::status()`.
- Packrat can be toggled on and off with `packrat::on()` and `packrat::off()`, respectively.
- To disconnect packrat and allow for package installation outside of your packrat project folder: `packrat::disable(project = NULL, restart = TRUE)`, where `project` refers to the current packrat project folder, and `restart = TRUE` will restart the R session.
- To re-initialize packrat run: `packrat::init("<path-to-packrat-project-folder>")`. This will automatically restart your R session.
- A package can be removed from packrat via: `remove.packages("viridis)`, but will remain in your packrat snapshot and can be restored with: `packrat::restore()`.
- The function `packrat::clean(dry.run=T)` will list any unused packages that were installed in your snapshot. You can remove them with: `packrat::clean()`.

Note: For most cases, having a single packrat directory is sufficient, unless you notice specific package conflicts or need different versions of the same package. A single packrat directory also saves from having to install the same dependencies multiple times in different locations.

If the installation location is not setting to your project folder you may need to turn off these environments. In some cases, these folders could also be present in your `/work/groupname/<project-name>` directory.

```
mv ~/.rstudio ~/.rstudio-off
mv ~/.local ~/.local-off
mv ~/ondemand ~/ondemand.off
mv ~/.Rprofile ~/.Rprofile.off
mv ~/.Rhistory ~/.Rhistory.off
```

CHAPTER

SIXTEEN

USING MPI

Message Passing Interface (MPI) is a standard for writing message-passing programs. MPI itself is not a language. It defines a library interface, aimed at establishing a practical and easy-to-use standard for message passing. There are several implementations of MPI, such as Open MPI and MVAPICH.

16.1 MPI libraries on Discovery

These are the current versions of Open MPI, MVAPICH, and MPICH that are available on Discovery as modules.

```
openmpi/4.1.0-zen2-gcc10.1
openmpi/4.1.0-amd-intel2021
openmpi/4.0.5-skylake-gcc7.3
openmpi/4.1.0-gcc10.1-cuda11.2
openmpi/4.0.4-amd-intel2020u2
openmpi/4.0.5
openmpi/4.0.5-skylake-gcc10.1
openmpi/4.0.3-cuda
mpich/3.3.2-skylake-gcc7.3
mvapich2/2.3.4-intel2020
```

Use the `module show` command to view information about the compilers you need to use with these libraries and if they support InfiniBand (IB) or not. For example, `module show openmpi/4.1.0-zen2-gcc10.1`.

For assistance with getting started with using MPI or troubleshooting using MPI libraries on Discovery, reach out to us at rchelp@northeastern.edu or schedule a consultation with one of our team members.

CHAPTER

SEVENTEEN

USING SLURM

Slurm (Simple Linux Utility Resource Management) is the software on Discovery that lets you do the following:

- view information about the cluster
- monitor your jobs
- schedule your jobs on Discovery
- view information about your account

Using srun and *Using sbatch* provide you with a few examples to help get you familiar with Slurm and be able to submit basic jobs on Discovery.

Important: Slurm commands have numerous options to help your jobs run efficiently by requesting specific resources. Options also usually have both short and verbose versions, such as `--nodes` and `-n` (both mean the same thing). The examples in this documentation all use the verbose version of the options for clarity, but you can use the short version if you prefer. For example, `srun -p short -N 1 -n 1` means the exact same thing as `srun --partition=short --nodes=1 --ntasks=1` Refer to the official Slurm documentation to get in-depth information about these commands and their options: Slurm documentation website.

17.1 Viewing Cluster Information

Use the following commands to view information about the cluster. This information can help you better understand the hardware that is available in order to customize your job scripts. Also see *Hardware overview* for more information.

Slurm Command	Function
`sinfo <options>`	View partition and node information. Use option -a to view all partitions.
`smap <options>`	View details about the cluster in a visual format

17.2 Submitting Jobs

There are two main commands for submitting jobs to Discovery: `srun` and `sbatch`. To run a job interactively, use `srun`. To submit a job to run in the background with a script, use `sbatch`.

Slurm Command	Function
`srun`	Run an interactive job on the cluster. See :ref:`using_srun`
`sbatch <scriptname.script>`	Submit a script to the scheduler for running a job. See :ref:`using_sbatch`
`scancel <jobid>`	Cancel a pending or running job on the cluster

17.3 Monitoring Jobs

Slurm Command	Function
`seff <jobid>`	Reports the computational efficiency of your calculations.
`squeue -u <your user name>`	Displays your job status in the job queue. Good to use with `sbatch`.
`scontrol show jobid -d <JOBID>`	Displays your job information. Good to use with `srun`.

17.4 Account information

Some Discovery users have more than one Discovery group account associated with their username. For example, a student might be in a class that is using Discovery, and also be in a student club that is using Discovery for a club project. In this case, the student would have two group accounts associated with their username. When running a job with either `srun` or `sbatch`, if you have more than one account associated with your username, we recommend that you use the `--account=` flag and specify the account that corresponds to the project you are working on. In the example with a student associated with a class and a student club, if the student is on Discovery submitting a job for a project for his or her class, set the `account=` flag to the name of the class account. If the student is working on a project for the club, set the `account=` flag to the name of the student club account.

To find out what account(s) your usesrname is associated with, use the following command:

```
sacctmgr show associations user=<yourusername>
```

After you have determined what accounts your username is associated with, if you have more than one account association, you can use the `account=` flag with your usual `srun` or `sbatch` commands.

For example, if you are associated with an account named `dataclub` and an account named `info7500`, and you're currently doing work that should be associated with the `dataclub` account, in your `srun` command, you can add the `--account=dataclub` flag to specify that account.:

```
srun --account=dataclub --partition=short --nodes=1 --ntasks=28 --mem=0 --pty /bin/bash
```

Note: If you do not have more than one account associated with your username, you do not need to use the `--account=` flag. Most users on Discovery have only one account associated with their username.

CHAPTER

EIGHTEEN

USING SBATCH

You use the `sbatch` command with a bash script to specify the resources you need to run your jobs, such as the number of nodes you want to run your jobs on and how much memory you'll need. Slurm then schedules your job based on the availability of the resources you've specified. The general format for submitting a job to the scheduler is as follows:

```
sbatch example.script
```

Where `example.script` is a script detailing the parameters of the job you want to run.

Note: The default time limit depends on the partition that you specify in your submission script using the `--partition=<partition name>` option. If your job does not complete within the requested time limit, Slurm will automatically terminate the job. See *Partitions* for the most up-to-date partition names and parameters.

18.1 SBATCH Examples

18.1.1 Job requesting one node

Run a job on one node for 4 hours on the short partition:

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=4:00:00
#SBATCH --job-name=MyJobName
#SBATCH --partition=short
<commands to execute>
```

18.1.2 Job requesting one node and additional memory

The default memory per allocated core is 1GB. If your calculations try to use more memory than what is allocated, Slurm automatically terminates your job. You should request a specific amount of memory in your job script if your calculations need more memory than the default. The example script below is requesting 100GB of memory (–mem=100G). Use one capital letter to abbreviate the unit of memory (K,M,G,T) with the `--mem=` option, as that is what Slurm expects to see.

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=4:00:00
```

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```
#SBATCH --job-name=MyJobName
#SBATCH --mem=100G
#SBATCH --partition=short
<commands to execute>
```

18.1.3 Job requesting one node with exclusive use of a node

If you need exclusive use of a node, such as when you have a job that has high I/O requirements, you can use the exclusive flag. The example script below specifies exclusive use of 1 node in the short partition for four hours.

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=4:00:00
#SBATCH --job-name=MyJobName
#SBATCH --exclusive
#SBATCH --partition=short
<commands to execute>
```

18.2 Example Parallel Job Scripts

Parallel jobs should be used with code that is configured to use the reserved resources. If your code is not optimized for running in parallel, your job could fail. The following script examples all allocate additional memory. The default memory per allocated core is 1GB. If your calculations try to use more memory than what is allocated, Slurm automatically terminates your job. You should request a specific amount of memory in your job script if your calculations need more memory than the default.

18.2.1 8-task job, one node and additional memory

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --cpus-per-task=1
#SBATCH --time=4:00:00
#SBATCH --job-name=MyJobName
#SBATCH --mem=100G
#SBATCH --partition=short
<commands to execute>
```

18.2.2 8-task job, multiple nodes and additional memory

```
#!/bin/bash
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=2
#SBATCH --cpus-per-task=1
#SBATCH --time=00:30:00
#SBATCH --job-name=MyJobName
#SBATCH --mem=100G
#SBATCH --partition=express
<commands to execute>
```

18.3 Using Arrays

Using a job array can often help in situations where you need to submit multiple similar jobs. To use an array with your jobs, in your `sbatch` script, use the `array=` option.

For example, if you want to run a 10 job array, one job at a time, you would add the following line to your sbatch script:

```
#SBATCH --array=1-10%1
```

For more information on this command, go to the Slurm documentation page.

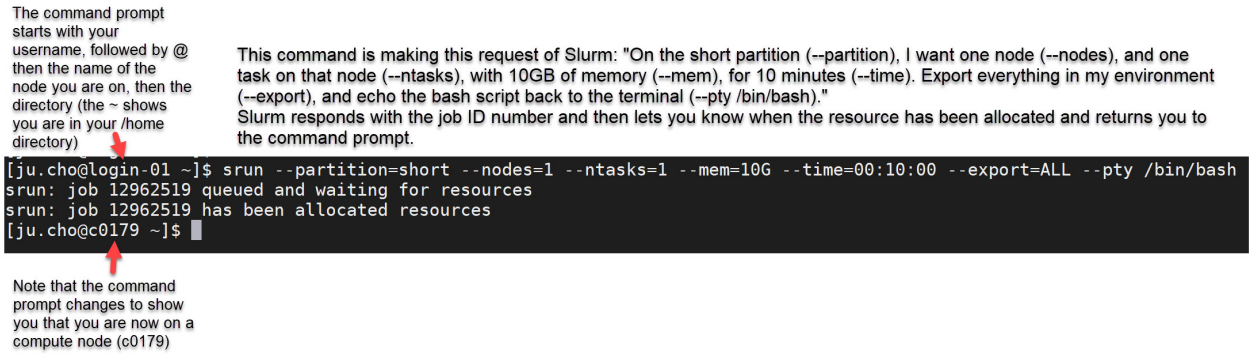
CHAPTER

NINETEEN

USING SRUN

You can use the Slum command `srun` to allocate an interactive job. This means you use specific options with `srun` on the command line to tell Slurm what resources you need to run your job, such as number of nodes, amount of memory, and amount of time. After typing your `srun` command and options on the command line and pressing enter, Slurm will find and then allocate the resources you specified. Depending on what you specified, it can take a few minutes for Slurm to allocate those resources. You can view all of the `srun` options on the Slurm documentation website.

The following image shows an example of an `srun` command as run on a command line.



19.1 srun examples

This section details a few examples using `srun`. You should first review the *Hardware overview* and *Partitions* sections to be familiar with the available hardware and partition limits on Discovery. This way, you can tailor your request to fit both the needs of your job and the limits of the partitions. For example, if you specify `--partition=debug` and `--time=01:00:00`, you'll get an error because the time you've specified exceeds the limit for that partition. Also keep in mind that while these examples are all valid, general examples, they might not work for your particular job.

simple `srun` example is to move to a compute node after you first log into Discovery.

```
srun --pty /bin/bash
```

To request one node and one task for 30 minutes with X11 forwarding on the short partition, type:

```
srun --partition=short --export=ALL --nodes=1 --ntasks=1 --x11 --mem=10G --time=00:30:00␣
↪--pty /bin/bash
```

To request one node, with 10 tasks and 2 CPUs per task (a total of 20 CPUs), 1GB of memory, for one hour on the express partition, type:

```
srun --partition=express  --nodes 1 --ntasks 10 --cpus-per-task 2 --pty --export=ALL --
↪mem=1G --time=01:00:00 /bin/bash
```

To request two nodes, each with 10 tasks per node and 2 CPUs per task (a total of 40 CPUs), 1GB of memory, for one hour on the express partition, type:

```
srun --partition=express  --nodes=2 --ntasks 10 --cpus-per-task 2 --pty --export=ALL --
↪mem=1G --time=01:00:00 /bin/bash
```

To allocate a GPU node, you should specify the gpu partition and use the –gres option:

```
srun --partition=gpu --nodes=1 --ntasks=1 --export=ALL --gres=gpu:1 --mem=1Gb --
↪time=01:00:00 --pty /bin/bash
```

For more information about working with GPUs, see *Working with GPUs*.

19.1.1 Monitor your jobs

You can monitor your jobs by using the Slurm `scontrol` command. Type `scontrol show jobid -d <JOBID>`, where `JOBID` is the number of your job. In the figure at the top of the page, you can see that when you submit your `srun` command, Slurm displays the unique ID number of your job (`job 12962519`). This is the number you use with `scontrol` to monitor your job.

CHAPTER

TWENTY

WORKING WITH GPUS

The Discovery cluster has various NVIDIA Graphics Processing Units (GPUs), as detailed in the table below.

Note: The tables on this page slide from left-to-right. Make sure to swipe to right to see the content on the right side of the table

GPU Type	GPU Memory	Tensor Cores	CUDA Cores	Nodes in Public GPUs	Nodes in Private GPUs
p100 (Pascal)	12GB	N/A	3,584	12 (x3-4 GPUs)	3 (x4 GPUs)
v100-pcie (Volta)	32GB	640	5,120	4 (x2 GPUs)	1 (x2 GPUs, 16GB)
v100-sxm2 (Volta)	32GB	640	5,120	24 (x4 GPUs)	10 (x4 GPUs, 16GB); 8 (x4 GPUs, 32GB)
t4 (Turing)	15GB	320	2,560	2 (x3-4 GPUs)	1 (x4 GPUs)
quadro (Quadro RTX 8000)	46GB	576	4,608	0	2 (x3 GPUs)
a30 (Ampere)	24GB	224	3,804	0	1 (x3 GPUs)
a100 (Ampere)	41 & 82GB	432	6,912	3 (x4 GPUs)	15 (x2-8 GPUs)
a5000 (Ampere RTX A5000)	24GB	256	8,192	0	6 (x8 GPUs)
a6000 (Ampere RTX A6000)	49GB	336	10,752	0	3 (x8 GPUs)

The public GPUs are available within two partitions, named `gpu` and `multigpu`. The differences between the two partitions are the number of GPUs that one can request per job and the time limit on each job. Both partitions give access to all the public GPU types mentioned above. The table below shows the differences between the two partitions. For more information about the partitions on the cluster, see *Partitions*.

Note: All user limits are subject to the availability of cluster resources at the time of submission and will be honored according to that.

Name	Requires Approval?	Time limit (Default/Max)	Submitted Jobs	GPU per job Limit	Max GPUs per user Limit
gpu	No	4 hours/8 Hours	50/100	1	8
multi-gpu	**Yes**	4 hours/24 Hours	50/100	12	12

Anyone with a Discovery account can use the `gpu` partition. However, you must submit a ServiceNow ticket to request

temporary access to multigpu for testing, or to request full access to the `multigpu` partition. Your request will be evaluated by members of the RC team to ensure that the resources in this partition will be used appropriately.

20.1 Requesting GPUs with Slurm

Use `srun` for interactive and `sbatch` for batch mode. The `srun` example below is requesting 1 node and 1 GPU with 4GB of memory in the `gpu` partition. You must use the `--gres=` option to request a gpu:

```
srun --partition=gpu --nodes=1 --pty --gres=gpu:1 --ntasks=1 --mem=4GB --time=01:00:00 /
↪bin/bash
```

Note: On the `gpu` partition, requesting more than 1 GPU (`--gres=gpu:1`) will cause your request to fail. Additionally, one cannot request all the CPUs on that gpu node as they are reserved for other GPUs.

The `sbatch` example below is similar to the `srun` example above, but it submits the job in the background, gives it a name, and directs the output to a file:

```
#!/bin/bash
#SBATCH --partition=gpu
#SBATCH --nodes=1
#SBATCH --gres=gpu:1
#SBATCH --time=01:00:00
#SBATCH --job-name=gpu_run
#SBATCH --mem=4GB
#SBATCH --ntasks=1
#SBATCH --output=myjob.%j.out
#SBATCH --error=myjob.%j.err

## <your code>
```

20.1.1 Specifying a GPU type

You can add a specific type of GPU to the `--gres=` option (with either `srun` or `sbatch`). For a list of available GPU types, refer to the GPU Types column in the table, at the top of this page, that are listed as `Public`. The following is an example for requesting a single p100 GPU:

```
--gres=gpu:p100:1
```

Note: Requesting a specific type of GPU could result in longer wait times, based on GPU availability at that time.

20.2 Using CUDA

There are several versions of CUDA Toolkits on Discovery, including:

```
cuda/9.0
cuda/9.2
cuda/10.0
cuda/10.2
cuda/11.0
cuda/11.1
cuda/11.2
cuda/11.3
cuda/11.4
cuda/11.7
cuda/11.8
cuda/12.1
```

Use the `module avail` command to check for the latest software versions on Discovery. To see details on a specific CUDA toolkit version, use `module show`. For example, `module show cuda/11.4`.

To add CUDA to your path, use `module load`. For example, type `module load cuda/11.4` to load version 11.4 to your path.

Use the command `nvidia-smi` (NVIDIA System Management Interface) inside a GPU node to get the CUDA driver information and monitor the GPU device.

20.3 GPUs for Deep Learning

PyTorch

You should use PyTorch with a conda virtual environment if you need to run the environment on the Nvidia GPUs on Discovery. The following example demonstrates how to build PyTorch inside a conda virtual environment for CUDA version 11.7.

Note: Make sure to be on a GPU node before loading the environment. Additionally, the latest version of PyTorch is not compatible with GPUs with CUDA version 11.7 or less. Hence, the installation does not work on k40m or k80 GPU's. In order to see what `non-Kepler` GPUs might be available execute the following command:

```
sinfo -p gpu --Format=nodes,cpus,memory,features,statecompact,nodelist,gres
```

This will indicate the state (idle or not) of a certain gpu-type that could be helpful in requesting an `idle` gpu. However, the command does not give real-time information of the state and should be used with caution.

Listing 1: PyTorch's installation steps (with a specific GPU-type):

```
srun --partition=gpu --nodes=1 --gres=gpu:v100-sxm2:1 --cpus-per-task=2 --mem=10GB --
↪time=02:00:00 --pty /bin/bash
module load anaconda3/2022.05 cuda/11.7
conda create --name pytorch_env python=3.9 -y
source activate pytorch_env
```

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```
conda install pytorch torchvision torchaudio pytorch-cuda=11.7 -c pytorch -c nvidia -y
python -c 'import torch; print(torch.cuda.is_available())'
```

Note: If the installation times out, please ensure that your `.condarc` file doesn't contain additional channels. Also, consider cleaning your conda instance using the `conda clean` command. See Conda best practices .

If CUDA is detected by PyTorch, you should see the result, `True`.

As the latest version of PyTorch often depends on the newest CUDA available, please refer to the PyTorch documentation page for the most up to date instructions on installation.

The above PyTorch installation instructions will not include `jupyterlab` and few other commonly used datascience packages in the environment. In order to include those one can execute the following command after activating the `pytorch_env` environment:

```
conda install pandas scikit-learn matplotlib seaborn jupyterlab -y
```

TensorFlow

We recommend that you use CUDA 11.2 (the latest supported version) when working on a GPU with the latest version of TensorFlow (TF). TensorFlow provides information on the compatibility of CUDA and TensorFlow versions, and detailed installation instructions.

For the latest installation, use the TensorFlow pip package, which includes GPU support for CUDA-enabled devices:

```
srun --partition=gpu --gres=gpu:1 --nodes=1 --cpus-per-task=2 --mem=10GB --time=02:00:00␣
↪--pty /bin/bash

module load anaconda3/2022.05 cuda/11.2
conda create --name TF_env python=3.9 -y
source activate TF_env
conda install -c conda-forge cudatoolkit=11.2.2 cudnn=8.1.0 -y

export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$CONDA_PREFIX/lib/
mkdir -p $CONDA_PREFIX/etc/conda/activate.d
echo 'export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$CONDA_PREFIX/lib/' > $CONDA_PREFIX/etc/
↪conda/activate.d/env_vars.sh
pip install --upgrade pip
pip install tensorflow==2.11.*
```

Verify the installation:

```
# Verify the CPU setup (if successful, then a tensor is returned):
python3 -c "import tensorflow as tf; print(tf.reduce_sum(tf.random.normal((1000, 1000))))
↪"

# verify the GPU setup (if successful, then a list of GPU device is returned):
python3 -c "import tensorflow as tf; print(tf.config.list_physical_devices('GPU'))"

# test if a GPU device is detected with TF (if successful, then True is returned):
python3 -c 'import tensorflow as tf; print(tf.test.is_built_with_cuda())'
```

To get the name of the GPU, type:

```
python -c 'import tensorflow as tf;  print(tf.test.gpu_device_name())'
```

If the installation is successful, then, for example, you should see the following as an output:

```
2023-02-24 16:39:35.798186: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1613\]␣
↪Created device /device:GPU:0 with 10785 MB memory:  -> device: 0, name: Tesla K80, pci␣
↪bus id: 0000:0a:00.0, compute capability: 3.7 /device:GPU:0
```

Note: Ignore the `Warning` messages that get generated after executing the above commands.

CHAPTER

TWENTYONE

TRANSFERRING DATA

The HPC has a dedicated transfer node that you must use to transfer data to and from the cluster. You are not allowed to transfer data from any other node to or from the HPC to your local machine. The node name is `<username>@xfer.discovery.neu.edu:` where `<username>` is your Northeastern username to login into the transfer node.

You can also transfer files using Globus. This is highly recommended if you need to transfer large amounts of data. See *Using Globus* for more information.

If you are transferring data from different directories on the HPC, you need to use a compute node (see *Using srun* or *Using sbatch*) with scp, rsync, or with the copy command to complete this tasks. You should use the `--constraint=ib` flag (see *Hardware Overview*) to ensure the fastest data transfer rate.

Caution: The `/scratch` space is for temporary file storage only. It is not backed up. If you have directed your output files to `/scratch`, you should transfer your data from `/scratch` to another location as soon as possible. See *Data Storage Options* for more information.

21.1 Transfer via Terminal

SCP

You can use `scp` to transfer files/directories to and from your local machine and the HPC. As an example, you can use this command to transfer a file to your `/scratch` space on the HPC from your local machine:

```
scp <filename> <username>@xfer.discovery.neu.edu:/scratch/<username>
```

where `<filename>` is the name of the file in your current directory you want to transfer and `<username>` is your Northeastern username. Note, this command is run on your local machine.

If you want to transfer a directory in your `/scratch` called `test-data` from the HPC to your local machine's currenting working directory, an example of that command would be:

```
scp -r <username>@xfer.discovery.neu.edu:/scratch/<username>/test-data .
```

where `-r` flag is for the recurssive transfer because it is a directory. Note, this command is run on your local machine.

Rsync

You can use the `rsync` command to transfer data to and from the HPC and local machine. You can also use `rsync` to transfer data from different directories on the cluster.

The syntex of `rsync` is

```
rsync [options] <source> <destination>
```

An example of using rsync to transfer a directory called `test-data` in your current working directory on your local machine to your `/scratch` on the HPC is

```
rsync -av test-data/ <username>@xfer.discovery.neu.edu:/scratch/<username>
```

where this command is run on your local machine in the directory that contains `test-data`.

Similarily, `rsync` can be used to copy from the current working directory on the HPC to your current working directory on your local machine:

```
rsync -av <username>@xfer.discovery.neu.edu:/scratch/<username>/test-data .
```

where this command is run on your local machine in the current directory that you want to save the directory `test-data`.

You can also use rsync to copy data from different directories on the HPC:

```
srun --partition=short --nodes=1 --ntasks=1 --time=01:05:00 --constraint=ib --pty /bin/
↪bash
rsync -av /scratch/<username>/source_folder /home/<username>/destination_folder
```

sbatch

You can use an sbatch job to complete data transfers by submitting the job to the HPC queue. An example of using `rsync` through an sbatch script is as follows:

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks=2
#SBATCH --time=0:05:00
#SBATCH --job-name=DataTransfer
#SBATCH --mem=2G
#SBATCH --partition=short
#SBATCH --constraint=ib
#SBATCH -o %j.out
#SBATCH -e %j.err

rsync -av /scratch/<username>/source_folder /home/<username>/destination_folder
```

where we are transfering the data from `source_folder` to the `destination_folder`.

SSHFS

If you want to use `sshfs`, you will need to use it with the dedicated transfer node `xfer.discovery.neu.edu`. It will not work on the login or compute nodes. On a Mac, you will also have to install macFUSE and sshfs (please refer to macFUSE) to use the `sshfs` command.

Use this syntax to perform file transfers with `sshfs`:

```
sshfs <username>@xfer.discovery.neu.edu:</your/remote/path> <your/local/path> -<options>
```

For example, this will mount a directory in your `/scratch` named `test-data` to a local directory on your machine `~/mount_point`:

```
sshfs <username>@xfer.discovery.neu.edu:/scratch/<username>/test-data ~/mount_point
```

where you can interact with the directory from your GUI or using the terminal to perform tasks on it.

21.2 Transfer via GUI Application

OOD's File Explorer

You can use OOD's File Explorer application to transfer data from different directories on the HPC and also to transfer data to and from your local machine to the HPC. For more information to complete this please see *OOD File Explorer*.

MobaXterm

You can use MobaXterm to transfer data to and from the HPC. Please checkout MobaXterm to download MobaXterm.

1. Open MobaXterm.
2. Click **Session**, then select **SFTP**.
3. In the **Remote host** field, type `xfer.discovery.neu.edu`
4. In the **Username** field, type your Northeastern username.
5. In the **Port** field, type 22.
6. In the **Password** box, type your Northeastern password and click **OK**. Click **No** if prompted to save your password.

You will now be connected to the transfer node and can transfer files through MobaXterm. Please refer to MobaXterm for further information.

FileZilla

You can use FileZilla to transfer data to and from the HPC. Please checkout FileZilla to download MobaXterm.

1. Open FileZilla.
2. In the **Host** field, type `sftp://xfer.discovery.neu.edu`
3. In the **Username** field, type your Northeastern username.
4. In the **Password** field, type your Northeastern password.
5. In the **Port** field, type 22.

You will now be connected to the transfer node and can transfer files through FileZilla. Please refer to FileZilla for further information.

CHAPTER

TWENTYTWO

USING GLOBUS

Globus is a data management system that you can use to transfer and share files. Northeastern has a subscription to Globus, and you can setup a Globus account with your Northeastern credentials. If you have another account, either personal or through another institution, you can also link your accounts.

To use Globus, you must first set up an account as detailed below. Then, you must install Globus Connect to create an endpoint on your local computer, as also detailed below. After you have completed these two initial setup procedures, you can then use the Globus web app to perform file transfers. See *Using the Northeastern endpoint* for a walkthrough of using the Northeastern endpoint on Globus.

22.1 Globus Account Set Up

Use the following instructions to setup an account with Globus using your Northeastern credentials.

1. Go to Globus.
2. Click **Log In**.
3. From the Use your existing organizational login, select **Northeastern University**, and then click **Continue**.
4. Enter your Northeastern username and password.
5. If you do not have a previous Globus account, click **Continue**. If you have a previous account, click Link to existing account.
6. Check the agreement checkbox, and then click **Continue**.
7. Click **Allow** to give Globus permissions to access your files.

You will then be able to access the Globus File Manager app.

Tip: If you received an account identity that includes your NUID number (for example 000123456@northeastern.edu), you can follow the "Creating and linking a new account identity" instructions below to get a different account identity if you want a more user-friendly account identity. You can then link the two accounts together.

22.1.1 Creating and linking a new account identity (Optional)

If you created an account through the Northeastern University existing organizational login and received a username that includes your NUID, you can create a new identity with a different username and then link the two accounts together. A username that you have selected, as opposed to one with your NUID, can make it easier for you to remember your login credentials.

1. Go to Globus.
2. Click **Log In**.
3. Click **Globus ID** to sign in.
4. Click **Need a Globus ID? Sign up**.
5. Enter your Globus ID information.
6. Enter the verification code that Globus sends to your email.
7. Click **Link to an existing account** to link this new account with your primary account.
8. Select Northeastern University from the dropdown box, and click **Continue** to be taken to the Northeastern University single sign on page.
9. Enter your Northeastern username and password.

You should now be able to see your two accounts linked in the Account section on the Globus web app.

22.2 Install Globus Connect Personal (GCP)

Use Globus Connect Personal (GCP) to use your personal laptop as an endpoint. You first need to install GCP using the following procedure. You need to be logged into Globus before you can install GCP.

1. Go to Globus File Manager.
2. Enter a name for your endpoint in the Endpoint Display Name field.
3. Click **Generate Setup Key** to generate a setup key for your endpoint.
4. Click the **Copy** icon next to the setup key that was generated to copy the key to your clipboard. You will need this key during the installation of GCP in step 6.
5. Click the appropriate OS icon for your computer to download the installation file.
6. After the installation file has been downloaded to your computer, double click on the file to launch the installer.

Accept the defaults on the install wizard. After the install completes, you can now use your laptop as an endpoint within Globus.

Note: You can't modify an endpoint after you have created it. If you need an endpoint with different options, you'll need to completely delete the endpoint and recreate it. Follow the instructions on the Globus website for deleting and recreating an endpoint.

22.3 Working with Globus

After you have an account and set up a personal endpoint using Globus Connect personal, you can perform basic file management tasks using the Globus File Manager interface such as transferring files, renaming files, and creating new folders. You can also download and use the Globus Command Line Interface (CLI) tool. Globus also has extensive documentation and training files for you to practice with.

22.3.1 Using the Northeastern endpoint

To access the Northeastern endpoint on Globus, on the Globus web app, click **File Manager**, then in the **Collection** text box, type Northeastern. The endpoints owned by Northeastern University display in the collection area. The general Northeastern endpoint is `northeastern#discovery`. Using the File Manager interface, you can easily change directories, switch the direction of transferring to and from, and specify options such as transferring only new or changed files. Below is a procedure for transferring files from Discovery to your personal computer, but with the flexibility of the File Manager interface, you can adjust the endpoints, file view, direction of the transfer, and many other options.

To transfer files from Discovery to your personal computer, do the following

1. Create an endpoint on your computer using the procedure above "Install Globus Connect", if you have not done so already.
2. In the File Manager on the Globus web app, in the **Collections** textbox, type Northeastern, then in the collection list click the `northeastern#discovery` endpoint.
3. In the right-pane menu, click **Transfer or Sync to**.
4. Click in the **Search** text box, and then in on the **Your Collections** tab, click the name of your personal endpoint. You now can see the list of your files on Discovery on the left and a list of your files on your personal computer on the right.
5. Select the file or files from the right-side list of Discovery files that you want to transfer to your personal computer.
6. Select the destination folder from the left-side list of the files on your personal computer.
7. (Optional) Click **Transfer & Sync Options** and select the transfer options that you need.
8. Click **Start**.

22.3.2 Connecting to Google Drive

The version of Globus currently on Discovery allows you to connect to Google Drive by first setting up the connection in GCP. This will add your Google Drive to your current personal endpoint. You'll need to first have a personal endpoint, as outlined in the procedure above.This procedure is slightly different from using the Google Drive Connector with Globus version 5.5. You'll need your Google Drive downloaded to your local computer.

To add Google Drive to your personal endpoint, do the following

1. Open the GCP app. On Windows, right click on the **G** icon in your taskbar and select **Options**. On Mac, click the **G** icon in the menu bar and select **Preferences**.
2. On the **Access** tab, click the + button to open the **Choose a directory** dialog box.
3. Navigate to your Google Drive on your computer and click **Choose**.
4. Click the **Shareable** checkbox to make this a shareable folder in Globus File Manager, and then click **Save**.

You can now go to Globus File Manager and see that your Google Drive is available as a folder on your personal endpoint.

22.3.3 Command Line Interface (CLI)

The Globus Command Line Interface (CLI) tool allows you to access Globus from a command line. It is a stand-alone app that requires a separate download and installation. Please refer to the Globus CLI documentation for working with this app.

22.3.4 Globus documentation and test files

Globus provides detailed instructions on using Globus and also has test files for you to practice with. These are free for you to access and use. We encourage you to use the test files to become familiar with the Globus interface. You can access the Globus documentation and training files on the Globus How To website.

CHAPTER

TWENTYTHREE

DATA STORAGE OPTIONS

RC is responsible for the procurement and ongoing maintenance of several data storage options, including active, and archive storage solutions. If you are affiliated with Northeastern, you can request one or more storage solutions to meet your storage needs. If you anticipate needing storage as part of a grant requirement, please schedule a storage consultation with an RC staff member to understand what storage options would best meet your research needs.

23.1 Active Storage

There are two main storage systems connected to Northeastern's HPC cluster: `/home` and `/scratch`; these options have specific quotas and limitations. The list below details the storage options available to you on the HPC cluster by having an account. Every individual with an account has both a `/home` and `/scratch`. While research groups can request additional storage on the `/work` storage system, `/work` storage is not currently provisioned to individuals.

Important: The `/scratch` space is only for temporary storage; this storage is not backed up, and there is a purge policy for data older than 28 days. Please review the `/scratch` policy on our Policy page.

$HOME: `/home/<username>` where `username` is your NU login, e.g., `/home/j.smith`

- **Description:** All users are given a `/home` automatically when their account is created. This storage is mainly intended for storing relatively small files such as script files, source code, and software installation files. While `/home` is permanent storage that is backed up and replicated, `/home` is not performant storage. `/home` also has a small quota, so you should frequently check your space usage (use a command such as, `du -h /home/<yourusername>` where `<yourusername>` is your username, to see the total space usage). For running jobs and directing output files, you should use your `/scratch`.
- **Quota:** 75GB

Scratch: `/scratch/<username>`

- **Description:** All users are given a `/scratch` automatically when their account is created. Scratch is a shared space for all users. The total storage available is 1.8PB; however, while this is performant storage, it is for temporary use only. **It is not backed up.** Data on `/scratch` should be moved as soon as possible to another location for permanent storage. You should run your jobs from and direct output to your `/scratch` for best performance. However, it is best practice to move your files off of scratch to avoid any potential data loss.
- **Quota:** N/A

Work: `/work/<groupname>`

- **Description:** Research groups can request additional storage on `/work`. A PI can request this extra storage through the New Storage Space request. This is a performant, persistent, and long-term storage that is meant for storing data being actively used for research. It can be accessed by all members of the research group who have necessary access permissions, facilitating collaboration and seamless sharing of data within the group.

- **Quota:** Each group can request up to **35TB** of free storage across all supplemental storage tiers: `/work/<groupname>` and `/nese`.
- **Access Request:** Students with research groups can request access to the PI's storage on `/work`. To expedite the request process, we recommend that you inform the group owner they will be receiving an email requesting their permission to grant you access to `/work` before you submit the request.

1. To request access to `/work`, students can either create a ServiceNow ticket with RC or email rchelp@northeastern.edu to automatically generate a ticket in ServiceNow. Please include both the storage space name and the PI's name.
2. Once you have been added to the unix group for the space on `/work`, please ensure to close all open connections to the HPC and login again for the changes to reflect on your end. Please note that UNIX groups are assigned at login time, and this step ensures that your access privileges are updated accordingly. To confirm you have been added to the group, you can run the command `groups`.

- **Default Permission:** By default, users are given read and write access when added to `/work`. However, specific permissions might be granted at the PI's request.

Attention: The `/research` storage tier is no longer provided. Please contact Research Computing if you are a former user of `/research` and have questions or issues related to `/research` by submitting a ticket. Other storage options include `/work`, Sharepoint, and OneDrive.

23.2 Archival Storage

Important: If you are not connected to the campus internet, you must be connected to the university's VPN (GlobalProtect) before you can access the `/nese` system. You can find detailed information about downloading and using the GlobalProtect VPN in the FAQ: VPN and remote access.

NAME: `/nese`

- **Description:** This is archival, non-performant storage intended for researchers who need to have a long-term storage option for their data.
- **Quota:** Each group can request up to **35TB** of free storage across all supplemental storage tiers: `/work/<groupname>` and `/nese`.

CHAPTER

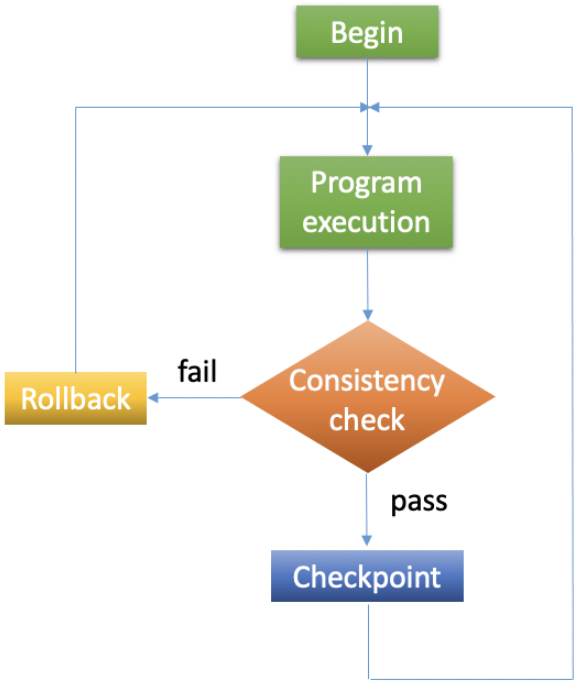
TWENTYFOUR

CHECKPOINTING JOBS

The complexity of HPC systems can introduce unpredictable behavior in hardware or software components, leading to job failures. Applying fault tolerance techniques to your HPC workflows can make your jobs more resilient to crashes, partition time limits, and hardware failures.

24.1 The Checkpointing technique

Checkpointing is a fault tolerance technique based on the Backward Error Recovery (BER) technique, designed to overcome "fail-stop" failures (interruptions during the execution of a job).



To implement checkpointing:

- Use data redundancy to create checkpoint files, saving all necessary calculation state data. Checkpoint files are generally created at constant time intervals during the run.
- If a failure occurs, start from an error-free state, check for consistency, and restore the algorithm to the previous error-free state.

Checkpointing allows you to:

- Create resilient workflows in the event of faults.
- Overcome most scheduler resource time limitations.
- Implement an early error detection approach by inspecting intermediate results.

24.2 Checkpointing types

Checkpointing can be implemented at different levels of your workflow:

- **Application-level** - This is the recommended approach for most Discovery users. Utilize the checkpointing tool that is already available in your software application. For example, most software designed for HPC has a checkpointing option, and information on proper usage is often available in the software user manual.
- **User-level** - This approach is suitable if you develop your code or possess sufficient knowledge of the application code to integrate checkpointing techniques effectively. We recommend this approach for some Discovery users with advanced proficiency and familiarity with checkpointing mechanisms.
- **System-level** - Checkpointing is done on the system side, where the user saves the state of the entire process. This option is less efficient than User-level or Application-level checkpointing as it introduces a lot of redundancy.
- **Model-level** - This approach is suitable for saving a model's internal state (its weights, current learning rate, etc.) so that the framework can resume the training from this point whenever desired. This is often the intent of users doing machine learning on Discovery.

24.2.1 Which checkpoint type to use?

There are several options for checkpointing, depending on the needs of your software.

- If your software already includes **built-in checkpointing**, this is often the preferred option, as it is the most optimized and efficient way to checkpoint.
- **Application-level** checkpointing is the easiest to use, as it exists within your application. It does not require significant changes to your scripts and saves only the relevant data for your specific application.
- **User-level** checkpointing is recommended if you are writing your own code. You can use DMTCP or implement your own checkpointing.
- **ML Model-level** checkpointing is specific to model training and deployment, as detailed in the `ML Model-level_` section.

Note: If you are developing in Python, Matlab or R, there are packages that can be used to implement checkpointing. Some examples include Python PyTorch checkpointing, TensorFlow checkpointing, MATLAB checkpointing and R checkpointing. Additionally, many Computational Chemistry and Molecular Dynamics software have built-in checkpointing options (e.g., GROMACS and LAMMPS).

Implementing checkpointing can be achieved by the following:

- Some save-and-load mechanism of your calculation state.
- The use of Slurm Job Arrays.

Note: To overcome partition time limits, replace your single long job with multiple shorter jobs. Then, use job arrays to set each job to run one after the other. If checkpointing, each job will write a checkpoint file. The following job will use the latest checkpoint file to continue from the latest state of the calculation.

24.3 Application-level checkpointing

24.3.1 GROMACS checkpointing example

The following example shows how to implement a 120-hour GROMACS job using multiple shorter jobs on the *short* partition. We use Slurm job arrays and the GROMACS built-in checkpointing option to implement checkpointing.

See also:

https://manual.gromacs.org/documentation/current/user-guide/managing-simulations.html

The following script `submit_mdrun_array.sh` creates a Slurm job array of 10 individual array jobs:

```
#!/bin/bash
#SBATCH --partition=short
#SBATCH --constraint=cascadelake
#SBATCH --nodes=1
#SBATCH --time=12:00:00
#SBATCH --job-name=myrun
#SBATCH --ntasks=56
#SBATCH --array=1-10%1  # execute 10 array jobs, 1 at a time
#SBATCH --output=myrun-%A_%a.out
#SBATCH --error=myrun-%A_%a.err

module load cuda/10.2
module load gcc/7.3.0
module load openmpi/4.0.5-skylake-gcc7.3
module load gromacs/2020.3-gpu-mpi
source /shared/centos7/gromacs/2020.3-gcc7.3/bin/GMXRC.bash

srun --mpi=pmi2 -n $SLURM_NTASKS gmx_mpi mdrun -ntomp 1 -s myrun.tpr -v -dlb yes -cpi␣
↪state
```

The script above sets checkpoint flag `-cpi state` preceding the filename to dump checkpoints. This directs `mdrun` to checkpoint to `state.cpt` when loading the state. The Slurm option `--array=1-10%1` creates 10 Slurm array tasks, and runs one task job serially for 12 hours. The variable `%A` denotes the main job ID, while `%a` denotes the task ID (i.e., spanning `1-10`).

To submit this array job to the scheduler, use the following command:

```
sbatch submit_mdrun_array.bash
```

24.3.2 DMTCP checkpoint example

DMTCP (Distributed MultiThreaded checkpointing) is a tool checkpoints without changing code. It works with most Linux applications such as Python, Matlab, R, GUI, and MPI.

The program runs in the background of your program, without significant performance loss, and saves the process states into checkpoint files. DMTCP is available on the cluster

```
module avail dmtcp
module show dmtcp
module load dmtcp/2.6.0
```

Since DMTCP runs in the background, it requires some changes to your shell script. See examples of checkpointing with DMTCP, which use DMTCP with a simple C++ program (scripts modified from RSE-Cambridge).

24.3.3 Application-level checkpointing tips

What data to save?

- Non-temporary application data
- Any application data that has been modified since the last checkpoint
- Delete checkpoints that are no longer useful - keep only the most recent checkpoint file.

How frequently to checkpoint?

- Too often – will slow down your calculation, maybe I/O heavy and memory-limited.
- Too infrequently – leads to large/long rollback times.
- Consider how long it takes to checkpoint and restart your calculation.
- In most cases a rate of every 10-15 minutes is ok.

24.4 ML Model-level Checkpointing

Model-level checkpointing is a technique used to periodically save the state of a machine learning (ML) model during training, enabling the training process to get resumed from the saved checkpoint in case of interruptions or premature termination. The saved state typically includes the model's parameters, optimizer state, and essential training information (e.g., the epoch number and loss value). Model checkpoints are especially critical for long-running training jobs.

24.4.1 Why is Checkpointing Important in Deep Learning?

Checkpointing is crucial in deep learning because the training process can be time-consuming and require significant computational resources. Additionally, the training process may be interrupted due to hardware or software issues. Checkpoints solve this problem by saving the model's current state to resume from where it left off.

Moreover, checkpointing also saves the best-performing model, which can then load for evaluation. For instance, the model's performance can vary based on the initialization and optimization algorithm, so checkpointing provides a way to select the best model based on a performance metric.

In summary, checkpointing is essential in deep learning as it provides a way to save progress, resume training, and select the best-performing model.

24.4.2 TensorFlow checkpoint example

The following example demonstrates how to implement a longer ML job using the *tf.keras* checkpointing API and multiple shorter Slurm job arrays on the gpu partition.

The following example of the `submit_tf_array.bash` script:

```
#!/bin/bash
#SBATCH --job-name=myrun
#SBATCH --time=00:10:00
#SBATCH --partition=gpu
#SBATCH --nodes=1
#SBATCH --gres=gpu:1
#SBATCH --mem=10Gb
#SBATCH --output=%A-%a.out
#SBATCH --error=%A-%a.err
#SBATCH --array=1-10%1  #execute 10 array jobs, 1 at a time.

module load miniconda3/2020-09
source activate tf_gpu

# Define the number of steps based on the job id:
numOfSteps=$(( 500 * SLURM_ARRAY_TASK_ID ))

# Run python and save outputs to a log file corresponding to the current job task ID
python train_with_checkpoints.py $numOfSteps &> log.$SLURM_ARRAY_TASK_ID
```

The following checkpoint example is given in the program `train_with_checkpoints.py`:

```
checkpoint_path = "training_2/{epoch:d}.ckpt"
checkpoint_dir = os.path.dirname(checkpoint_path)
cp_callback = tf.keras.callbacks.ModelCheckpoint(
   filepath=checkpoint_path,
   verbose=1,
   save_weights_only=True,
   period=5)
```

See scripts, which are modified from TensorFlow Save and load models.

The Slurm option `--array=1-10%1` will create 10 Slurm array tasks, and will run one task job at a time. Note that the saved variable `%A` denotes the main job ID, while variable `%a` denotes the task ID (spanning values 1-10). Note that also the output/error files are unique in order to prevent different jobs writing to the same files. The Shell variable `SLURM_ARRAY_TASK_ID` holds the unique task ID value and can be used within the Slurm Shell script to point to different files or variables.

To submit this job to the scheduler, use the command:

```
sbatch submit_tf_array.bash
```

24.4.3 PyTorch checkpointing

Model-level tips and tricks

Save only the model's State_dict

Save only the model's state_dict and optimizer state, allowing us to save only information needed to resume training. By this, we reduce the checkpoint file's size and make it easier to load the model. Hence, avoid keeping unnecessary information in the checkpoint file, such as irrelevant metadata or tensors we can define during training.

Save regularly

To prevent losing progress in case of a crash or interruption, save the checkpoint file regularly (i.e., after each epoch).

Save to multiple locations

Save the checkpoint file to multiple locations, such as a local drive and the cloud, to ensure that the checkpoint is recovered in case of failure.

Use the latest versions of libraries

Use the latest version of PyTorch and other relevant libraries is vital; changes in these libraries may cause compatibility issues with older checkpoints. With these best practices, you can ensure that your PyTorch models are saved efficiently and effectively and that your progress is not lost in case of a crash or interruption.

Naming conventions

Use a consistent naming convention for checkpoint files; include information such as the date, time, and epoch number in the file name to make tracking multiple checkpoint files easier and ensure you are choosing the proper checkpoint to load.

Checkpoint Validation

Validate the checkpoint after loading it to ensure that the model's state_dict and the state of the optimizer are correctly loaded by making a prediction using the loaded model and checking that the results are as expected.

Periodic clean-up

Periodically, remove old checkpoint files to avoid filling up storage. This can be done by keeping only the latest checkpoint or keeping only checkpoint files from the last few epochs.

Document checkpoints

Document the purpose of each checkpoint and what it contains: include the model architecture, the training data, the hyperparameters, and the performance metrics. This will help to keep track of the progress and make it easier to compare different checkpoints. With these additional best practices, you can ensure that your checkpointing process is efficient, effective, and well-organized.

CHAPTER

TWENTYFIVE

HOME DIRECTORY STORAGE QUOTA

There are strict quotas for each home directory (i.e., /home/<username>), and staying within the quota is vital for preventing issues on the HPC. This page provides some best practices for keeping within the quota. For more information about data storage on the HPC, see *Data Storage Options*.

Important: All commands on this page should be run from a compute node because they are cpu intensive. You can find more information on getting a job on a compute node from *Using srun*.

25.1 Analyze Disk Usage

From a compute node, run the following command from your /home/<username> directory:

```
du -shc .[^.]* ~/*
```

This command will output the size of each file, directory, and hidden directory in your /home/<username> space, with the total of your /home directory being the last line of the output. After identifying the large files and directories, you can move them to the appropriate location, (e.g., /work for research) or you can back up and delete the files and directories if they are no longer required. An example output would look like:

```
[<username>@<host> directory]$  du -shc .[^.]* ~/*
39M     .git
106M    discovery-examples
41K     README.md
3.3M    software-installation
147M    total
```

25.2 Utlilize /work and /scratch

Use /work for long-term storage. PIs can request a folder in /work via New Storage Space Request, and they can request additional storage via Storage Space Extension Request. Utilize /scratch/<username> for temporary or intermediate files. Then, move files from /scratch to /work for persistent storage (i.e., the recommended work flow).

Note: Please be mindful of the /scratch purge policy, which can be found on the Research Computing Policy Page. See *Data Storage Options* for information on /work and /scratch.

25.3 Cleaning Directories

25.3.1 Conda

Note: Conda environments are part of your research and should preferably be stored in your PI's `/work` directory.

Here are some suggestions to reduce the storage size of the environments for those using the `/home/<username>/.conda` directory.

Remove unused packages and clear caches of conda by loading an anaconda module and running the following:

```
source activate <your environment>
conda clean --all
```

This will only delete unused packages in your `~/.conda/pkgs` directory.

To remove any unused conda environments, run:

```
conda env list
conda env remove --name <your environment>
```

25.3.2 Singularity

If you have pulled any containers to the HPC using Singularity, you can clean your container cache in your `/home/<username>` directory by running the following command from a compute node:

```
module load singularity/3.5.3
singularity cache clean all
```

To avoid your `~/.singularity` directory filling up, you can set a temporary directory for when you pull containers to store the cache in that location; an example of this procedure, (where `<project>` is your PI's `/work` directory) is the following:

```
mkdir /work/<project>/singularity_tmp
export SINGULARITY_TMPDIR=/work/<project>/singularity_tmp
```

Then, pull the container using singularity as usual.

25.3.3 Cache

The `~/.cache` directory can become large over time with general use of the HPC and Open OnDemand. Make sure you are not running any processes or jobs at the time by running the following:

```
squeue -u <username>
```

which prints a table with `JOBID`, `PARTITION`, `NAME`, `USER ST`, `TIME`, `NODES`, and `NODELIST (REASON)` which is empty when no jobs are running (i.e., it is safe to remove `~/.cache` when no jobs are running).

25.4 Storing research environments

25.4.1 Conda environments

Use conda environments for python on HPC. To create an environment in `/work`, use the `--prefix` flag as follows: (where `<project>` is your PI's `/work` directory and `<my conda env>` is an empty directory to store your conda environment):

```
conda create --prefix=/work/<project>/<my conda env>
```

More information about creating custom conda environments can be found here *Using Conda*.

Utilize the same conda environment to save storage space and time (i.e., avoiding duplicate conda environments). Hence, shared environments can be easily done for a project accessing the same `/work` directory. For more information about creating custom conda environments, see *Using Conda*.

25.4.2 Singularity containers

Containers that are pulled, built and maintained for research work should be stored in your PI's `/work` directory, not in your `/home/<username>` directory.

CHAPTER

TWENTYSIX

INTRODUCTION TO OOD

Open OnDemand (OOD) is a web portal to the Discovery cluster. A Discovery account is necessary for you to access OOD. If you need an account, see *Request an account*. If you already have an account, in a web browser, go to http://ood.discovery.neu.edu and sign in with your Northeastern username and password.

OOD provides you with a number of resources for interacting with the Discovery cluster:

- Launch a terminal that runs within your web browser without needing a separate terminal program. This is an advantage if you use Windows, as otherwise you need to download and use a separately installed program, such as MobaXterm.
- Use software applications, such as SAS Studio, that run in your browser without needing any further configuration. See *Using OOD's Interactive Apps* for more information.
- View, download, copy, and delete files using the File Explorer feature. See *Using OOD's FIle Explorer* for more information.

Note: OOD is a web-based application. You access it by using a web browser. Like many web-based applications, it has compatibility issues with certain web browsers. For optimal results, use OOD with newer versions of Chrome, Firefox, or Internet Explorer. OOD does not currently have support for Safari or mobile devices (phones and tablets).

CHAPTER

TWENTYSEVEN

OOD FILE EXPLORER

When working with the resources in OOD, your files are stored in your home directory on the storage space on the Discovery cluster. Similar to any file navigation system, you can work with your files and directories through the OOD Files feature as detailed below. For example, you can download a Jupyter Notebook file in OOD that you've been working on to your local hard drive, rename a file, or delete a file that you no longer need.

Note: Your home directory has a file size limit of 75GB. Be sure to check your home directory regularly, and remove any files you do not need to ensure you do not run out of space.

---

1. In a web browser, go to ood.discovery.neu.edu. If prompted, enter your myNortheastern username and password.
2. Select **Files > Home Directory**. The contents of your home directory display in a new tab.
3. To download a file to your hard drive, navigate to the file you want to download, select the file, and click **Download**. If prompted by your browser, click **OK** to save your file to your hard drive.
4. To navigate to another folder on the Discovery file system, click **Go To**, enter the path to the folder you want to access, and click **OK**.

Note: From the **Files > Home Directory** view, the **Edit** button will not launch your .ipynb file in a Jupyter Notebook. It will open the file in a text editor. You have to be in Jupyter Notebook in order to launch a .ipynb file from your /home directory. See *Using OOD's Interactive Apps* for how to access a Jupyter Notebook through OOD.

CHAPTER

TWENTYEIGHT

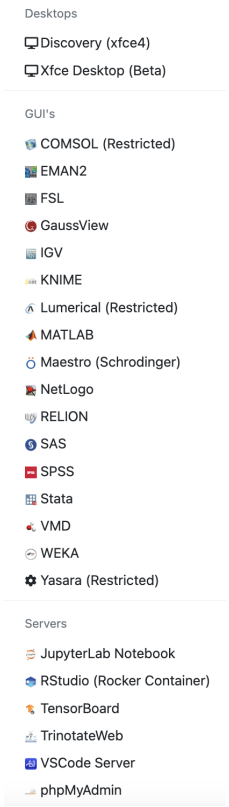
OOD INTERACTIVE APPS

The OOD web portal offers a variety of applications. When you click launch, the scheduler (Slurm) assigns a compute node with a set number of cores and memory. By default, applications run for one hour. If you request more than one hour, you may need to wait for Slurm to assign resources to accommodate your requested time.

If you are trying to run a job on one of the interactive apps on OOD that launches a graphical user interface (GUI), such as Maestro, you may encounter an error if your passwordless ssh is improperly set up. Check out {ref}using-x11 for tips and troubleshooting information on opening applications that use X11 forwarding.

28.1 Available Apps (June 2023)

On the Interactive Apps tab, you can view the list of available interactive apps through the OOD web interface.



Note: Some apps are reserved for specific research groups and are not for public access, denoted by Restricted next

to the application name. If you get an access error when attempting to open an app, and you believe that you should have access to it, please email rchelp@northeastern.edu with your username, research group, the app you are trying to access, a screenshot of the error that you are getting, and we will look into the issue.

1. Go to Open On Demand in a web browser. If prompted, enter your myNortheastern username and password.
2. Select **Interactive Apps**, then select the application you want to use.
3. Keep the default options for most apps, then click **Launch**. You might have to wait a minute or two for a compute node to be available for your requested time and resource.

28.2 Jupyter Notebook

JupyterLab Notebook is one of the interactive apps on OOD. This section will provide a walkthrough of setting up and using this app. The general workflow is to create a virtual Python environment, ensure that JupyterLab Notebook uses your virtual environment, and reference this environment when you start the JupyterLab Notebook OOD interactive app.

You can find the JupyterLab notebook on OOD by following these steps:

1. Go to Open On Demand
2. Click on Interactive Apps
3. Select JupyterLab Notebook from the dropdown list

The OOD form for launching JupyterLab Notebook will appear.

28.2.1 Conda virtual environment

You can import Python packages in your JupyterLab Notebook session by creating a conda virtual environment and activating that environment when starting a JupyterLab Notebook instance.

1. First, set up a virtual Python environment. See *Creating an Environment* for how to set up a virtual Python environment on the HPC using the terminal.
2. Type `source activate <yourenvironmentname>` where `<yourenvironmentname>` is the name of your custom environment.
3. Type `conda install jupyterlab -y` to install jupyterlab in your environment.

28.2.2 Using OOD to launch Jupyter Notebook

1. Go to Open On Demand.
2. Click **Interactive Apps**, then select **JupyterLab Notebook**.
3. Enter your **Working Directory** (e.g., `/home/<username>` or `/work/<project>`) that you want JupyterLab Notebook to launch in.
4. Select from the **Partition** dropdown menu the partition you want to use for your session. Refer to *Partitions* for the resource restrictions for the different partitions. If you need a GPU, select the `gpu` partition.
5. Select the compute node features for the job:
    - In the **Time** field, enter the number of hour(s) needed for the job.
    - Enter the memory you need for the job in the **Memory (in Gb)** field.

- If you selected the `gpu` partition from the dropdown menu, select the GPU you would like to use and the version of CUDA that you would like to use for your session under the respective dropdown menus.

6. Select the Anaconda version you used to create your virtual Python environment in the **System-wide Conda Module** field.
7. Check the **Custom Anaconda Environment** box, and enter the name of your custom virtual Python environment in the **Name of Custom Conda Environment** field.
8. Click **Launch** to join the queue for a compute node. This might take a few minutes, depending on your requested resources.
9. When you have been allocated a compute node, click **Connect to Jupyter**.

When your Jupyter Notebook is running and open, type `conda list` in a cell and run the cell to confirm that the environment is your custom conda environment (you should see this on the first line). This command will also list all of your available packages.

28.3 Xfce Desktop (Beta)

This Open OnDemand application is a containerized desktop running on the HPC cluster. It has access to these tools/programs:

- Slurm (for running Slurm commands via the terminal in the desktop and interacting on compute nodes)
- Module command (for loading and running HPC-ready modules)
- File explorer (able to traverse and view files that you have access to on the HPC)
- Firefox web browser
- VLC media player
- Office Libre suite of applications (word processing, spreadsheets, presentation applications)

Note: The desktop application is a Singularity container: a Singularity container cannot run inside. It will fail if a user tries to run a module or program that runs a container inside this application.

CHAPTER

TWENTYNINE

CLASSROOM HPC: FAQ

There are several use cases for teaching and learning with the Discovery cluster in a classroom. Discovery offers both a command line and web interface, allowing flexibility in access and instruction level. Using Discovery gives you and your students access to many popular scientific applications, and also allows you and your students to install other packages as needed. The easy-to-use Open onDemand web portal also offers a built-in visual file explorer for file viewing and transfer.

The following Frequently Asked Questions section should help to answer most of your questions about how you can use the Discovery cluster for classroom use. You can also reach out to us at rchelp@northeastern.edu or submit a ServiceNow ticket if you need further information.

How can I use Discovery with my class?

There are several ways you can use Discovery in your classroom. Your class can use Discovery for accessing specific software packages and working environments, as well as learning how to utilize high performance computing (HPC) resources for large and complex data processing, such as machine learning; AI and molecular simulations; and more.

How do I get my class access to Discovery?

You fill out a Discovery Classroom Use Request ticket. The form asks you to submit a list of your students' names and emails. We will create accounts on Discovery for them. Follow the steps in the article How to Download a List of Student Email Addresses from Canvas to get a list of your students' emails. If your class roster is not complete, you can attach a preliminary list to the ticket, and then follow up with us on the same ticket with an updated roster when the add/drop period is over.

Is there any training on Discovery for my class?

Yes, we currently provide online training for your class on using Discovery. In the past, we have also given in-person presentations during a class period on the Boston campus. We hope to provide in-person training again in 2021. We can customize the training to focus on the resources you will be using with them for the class. Email us at rchelp@northeastern.edu and provide us with some details about your class and what training you would like us to provide.

Do my students have to learn Linux to work with Discovery?

Depending on your class assignments, many students can work with the Open onDemand web portal, which does not require any knowledge of Linux to use. In cases where you want them to work on the command line, they should have a basic understanding of Linux commands. Please see the question "Is there any training on Discovery for my class" above if you would like us to provide your class with a basic training course prior to using Discovery.

What software is available to use with my class on Discovery?

There are many software packages available, including popular software apps such as Jupyter Notebook, RStudio, and MATLAB. If you have an account on Discovery, you can see the list of available software by using the `module avail` command. See *Using Module* for more information. Students have access to all the modules on Discovery. They can also use the interactive apps available on Open onDemand. See *Introduction to Open OnDemand (OOD)* for more information. We can also install additional modules and libraries specifically for your class as needed.

My class needs access to a specific software application that I do not see installed on Discovery or Open onDemand (OOD). What should I do?

If you class requires software not currently installed on Discovery or OOD, follow the procedure below to request that software be installed on Discovery. You must be a professor or instructor to initiate this request. Students in your class should not make this request. If your students need a specific software application, you must complete the form for them. This is to ensure that we only get one request for the software. Students in one class often make multiple requests for the same software, so having all requests go through the professor or instructor reduces this overlap.

To request additional software (instructors only):

1. Go to the Discovery Cluster Software Request. If prompted, sign in to ServiceNow with your Northeastern username and password to access the form.
2. In the Sponsor's Name field, enter your name.
3. Make sure to follow the instructions on the form regarding either providing the URL of the open source software library or uploading the installation package in your home directory if it requires you to register it first. The request will not be completed without this information.
4. Select the acknowledgement checkbox, and click **Submit**.

Note: Software requests can take up to 24 hours to verify, and then additional time is needed to complete the installation. We might not be able to install every software application requested. If this is the case we will notify you and try to provide alternative software to meet your needs.

Tip: You and your students can install software locally to your PATH on Discovery, which may be a better option in some cases, such as installing multiple conda environments. See *Software Overview* for more information.

I just need my class to access Open onDemand. How do I request that?

Open onDemand is a web portal that lets you access the resources on Discovery through an easy-to-navigate web browser interface. You request course access the same way you would to get access to Discovery, as outlined above. Please specify that you'd like your course to be on Open onDemand for your students, in addition to the information we request above.

I'd like my class to use specific resources on Discovery. Can you create a reservation on Discovery for my class?

In many cases, we will create a reservation on Discovery for your class for specific hardware resources. For example, if you course assignments require the use of GPUs or nodes with a large amount of memory, we can create a reservation on specific nodes that only your class can access for the duration of the course. However, Discovery is a shared resource, so we ask that you test out your assignments on Discovery so that you are requesting an appropriate amount of resources for your class. If a class needs an increase in resources due to higher than expected use, we can always increase your reservation. But, if a reservation is not being used to capacity, we will ask you to review the need for the requested resources, and adjust the reservation accordingly. We understand that sometimes it is difficult to determine exactly what your resource needs will be, but we do need to keep a reservation to a reasonable limit so that we keep the shared resources available to all users.

How long do my students have access to Discovery?

Students will have access to Discovery for the full duration of the class. If they want to continue to have access to Discovery after that time period, they'll need to request an individual account.

How do I get an account on Discovery?

If you are a professor or instructor at Northeastern, you can request an account on Discovery. See *Sponsor Approval Process* for more information.

How do my students get help with Discovery?

You and/or your students can either submit a Get Assistance with Research Computing ticket or email rchelp@northeastern.edu.

CHAPTER

THIRTY

CPS CLASS INSTRUCTIONS

Caution: Note - The following instructions will only work for CPS classes.

These instructions describe the process of opening a CPS JupyterLab environment on the Open OnDemand (OOD) Discovery web portal and accessing class work directories.

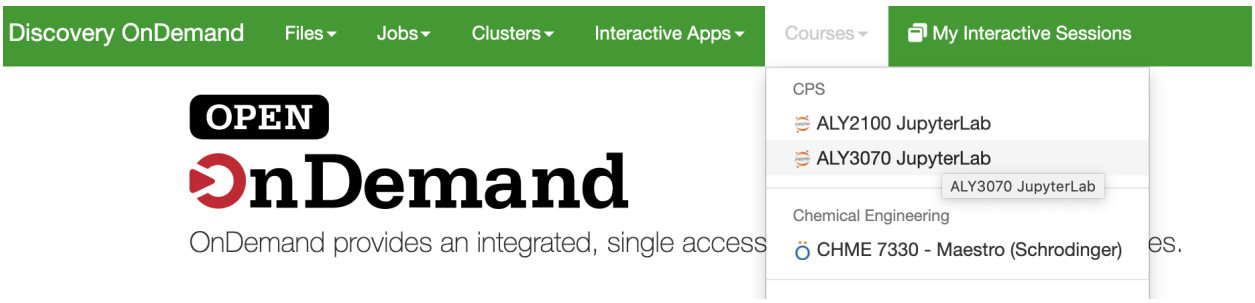
Note: Due to problems with launching OOD on **Safari**, we recommend using **Google Chrome**, **Mozilla Firefox** or **Microsoft Edge** browsers instead for best experience.

30.1 Open the CPS JupyterLab environment

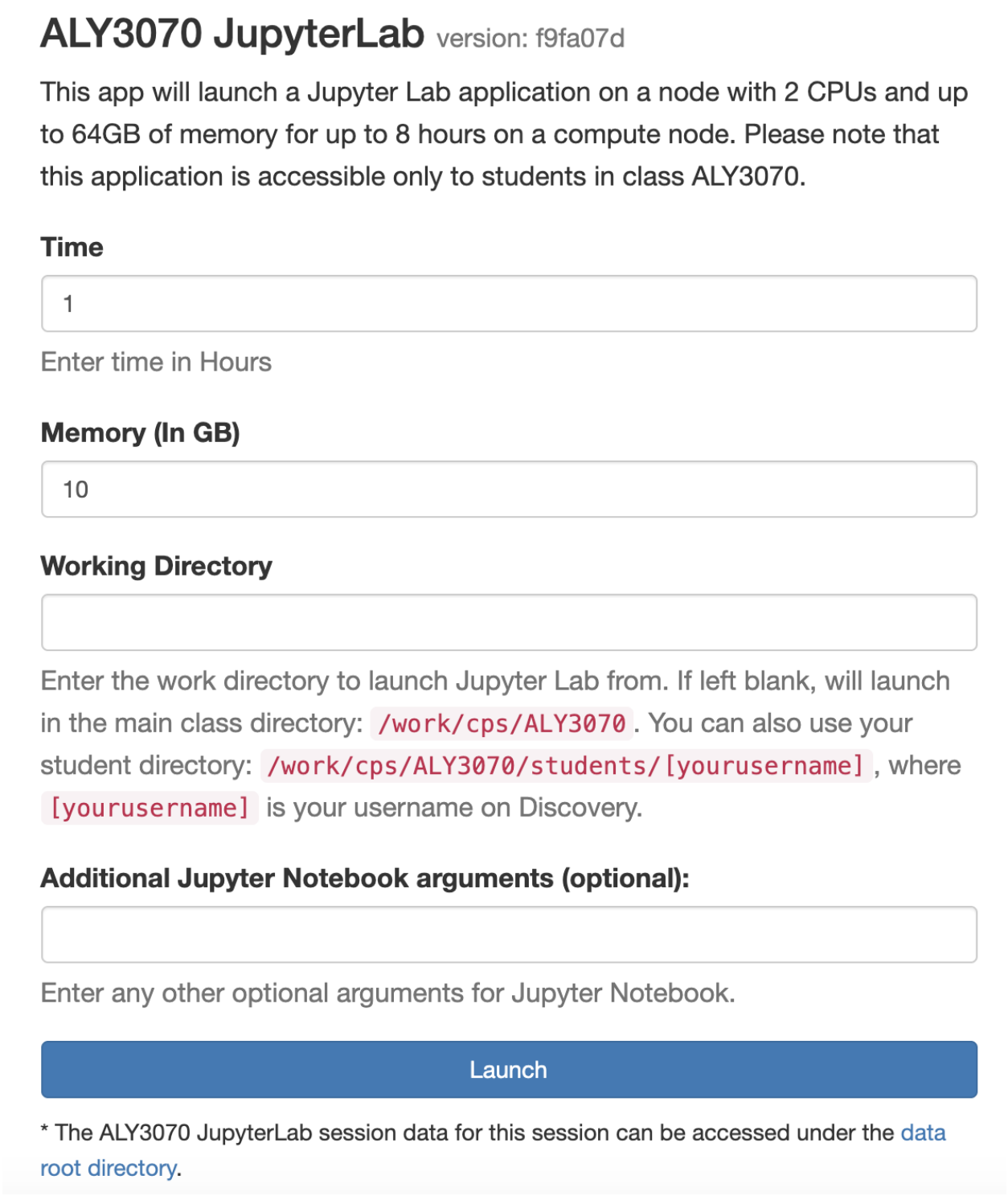
Important: The class instructor needs to fill in the: Discovery Classroom Use Request You will only be able to find your class resources if a request was already made.

In a web browser, go to http://ood.discovery.neu.edu. Login with your NU credentials.

Under the **Courses** menu, select your Class Name (For example: **ALY3070 JupyterLab**):



Select the default options and click **Launch**. Wait until the session is successfully created and ready to be launched (turns green).

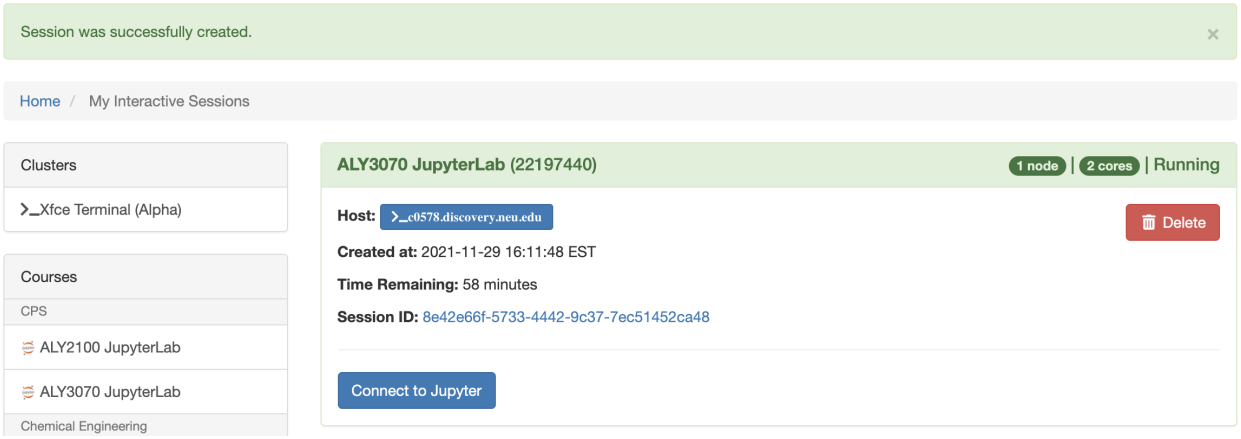


For more control of the session, modify **Time** for the session time (in hours), **Memory** to get more memory in GB, and the **Working Directory** where JupyterLab will launch.

Note: If **Working Directory** is left blank, the session will launch in the main class folder (in this example `/work/cps/ALY3070`). Alternatively, start the session directly from your personal working directory by entering: `/work/cps/ALY3070/students/[username]`, where `[username]` is your username on Discovery. The instructions below

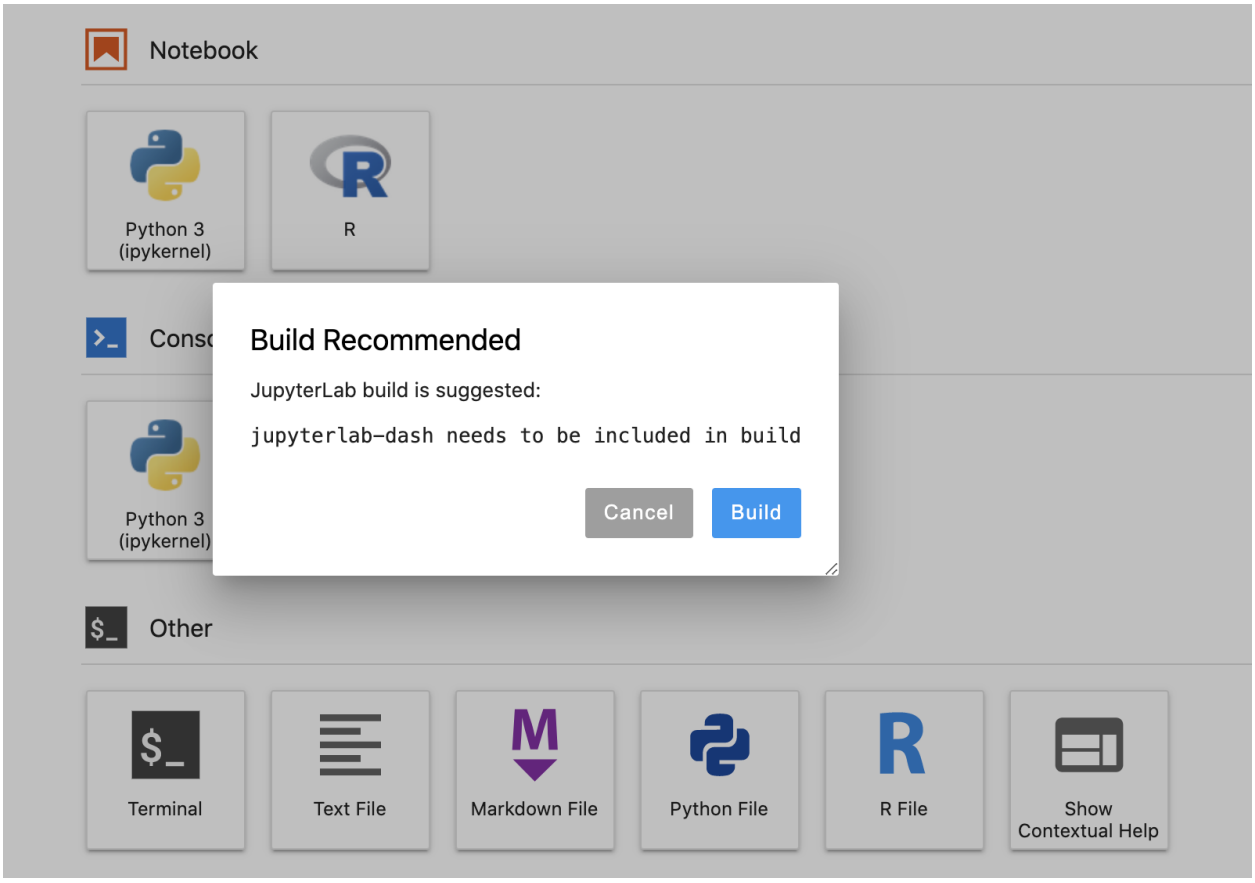
assume the field is left blank.

Click **Connect to Jupyter** to open JupyterLab:



This will open a JupyterLab interface in another tab.

Select **Cancel** when prompted with the **Build Recommended** option:

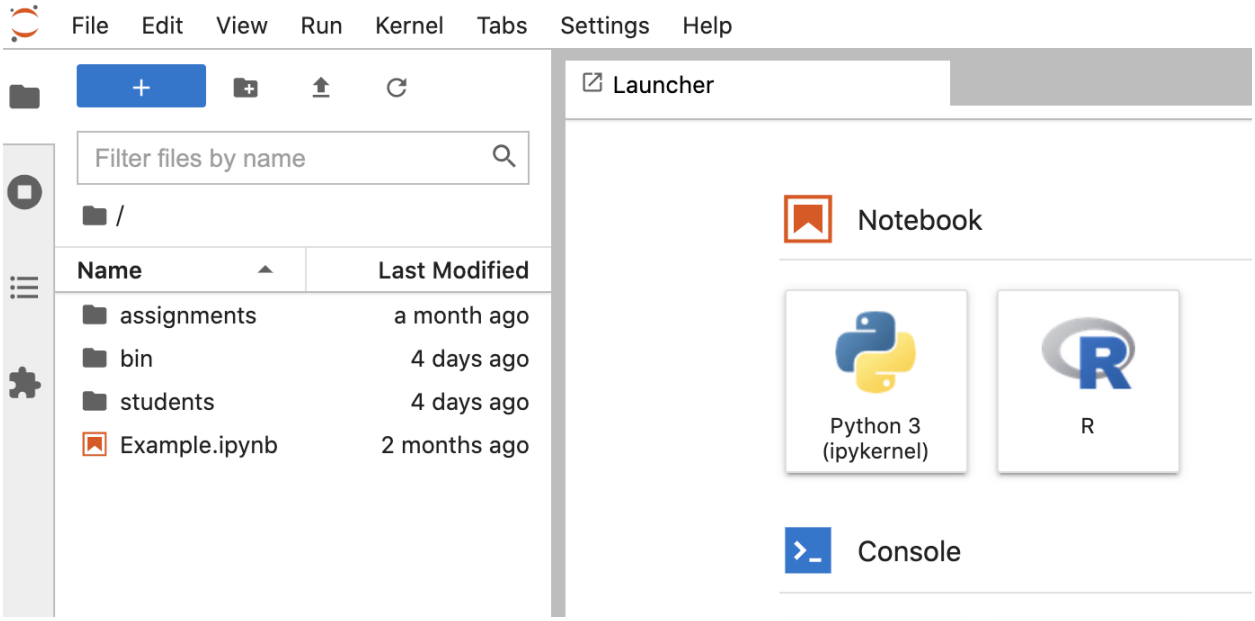


The package jupyterlab-dash does not require a build, and will not work when build is enabled.

30.2 Access CPS class directories

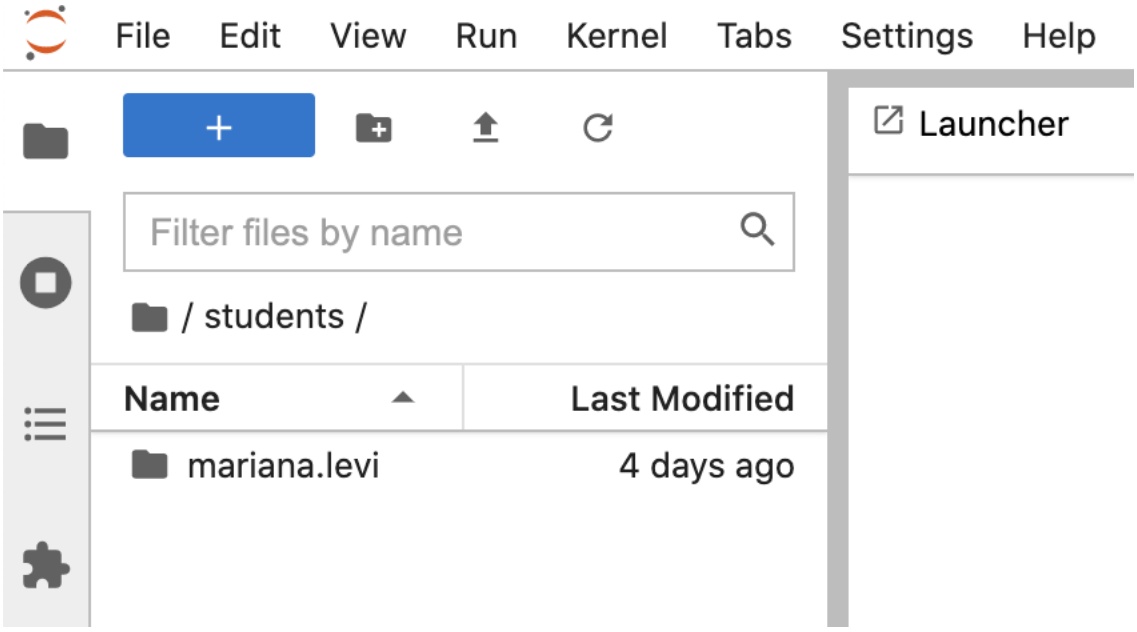
After you are connected to a CPS JupyterLab session on OOD, you can access any shared class directories and your private class directory.

You can navigate between the class folders using the left menu. Your instructor may share files in this directory:

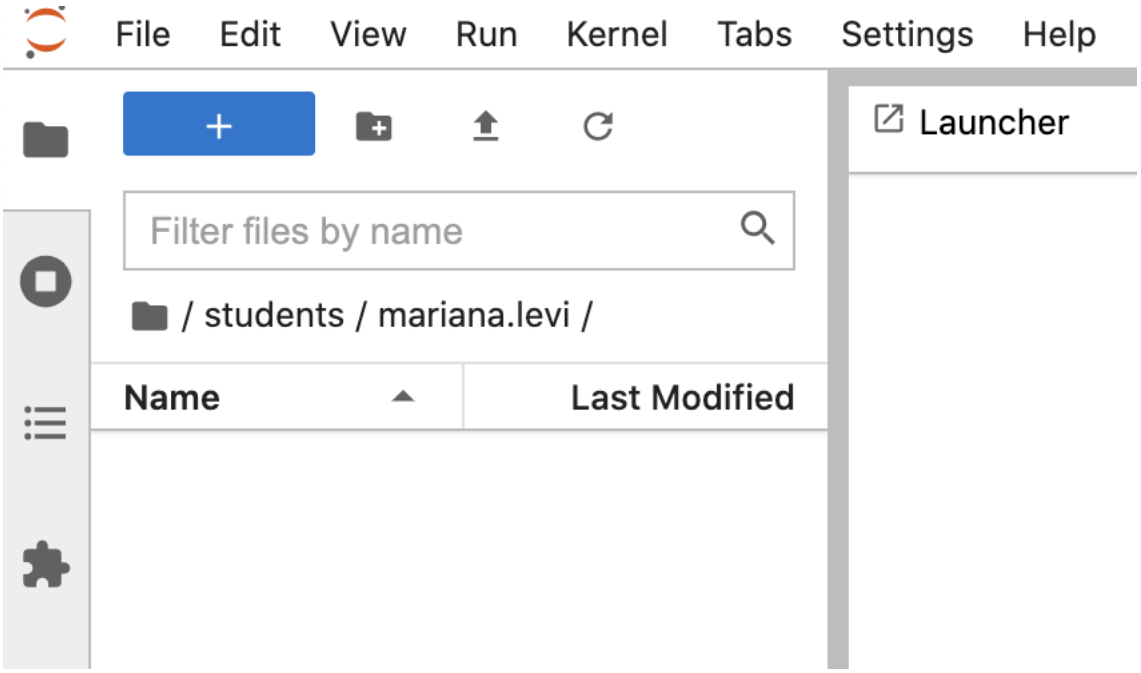


For instance, file **Example.ipynb** can be viewed using Python Jupyter Notebook (but not edited or removed).

Navigate to the **students** directory, where you will see another directory under your username:

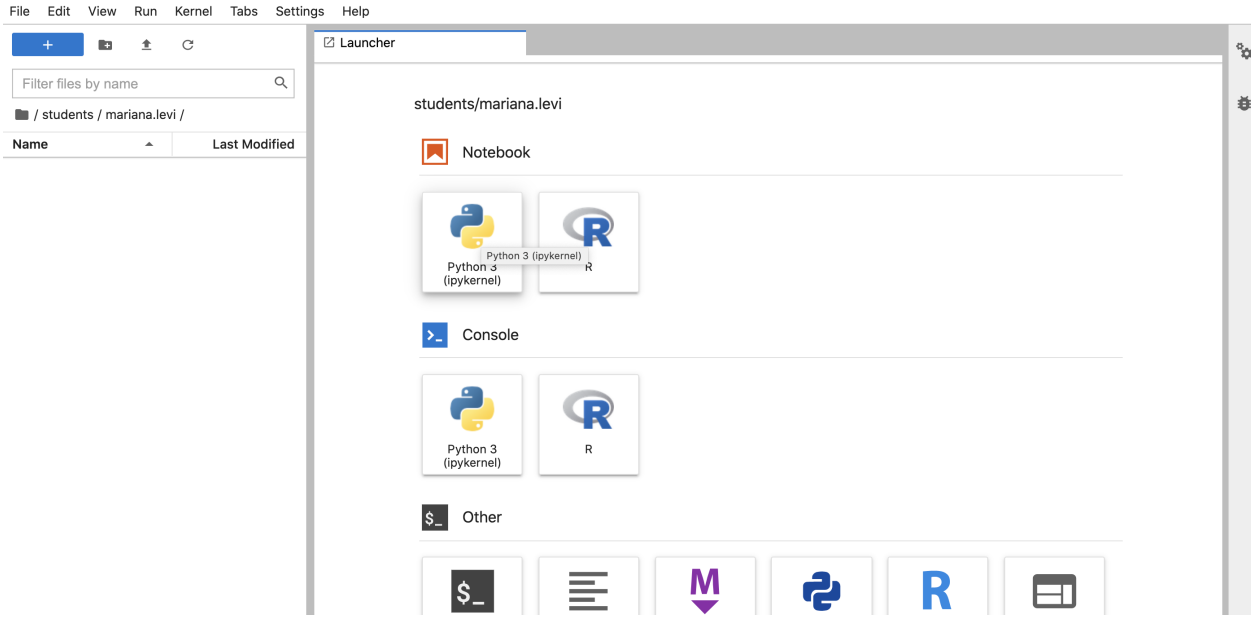


Enter your personal class directory (here, username `mariana.levi` is shown):

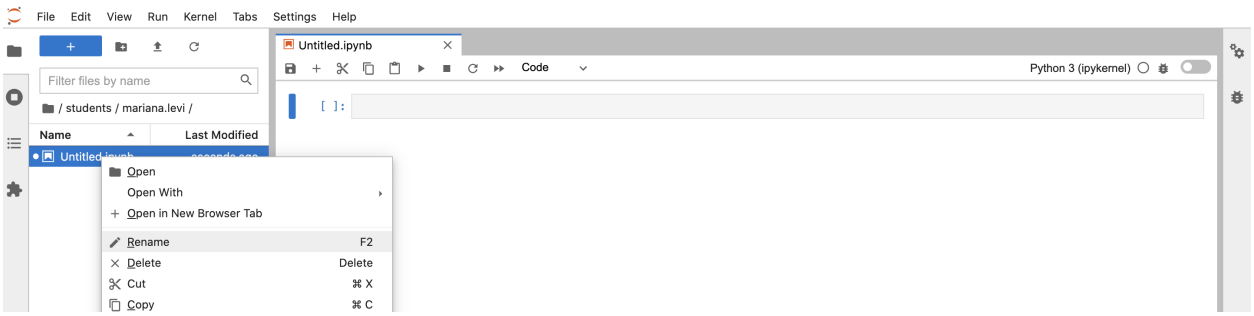


Now you can create and edit Jupyter Notebook files.

Open a new Python Notebook session from the Launcher menu by clicking the **Python 3 (ipykernel)**:



A new file will be created inside your directory called **Untitled.ipynb**. You can rename it by right-clicking on it and using the Rename option:



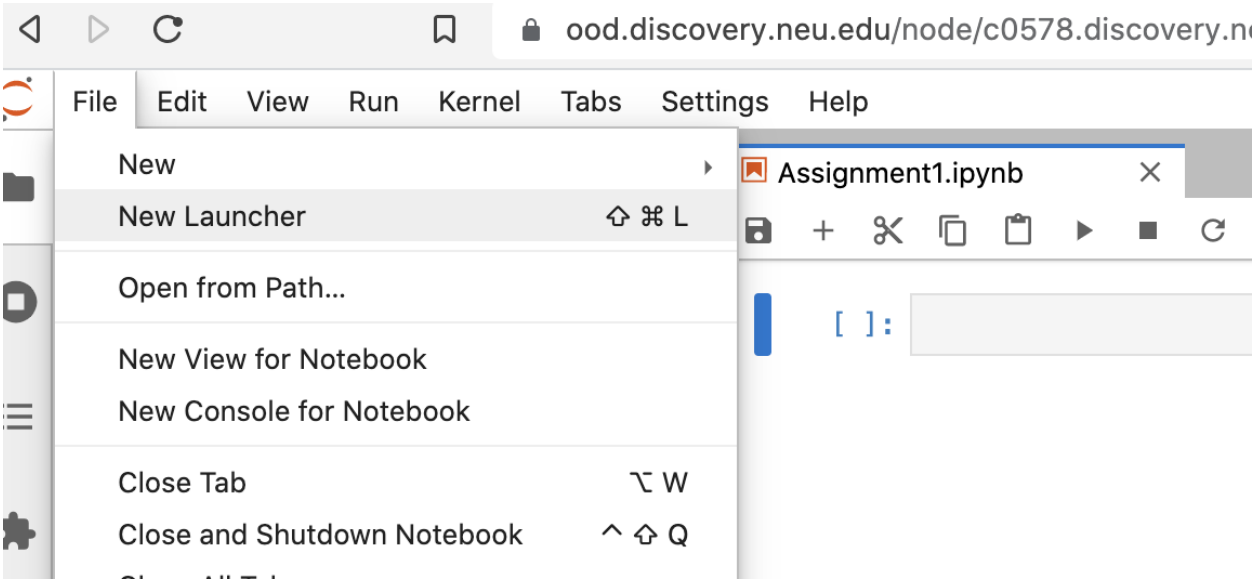
This Python notebook has ready-to-use Python packages needed for your class.

Note: Permission Denied errors: Do not attempt to create, edit or write files that are outside of your personal student directory. Most "Permission Denied" errors are due to directories or files having read-only access permissions.

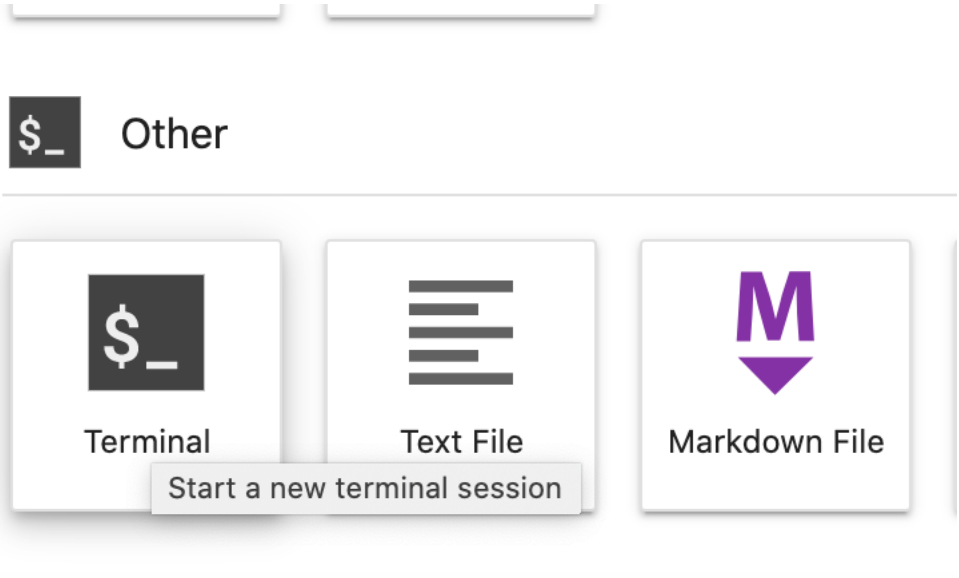
30.3 Submit CPS class assignments

Important: Due to the write-only access permissions on the **assignments** directory, it is required to use the command line interface (Linux Terminal) to submit assignments. **Using other methods, such as the JupyterLab interface or OOD File Explorer, currently does not work**.

To submit your assignment (for example, named: **Assignment1.ipynb**) to the **assignments** directory, open the JuypterLab New Launcher by clicking the **File** top menu option, and then selecting **New Launcher**:



Click on the **Terminal** option under **Other** to open a Linux terminal:



Navigate to your personal directory by typing the following command (change the class name from `ALY3070` to your class name accordingly):

```
cd /work/cps/ALY3070/students/$USER
```

Where `$USER` is a saved shell variable for your username. You can optionally also replace it with your username.

Check that your assignment file is visible in the command line by typing `ls`. Then, Copy the assignment file to the **assignments** directory with this command (replace **Assignment1.ipynb** with your file name):

```
cp Assignment1.ipynb ../../assignments
```

To remove an existing assignment, type (replace **Assignment1.ipynb** with your file name):

```
rm ../../assignments/Assignment1.ipynb
```

Close the Terminal tab when done.