

# Quick Intro to MSI

Ju Sun (Computer Science & Engineering)

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UNIVERSITY OF MINNESOTA

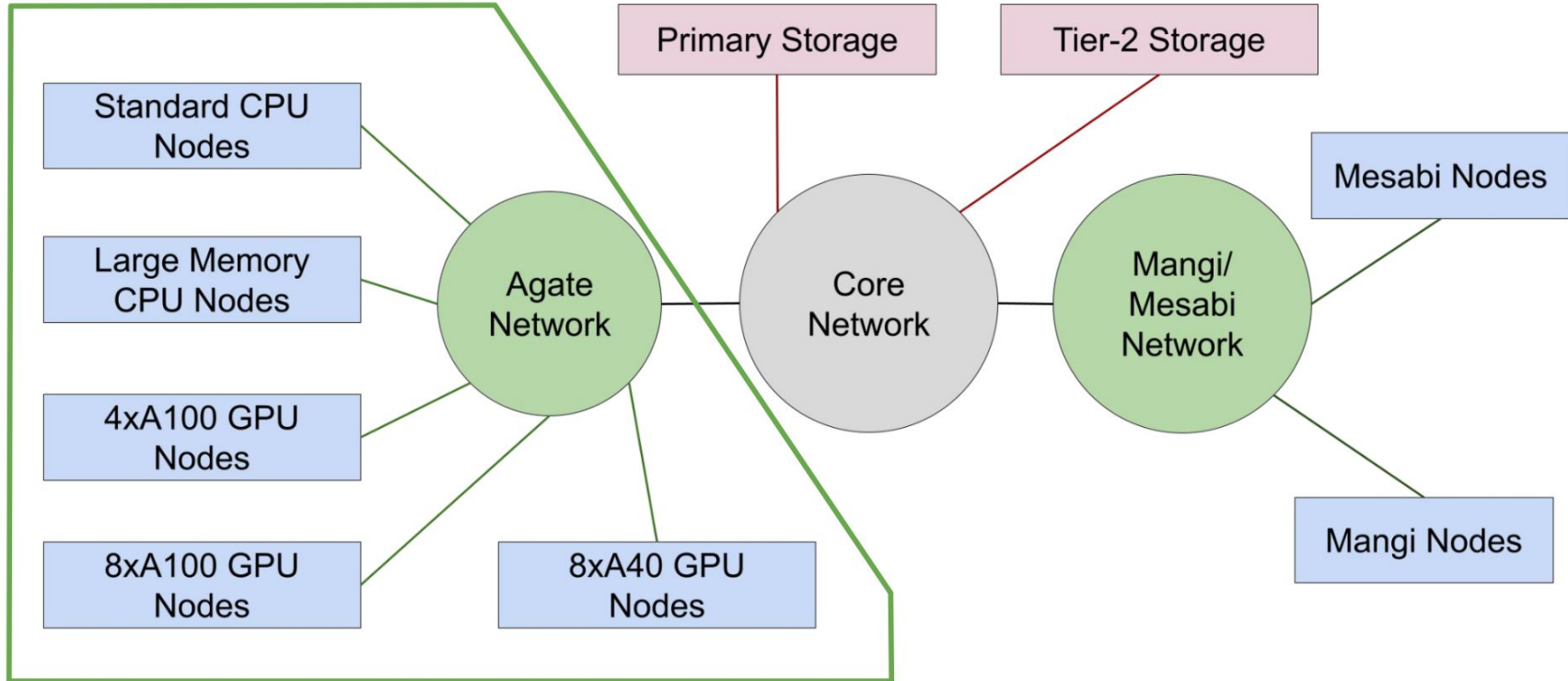
Driven to Discover<sup>SM</sup>

# Disclaimer

Many of the slides are taken from MSI's tutorial slides below, as well introductory slides made by **Dr. Ben Lynch, MSI Director**.

- Introduction to Minnesota Supercomputing Institute (MSI)  
<https://youtu.be/bNBfh2Q9l1E>
- Job submission and scheduling at MSI  
<https://youtu.be/r4m4WK4LfPY?si=BxtSrhzofEcYCTH6>
- Interactive computing at MSI  
[https://youtu.be/D6D77\\_gEmhw?si=PlMJigp-GYO\\_3bcF](https://youtu.be/D6D77_gEmhw?si=PlMJigp-GYO_3bcF)

# What's MSI?



# What's MSI?



## Mesabi

- Over 700 nodes
  - Memory configuration
    - 616 nodes have 64GB RAM
    - 24 nodes have 256GB RAM
    - 16 nodes have 1TB RAM
    - 40 k40 GPU nodes with 128GB RAM
- 17,784 cores provided by Intel Haswell Processors
- 480GB SSD available on 32 nodes



## Agate

- 412 nodes
- AMD processors with 64-128 CPU cores per node
- 344 CPU compute node
  - 244 have 512G mem
  - 100 have 2TB mem
- 58 GPU compute nodes
  - 50 A100 512G mem
  - 8 A100 1TB mem
- 10 GPU interactive nodes
  - 8 A40 GPUs 512G mem each

Basic access

# Prerequisite to connect

## Campus VPN

<https://it.umn.edu/services-technologies/virtual-private-network-vpn>

- MSI services are only available to on-campus network addresses
- Especially during the pandemic, many users are working off-campus
- VPN clients and instructions are available from OIT for most operating systems and mobile devices

## DUO Authentication

<https://it.umn.edu/services-technologies/self-help-guides/duo-set-use-duo-security>

- DUO 2-factor authentication is required for most MSI services
- DUO is also required to connect to the campus VPN

# Two way to access

- GUI interactive access
- Command-line access (please check their tutorial details)

## **Job submission and scheduling at MSI**

<https://youtu.be/r4m4WK4LfPY?si=BxtSrhzofEcYCTH6>

## **Interactive computing at MSI**

[https://youtu.be/D6D77\\_gEmhw?si=PlMJi9p-GYO\\_3bcF](https://youtu.be/D6D77_gEmhw?si=PlMJi9p-GYO_3bcF)

# GUI interactive access: OnDemand

<https://ondemand.msi.umn.edu/>


Open OnDemand


Files ▾


Jobs ▾


Clusters ▾


Interactive Apps ▾




 ▾

 ▾







Minnesota

Supercomputing Institute

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**Driven to Discover®**

OnDemand provides an integrated, single access point for all of your HPC resources.

### Message of the Day

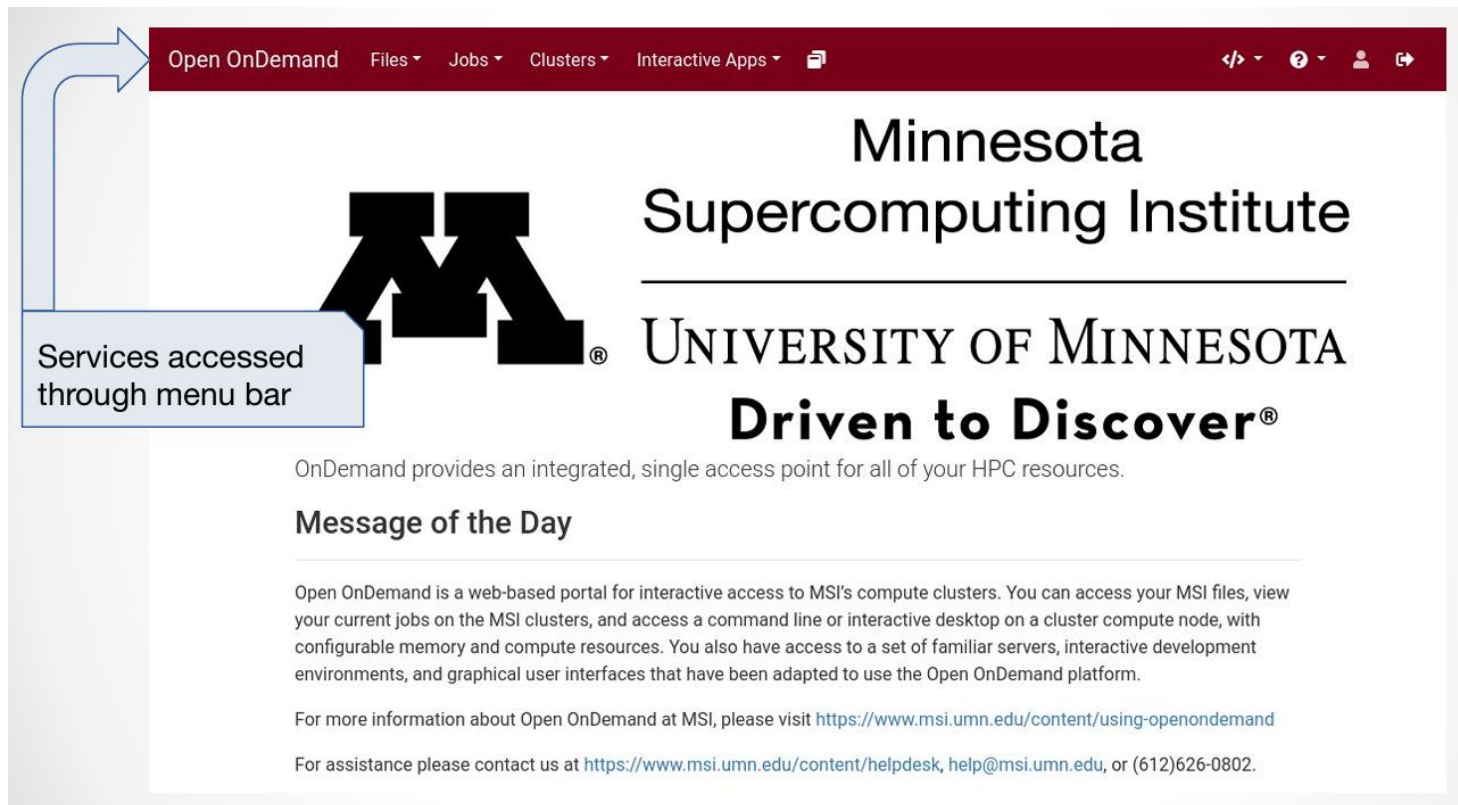
Open OnDemand is a web-based portal for interactive access to MSI's compute clusters. You can access your MSI files, view your current jobs on the MSI clusters, and access a command line or interactive desktop on a cluster compute node, with configurable memory and compute resources. You also have access to a set of familiar servers, interactive development environments, and graphical user interfaces that have been adapted to use the Open OnDemand platform.

For more information about Open OnDemand at MSI, please visit <https://www.msi.umn.edu/content/using-openondemand>

For assistance please contact us at <https://www.msi.umn.edu/content/helpdesk>, [help@msi.umn.edu](mailto:help@msi.umn.edu), or (612)626-0802.



# OnDemand walkthrough



The screenshot shows the Open OnDemand web portal. At the top is a dark red navigation bar with the text "Open OnDemand" and several dropdown menus: "Files", "Jobs", "Clusters", and "Interactive Apps". To the right of these menus are icons for code, help, user, and share. Below the navigation bar, the page features the Minnesota Supercomputing Institute logo (a stylized 'M' with three upward-pointing arrows) and the text "Minnesota Supercomputing Institute" followed by "UNIVERSITY OF MINNESOTA" and "Driven to Discover®". A light blue callout box with a curved arrow pointing to the navigation bar contains the text "Services accessed through menu bar". Below the header, a paragraph states: "OnDemand provides an integrated, single access point for all of your HPC resources." This is followed by a section titled "Message of the Day" which describes the portal's capabilities: "Open OnDemand is a web-based portal for interactive access to MSI's compute clusters. You can access your MSI files, view your current jobs on the MSI clusters, and access a command line or interactive desktop on a cluster compute node, with configurable memory and compute resources. You also have access to a set of familiar servers, interactive development environments, and graphical user interfaces that have been adapted to use the Open OnDemand platform." At the bottom, two lines of text provide contact information: "For more information about Open OnDemand at MSI, please visit <https://www.msi.umn.edu/content/using-openondemand>" and "For assistance please contact us at <https://www.msi.umn.edu/content/helpdesk>, [help@msi.umn.edu](mailto:help@msi.umn.edu), or (612)626-0802."

Services accessed through menu bar

Open OnDemand Files Jobs Clusters Interactive Apps

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**Driven to Discover®**

OnDemand provides an integrated, single access point for all of your HPC resources.

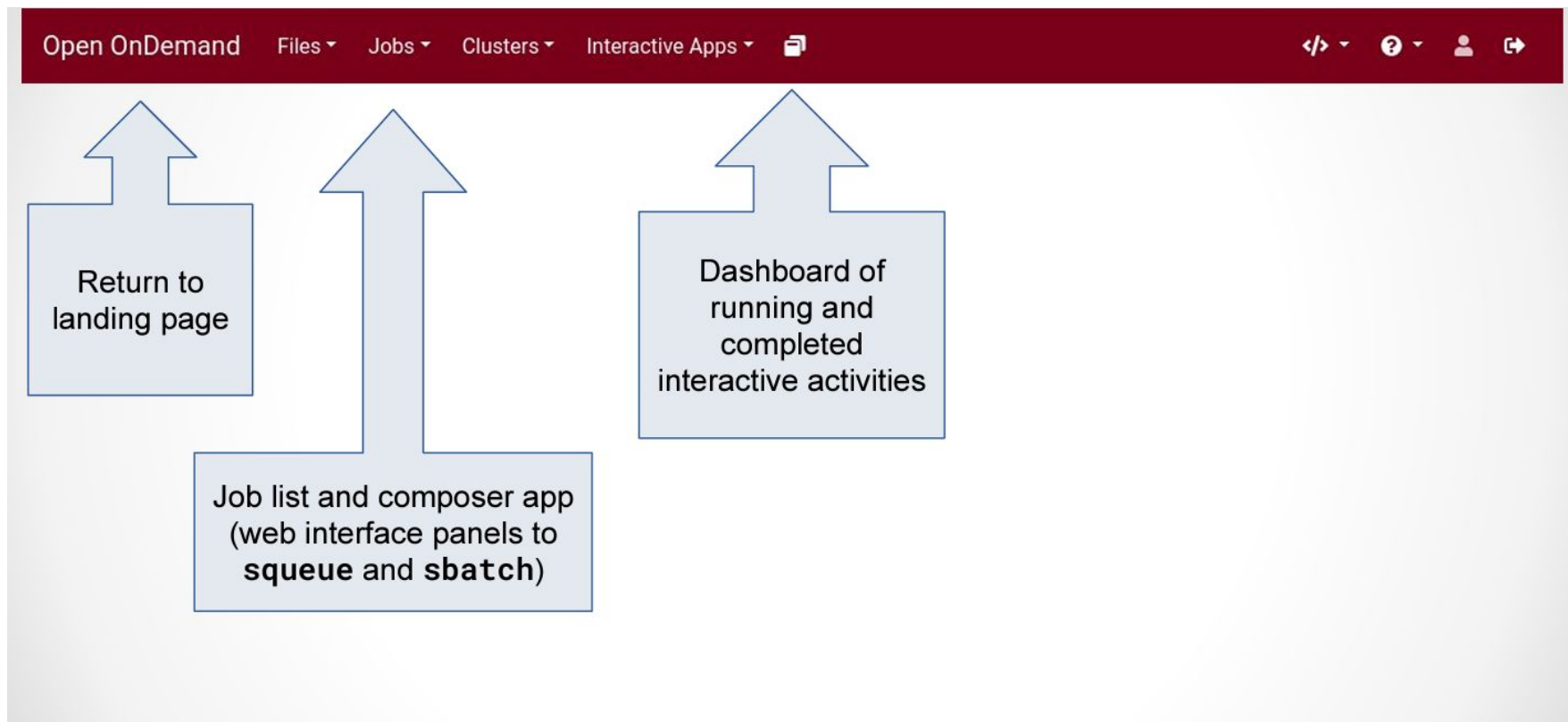
### Message of the Day

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# OnDemand walkthrough



# OnDemand walkthrough

The screenshot shows the OnDemand web interface. At the top is a dark red navigation bar with links: "Open OnDemand", "Files" (highlighted in yellow), "Jobs", "Clusters", "Interactive Apps", and "My Interactive Sessions". Below the "Files" link, a dropdown menu is open, showing "Home Directory" with a house icon and "/home/support" with a folder icon. A blue box with the text "File browser access" and a large blue arrow points from below to the "/home/support" option. To the right of this, another blue box titled "File browser:" contains a list of capabilities: "browse/navigate/manage files", "upload/download files up to few GB size", and "access different starting dirs if you have multiple groups/projects". Below the navigation bar, a toolbar contains buttons: "Open in Terminal", "New File", "New Directory", "Upload", "Download", "Copy/Move", and "Delete". The main content area shows a breadcrumb path: "/ home / support / milligan /", followed by a "Change directory" button and a "Copy path" button. Below the path, there are checkboxes for "Show Owner/Mode" and "Show Dotfiles", and a "Filter:" input field. At the bottom, a table header is visible with columns: "Type", "Name", "Size", and "Modified at".

Open OnDemand Files Jobs Clusters Interactive Apps My Interactive Sessions

Home Directory  
/home/support

File browser access

File browser:

- browse/navigate/manage files
- upload/download files up to few GB size
- access different starting dirs if you have multiple groups/projects

Open in Terminal New File New Directory Upload Download Copy/Move Delete

/ home / support / milligan / Change directory Copy path

Show Owner/Mode Show Dotfiles Filter:

Showing 92 of 236 rows - 0 rows selected

Type	Name	Size	Modified at
------	------	------	-------------

# OnDemand walkthrough

The screenshot shows the OnDemand web interface. The top navigation bar includes links for 'Open OnDemand', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. The 'Clusters' menu is expanded, showing options for '\_Agate Shell Access' and '\_Mesabi Shell Access'. A blue box labeled 'Command line terminal access' has an arrow pointing to the '\_Mesabi Shell Access' option. Another blue box titled 'Command line terminal:' contains a list of instructions: 'SSH in a web browser (almost)', 'Launch terminal on cluster headnode', 'Roughly equivalent to e.g. ssh <username>@agate.msi.umn.edu', and 'Also launch in specific directory via file browser pane'. A blue arrow points from this box to the 'Open in Terminal' button in the file browser pane, which is circled in red. The file browser pane also includes buttons for 'New File', 'New Directory', 'Upload', 'Download', 'Copy/Move', and 'Delete'. The bottom status bar shows the current path as '/ home / support / milligan /' and a 'Change directory' button.

Open OnDemand Files Jobs Clusters Interactive Apps My Interactive Sessions

>\_Agate Shell Access  
>\_Mesabi Shell Access

Command line terminal access

Command line terminal:

- "SSH" in a web browser (almost)
- Launch terminal on cluster headnode
- Roughly equivalent to e.g. `ssh <username>@agate.msi.umn.edu`
- Also launch in specific directory via file browser pane

>\_ Open in Terminal New File New Directory Upload Download Copy/Move Delete

/ home / support / milligan / Change directory Copy path

# OnDemand walkthrough

The screenshot displays the OnDemand web interface. At the top is a dark red navigation bar with the following items: "Open OnDemand", "Files", "Jobs", "Clusters", "Interactive Apps" (highlighted in yellow), and "My Interactive Sessions". The "Interactive Apps" dropdown menu is open, showing categories and their respective launchers:

- Desktops
  - Desktop
  - Persistent Desktop
- GUIs
  - ANSYS Workbench
  - IGV
  - MATLAB
- IDEs
  - Abaqus
  - COMSOL Multiphysics
  - IDL
  - Mathematica
- Servers
  - Jupyter
  - RStudio Server

On the left side of the interface, there is a light blue box containing the following text:

- Interactive Apps menu lists available application launchers
- Each launcher leads to a session options page
- Each session runs as an interactive job on a cluster resource
- Launchers also available via the Interactive Sessions dashboard

Red arrows indicate the flow of information: three arrows point from the text box to the "Desktops", "GUIs", and "IDEs" sections of the dropdown menu, and one arrow points from the text box to the "My Interactive Sessions" link in the top navigation bar.

# OnDemand walkthrough

Session was successfully created. ×

Home / My Interactive Sessions

Interactive Apps

Desktops

- Desktop
- Persistent Desktop

GUIs

- ANSYS Workbench
- IGV
- MATLAB

IDEs

- Abaqus
- COMSOL Multiphysics
- IDL
- Mathematica

Servers

- Jupyter
- RStudio Server

**Desktop (71087165)** 1 node | 2 cores | Running

Host: `>_acn23.agate.msl.umn.edu` Delete

Created at: 2023-02-16 12:31:57 CST

Time Remaining: 3 hours and 58 minutes

Session ID: `a2a0db19-7a3a-45a0-9e90-eddca9bfd03b`

Compression 0 (low) to 9 (high)

Image Quality 0 (low) to 9 (high)

Launch Desktop View Only (Share-able Link)

**RStudio Server (71064307)** Completed

Created at: 2023-02-13 23:32:26 CST

Session ID: `713d240a-60e3-488d-a2a4-3d5d80dcfd9a`

For debugging purposes, this card will be retained for 5 more days

**RStudio Server (71061783)** Completed

**My Interactive Sessions**

List job status for interactive sessions:  
queued, running, finished

Launch into a running session (usually opens new browser tab)

Access full menu of interactive launchers



# Setting up your deep learning environment

# Put everything inside a virtual environment

## Conda



*Package, dependency and environment management for any language—Python, R, Ruby, Lua, Scala, Java, JavaScript, C/ C++, Fortran, and more.*

## Miniconda Highly recommended!

Miniconda is a free minimal installer for conda. It is a small bootstrap version of Anaconda that includes only conda, Python, the packages they both depend on, and a small number of other useful packages (like pip, zlib, and a few others). If you need more packages, use the `conda install` command to install from thousands of packages available by default in Anaconda's public repo, or from other channels, like conda-forge or bioconda.

Is Miniconda the right conda install for you? The [Anaconda](#) or [Miniconda](#) page lists some reasons why you might want one installation over the other.

Check out how to use conda to manage virtual environments, e.g.,

<https://conda.io/projects/conda/en/latest/user-guide/getting-started.html>

<https://docs.conda.io/projects/miniconda/en/latest/>



# Install PyTorch inside Conda

## INSTALL PYTORCH

Select your preferences and run the install command. Stable represents the most currently tested and supported version of PyTorch. This should be suitable for many users. Preview is available if you want the latest, not fully tested and supported, builds that are generated nightly. Please ensure that you have **met the prerequisites below (e.g., numpy)**, depending on your package manager. Anaconda is our recommended package manager since it installs all dependencies. You can also **install previous versions of PyTorch**. Note that LibTorch is only available for C++.

PyTorch Build	Stable (2.1.0)		Preview (Nightly)	
Your OS	Linux	Mac	Windows	
Package	Conda	Pip	LibTorch	Source
Language	Python		C++ / Java	
Compute Platform	CUDA 11.8	CUDA 12.1	ROCm 5.6	CPU
Run this Command:	<pre>conda install pytorch torchvision torchaudio pytorch-cuda=11.8 -c pytorch -c nvidia</pre>			

<https://pytorch.org/>

Be careful of the CUDA version!

\*\* **A100**: this gpu **ONLY WORKS** with cuda  $\geq 11.3$ . (

\*\* **V100**: this gpu **DOES NOT** work with cuda  $\geq 11.3$ .

# Prepare a job script

```
#!/bin/bash -l
#SBATCH --time=8:00:00    ## Specify your request computing time
                        ## 24:00:00 max for public queues
#SBATCH --nodes=1        ## Specify number of computing nodes to request
                        ## For most jobs in our research, we just need 1
#SBATCH --ntasks-per-node=4  ## Number of cpu cores to request.
                        ## Request more if:
                        ## 1) you need many cpu cores
                        ## for multi-thred computing
                        ## (e.g., parallelize for loops
                        ## for data pre-processing)
                        ## 2) multi-GPU (there may be min number of
                        ## cpu core requires for gpu connection
                        ## visit MSI website for detailed info.)

#SBATCH --mem=10g
#SBATCH --tmp=10g        ## Requesting storage (like cache and RAM)
                        ## to support your job computation

#SBATCH --mail-type=ALL    ## Receive all job notifications by email
#SBATCH --mail-user=$your_x500$@umn.edu  ## Your email address
                        ## to view the notifications
```

```
#SBATCH --partition=interactive-gpu      ## Job queue to submit your job
#SBATCH --gres=gpu:a40:1                ## Number and type of gpu to request
                                         ## Without this line,
                                         ## you are not requesting any gpu
```

```
cd /home/csci5527/your_x500/your_working_folder
                                         ## Direct your working directory

export PATH=/home/csci5527/$your_x500$/$your_conda$/
envs/$your_venv_name$/bin:$PATH         ## Load your conda env

python autoencoder_train.py             ## Execute your job
```

<https://www.msi.umn.edu/content/job-submission-and-scheduling-slurm> for more details

# Which partition?

Partition Name	Max cores per node	Maximum walltime	Max available node memory <sup>3</sup> (GB)	Memory per core (MB)	Local scratch per node (GB)	Max nodes per job	Max jobs per user
msismall	128	96:00:00	248-755	3900	850	1	4000 <sup>4</sup>
msilarge	128	24:00:00	248-755	3900	850	32	4000 <sup>4</sup>
msibigmem	128	24:00:00	1995	15950	850	1	4000 <sup>4</sup>
msigpu <sup>1</sup>	24-128	24:00:00	374-1002	3900-8000	850	4	4000 <sup>4</sup>
msilong	32	37-0	248-755	3900	850	*** <sup>5</sup>	*** <sup>5</sup>
interactive	128	24:00:00	499	3900	850	2	1
interactive-gpu <sup>1,6</sup>	64-128	24:00:00	499-755	5120	850	1	1
interactive-long	64-128	37-0	499	3900	850	1	1
preempt <sup>2</sup>	128	24:00:00	248-755	3900	850	1	4000 <sup>4</sup>
preempt-gpu <sup>1,2</sup>	64-128	24:00:00	499-755	3900-8000	850	1	4000 <sup>4</sup>

```
#SBATCH --partition=interactive-gpu
```

<https://www.msi.umn.edu/partitions>

# Frequently used commands

## Step 5: Submit your job

```
sbatch XXX.slurm # XXX.slurm is your job script name
```

## Step 6: Useful commands after submitting your job

(1) Checking the status of the MSI queue:

```
squeue -p interactive-gpu # Lists all job statuses on the  
                           # interactive-gpu partition (not only you)
```

Or simply checking your own queue status by:

```
squeue --me # chek your own jobs
```

(2) Canceling a submitted job:

```
scancel jobIDnumber
```

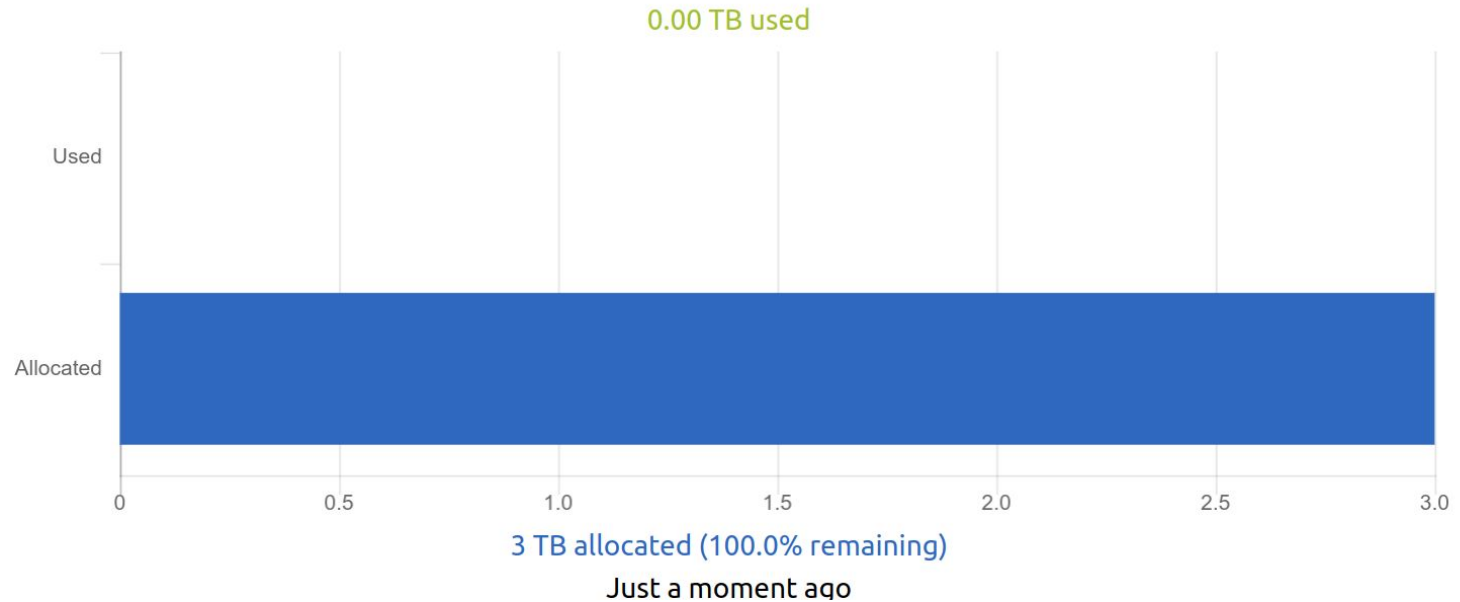
(3) Canceling all your submitted jobs:

```
scancel --user=your_x500
```

Save the class storage

# Storage/file counts shared for the whole class

## Storage



# Three levels of storage

## Primary Storage

- Primary storage is where you will do most of your work
  - GNU/Linux filesystem
- Watch your disk usage:

Impo  
/hon  
Your

## Second Tier Storage

- Sometimes referred to as “Ceph”, the name of the software defined storage utility in use in this storage layer.
- Second tier storage is separate from primary storage, it is an “object store” - you must use special tools to access it.
- From the command line, you can use the “s3cmd” software package to interact with your storage:
  - See: <https://www.msi.umn.edu/support/faq/how-do-i-use-second-tier-storage-command-line>
- For a graphical interface, you can use Globus
  - See: <https://www.msi.umn.edu/support/faq/how-do-i-use-globus-transfer-data-msi-0>
- **Not** backed up, so if you delete a file, it will be gone for good
  - Quotas are much more relaxed on second tier storage
  - **Resilient system to store data**

## Primary Storage Scratch

- Quotas are large, so there should be leeway to make very large files here
  - Use it for intermediate/temporary files in analytical workflows
- Files are kept for 30 days, so be sure to copy important files to your group directory

space is also not backed up by snapshot  
**the tricks that exist to keep data in scratch for an 30 days. Consider data on scratch as having no**

**Required: use  
scratch storage to  
store your large  
datasets and  
immediate results**