High Performance Computing in GW

Shuyue (Frank) Guan

The Medical Imaging & Image Analysis (MIA) Laboratory

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Outline

- Introduce to the new HPC: PEGASUS
- How to get an account
- How to upload files
- How to log in the HPC system
- To run jobs by SLURM

New HPC in GW

GW COLONIAL ONE

GW PEGASUS

- One CPU node
  - Dual 20-Core 3.70GHz Intel Xeon processors
  - 192GB RAM
  - 800 GB SSD
- One GPU node
  - 2 NVIDIA **Tesla V100** GPU (4 for large nodes)
  - Dual 20-Core 3.70GHz Intel Xeon (18-Core Xeon for large nodes)
  - 192GB RAM (384GB for large nodes)
  - 800 GB SSD
- High throughput node, High memory node (3TB RAM!),…

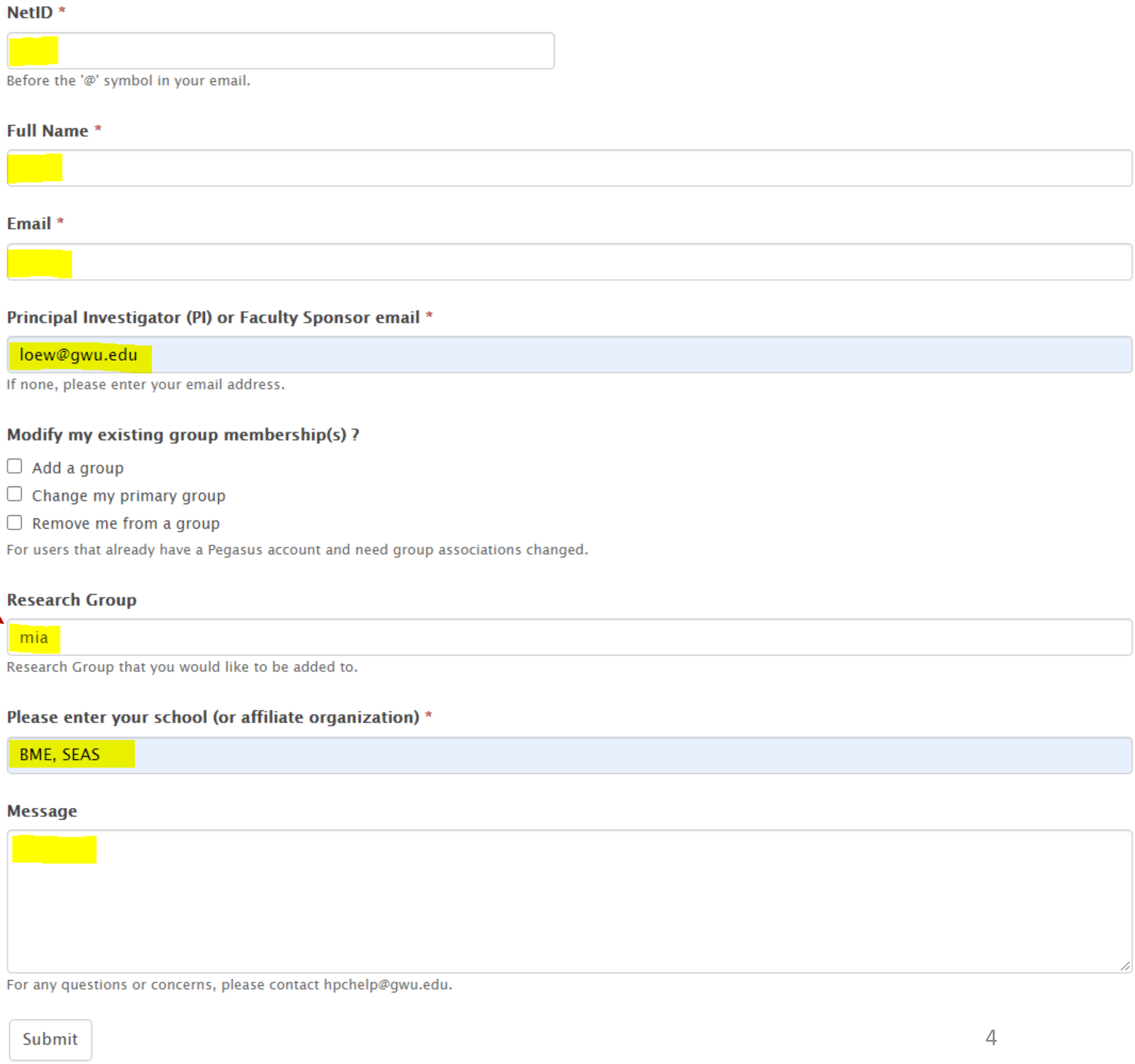
Tesla V100 highlight

640	**Tensor Cores**
5120	**CUDA Cores**
16 GB	**Memory**

First: request for an account

https://colonialone.gwu.edu/getting-access/

mia



NetID *

Before the '@' symbol in your email.

Full Name *

Email *

Principal Investigator (PI) or Faculty Sponsor email *

loew@gwu.edu

If none, please enter your email address.

Modify my existing group membership(s) ?

- ☐ Add a group
- ☐ Change my primary group
- ☐ Remove me from a group

For users that already have a Pegasus account and need group associations changed.

Research Group

mia

Research Group that you would like to be added to.

Please enter your school (or affiliate organization) *

BME, SEAS

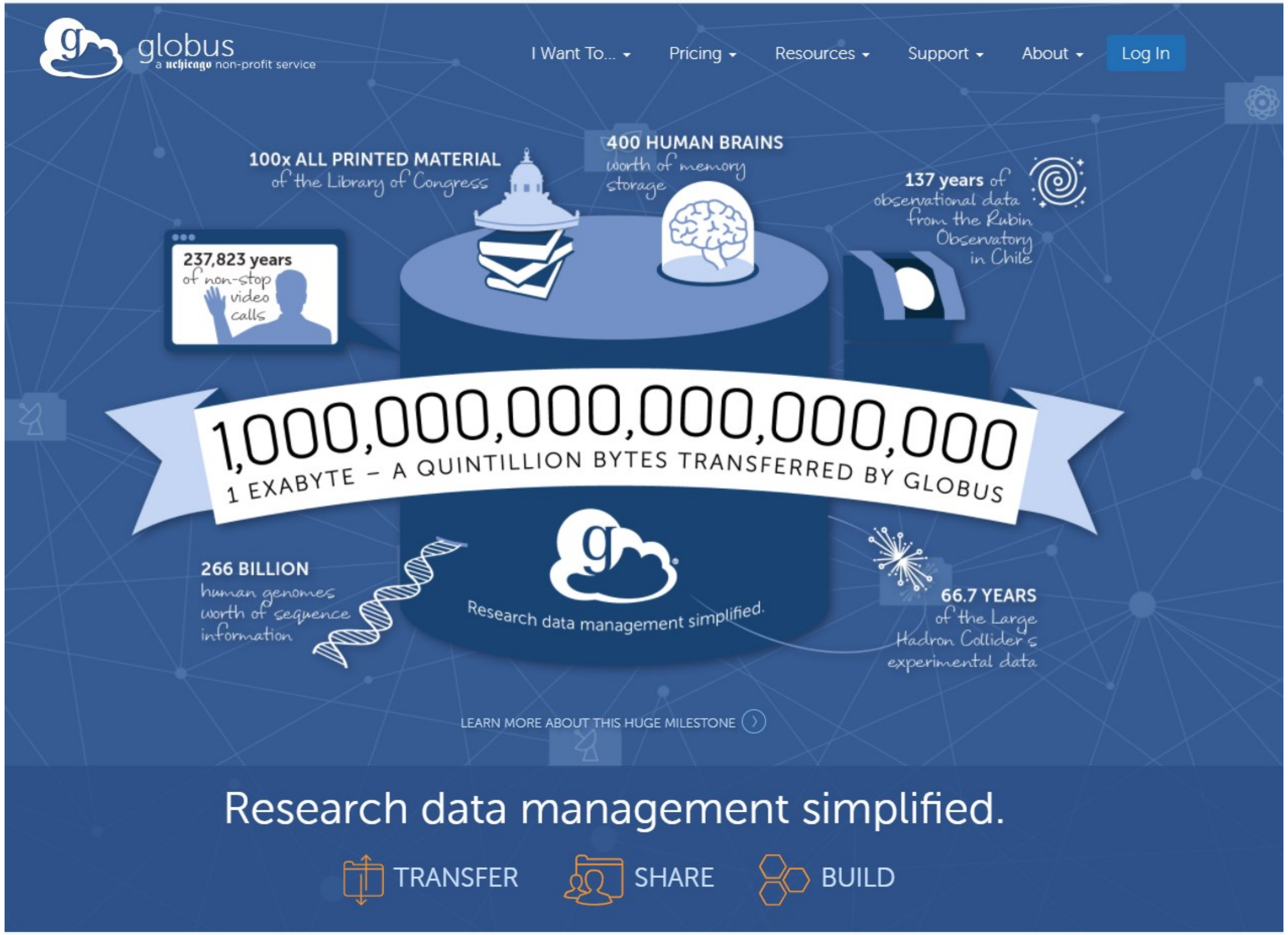
Message

For any questions or concerns, please contact hpchelp@gwu.edu.

File Transfer with Globus

Globus is used literally everywhere by everyone transferring data in the HPC world. AWS, National Labs, Universities ,…, and GWU.

https://www.globus.org/



100x ALL PRINTED MATERIAL of the Library of Congress

400 HUMAN BRAINS worth of memory storage

137 years of observational data from the Rubin Observatory in Chile

237,823 years of non-stop video calls

1,000,000,000,000,000,000

1 EXABYTE – A QUINTILLION BYTES TRANSFERRED BY GLOBUS

266 BILLION human genomes worth of sequence information

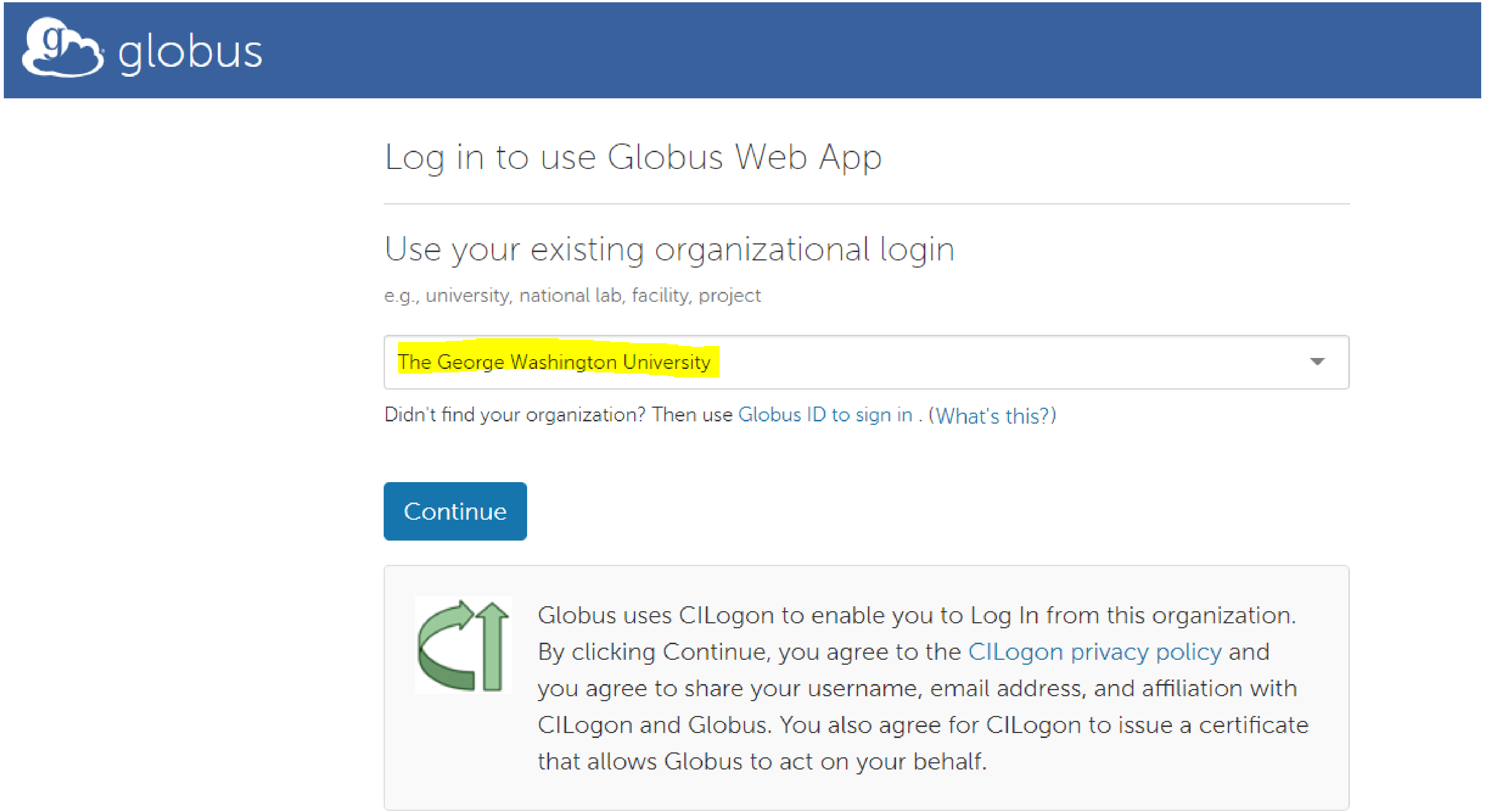
Research data management simplified.

66.7 YEARS of the Large Hadron Collider's experimental data

LEARN MORE ABOUT THIS HUGE MILESTONE

Research data management simplified.

When log in



Log in to use Globus Web App

Use your existing organizational login

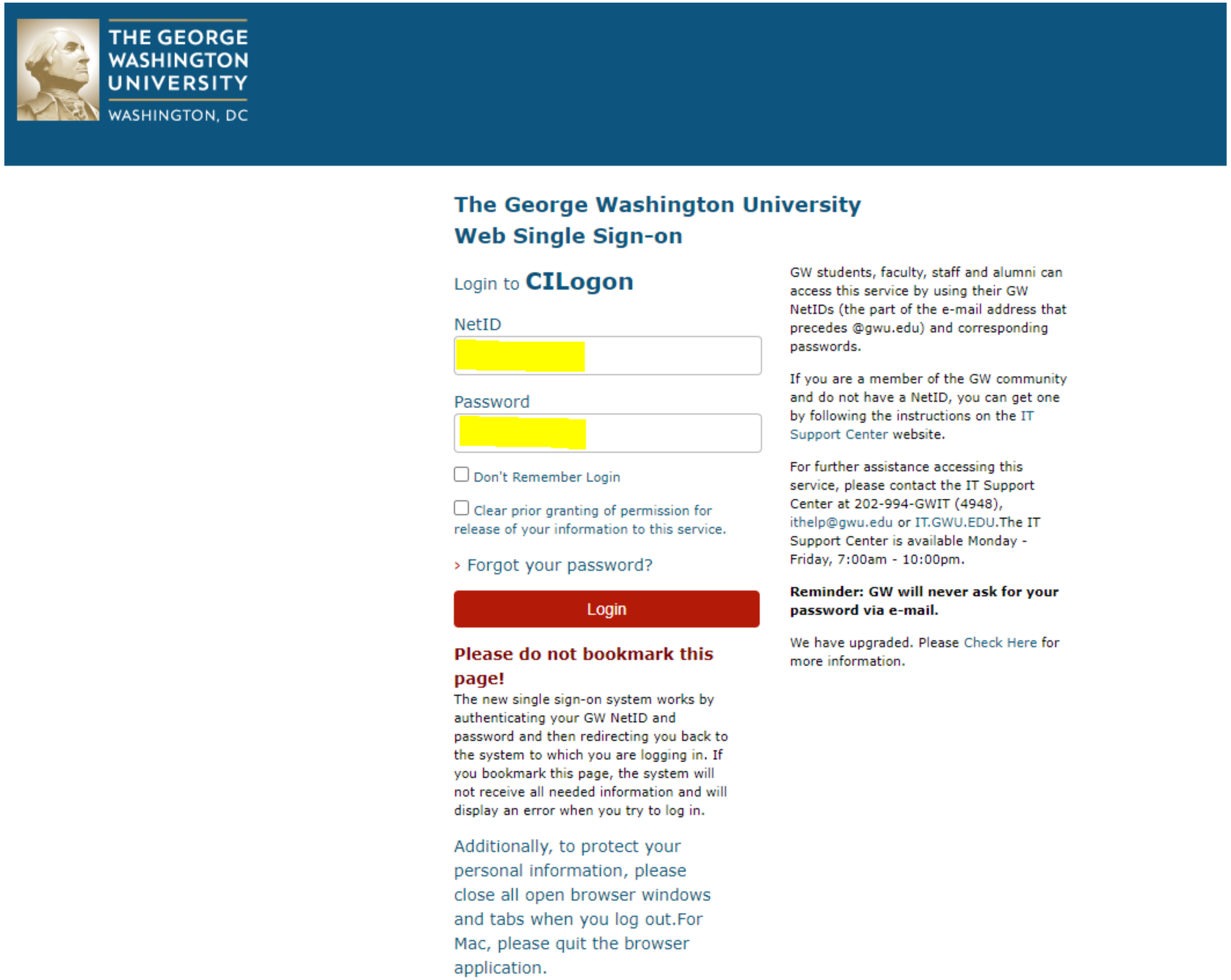
e.g., university, national lab, facility, project

The George Washington University

Didn't find your organization? Then use Globus ID to sign in . (What's this?)

Globus uses CILogon to enable you to Log In from this organization. By clicking Continue, you agree to the CILogon privacy policy and you agree to share your username, email address, and affiliation with CILogon and Globus. You also agree for CILogon to issue a certificate that allows Globus to act on your behalf.

Log in using GW NetID



The George Washington University Web Single Sign-on

Login to **CILogon**

NetID

[redacted]

Password

[redacted]

☐ Don't Remember Login

☐ Clear prior granting of permission for release of your information to this service.

› Forgot your password?

Login

Please do not bookmark this page!

The new single sign-on system works by authenticating your GW NetID and password and then redirecting you back to the system to which you are logging in. If you bookmark this page, the system will not receive all needed information and will display an error when you try to log in.

Additionally, to protect your personal information, please close all open browser windows and tabs when you log out.For Mac, please quit the browser application.

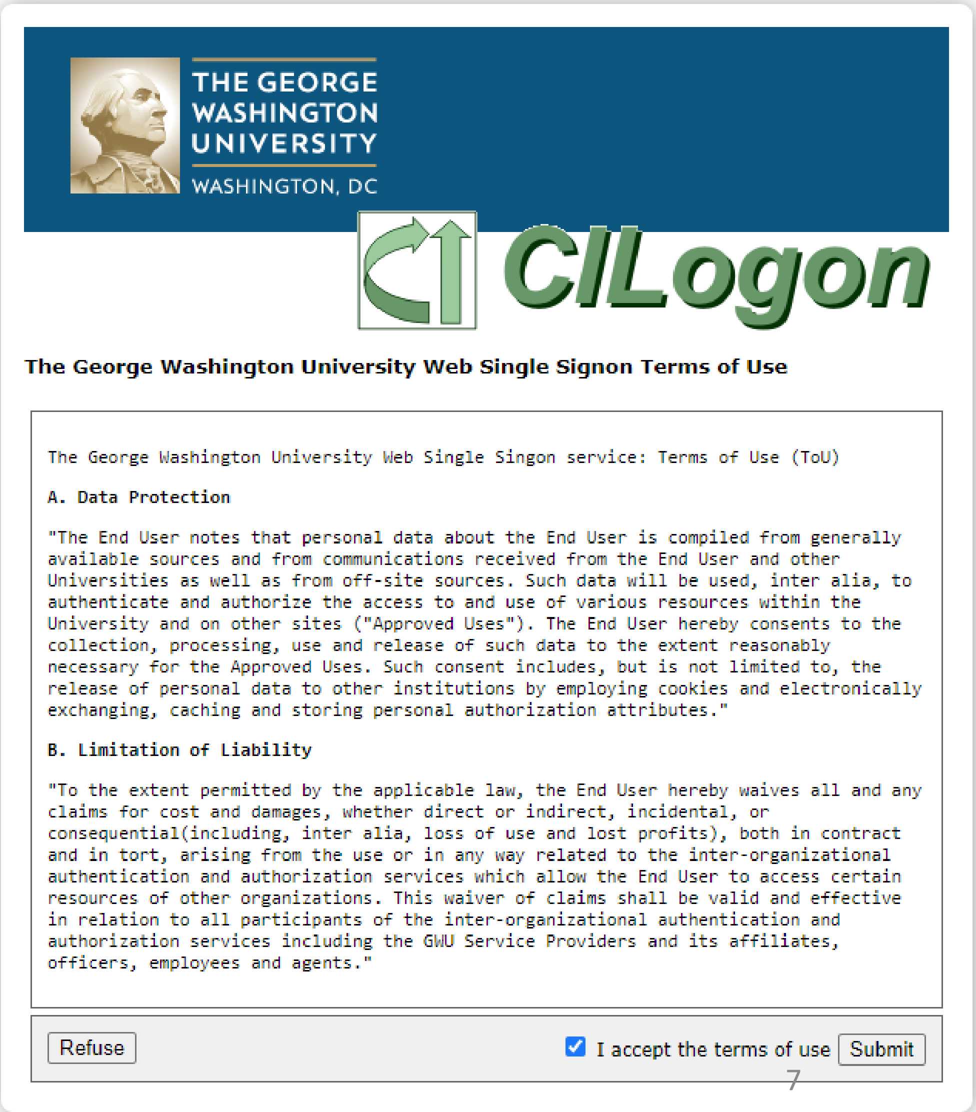
GW students, faculty, staff and alumni can access this service by using their GW NetIDs (the part of the e-mail address that precedes @gwu.edu) and corresponding passwords.

If you are a member of the GW community and do not have a NetID, you can get one by following the instructions on the IT Support Center website.

For further assistance accessing this service, please contact the IT Support Center at 202-994-GWIT (4948), ithelp@gwu.edu or IT.GWU.EDU.The IT Support Center is available Monday - Friday, 7:00am - 10:00pm.

Reminder: GW will never ask for your password via e-mail.

We have upgraded. Please Check Here for more information.



The George Washington University Web Single Signon Terms of Use

The George Washington University Web Single Singon service: Terms of Use (ToU)

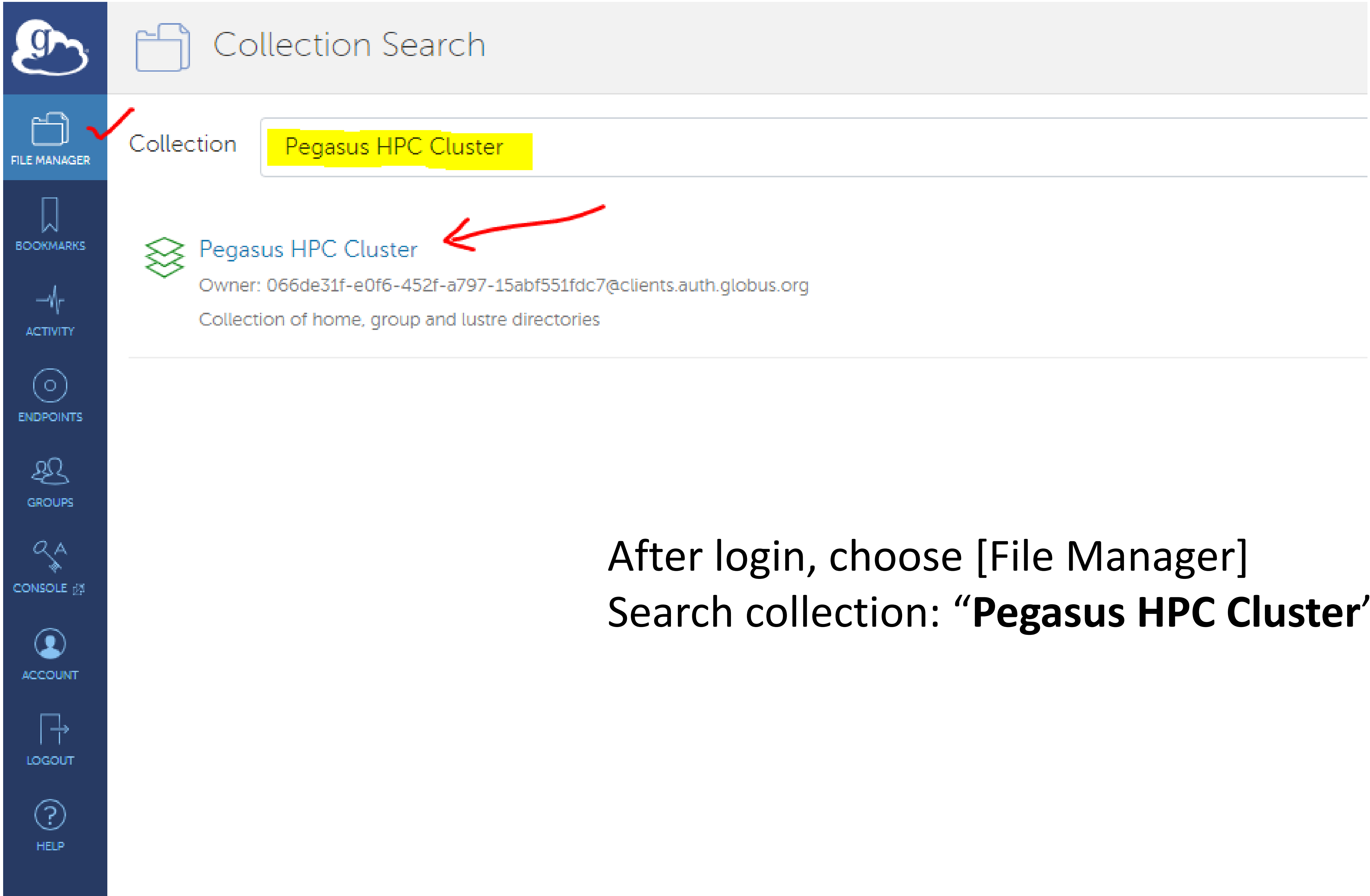
A. Data Protection

"The End User notes that personal data about the End User is compiled from generally available sources and from communications received from the End User and other Universities as well as from off-site sources. Such data will be used, inter alia, to authenticate and authorize the access to and use of various resources within the University and on other sites ("Approved Uses"). The End User hereby consents to the collection, processing, use and release of such data to the extent reasonably necessary for the Approved Uses. Such consent includes, but is not limited to, the release of personal data to other institutions by employing cookies and electronically exchanging, caching and storing personal authorization attributes."

B. Limitation of Liability

"To the extent permitted by the applicable law, the End User hereby waives all and any claims for cost and damages, whether direct or indirect, incidental, or consequential(including, inter alia, loss of use and lost profits), both in contract and in tort, arising from the use or in any way related to the inter-organizational authentication and authorization services which allow the End User to access certain resources of other organizations. This waiver of claims shall be valid and effective in relation to all participants of the inter-organizational authentication and authorization services including the GWU Service Providers and its affiliates, officers, employees and agents."

Refuse ☑ I accept the terms of use Submit



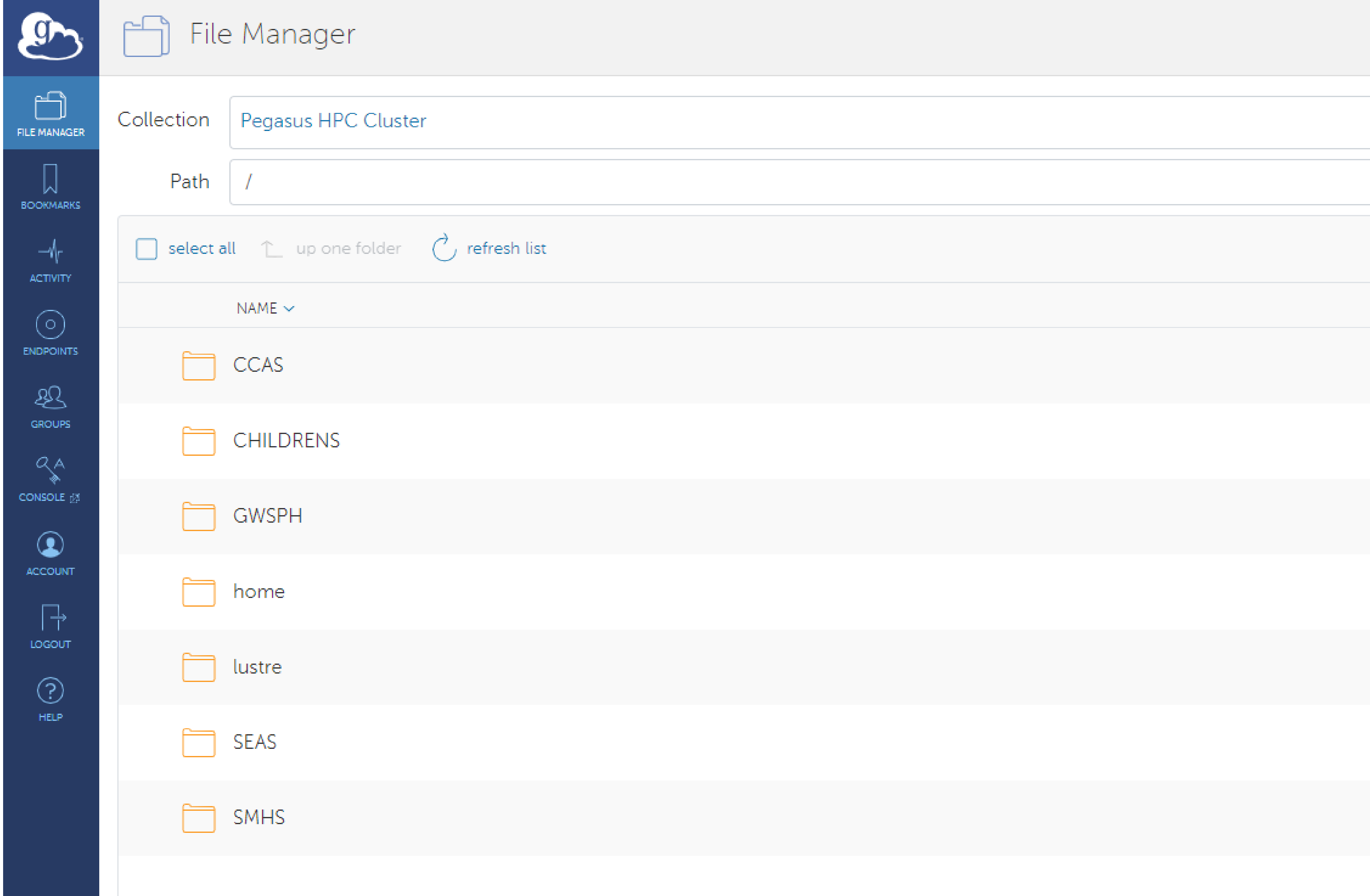
Collection: Pegasus HPC Cluster

Pegasus HPC Cluster

Owner: 066de31f-e0f6-452f-a797-15abf551fdc7@clients.auth.globus.org

Collection of home, group and lustre directories

After login, choose [File Manager]
Search collection: “**Pegasus HPC Cluster**”



File Manager

Collection: Pegasus HPC Cluster

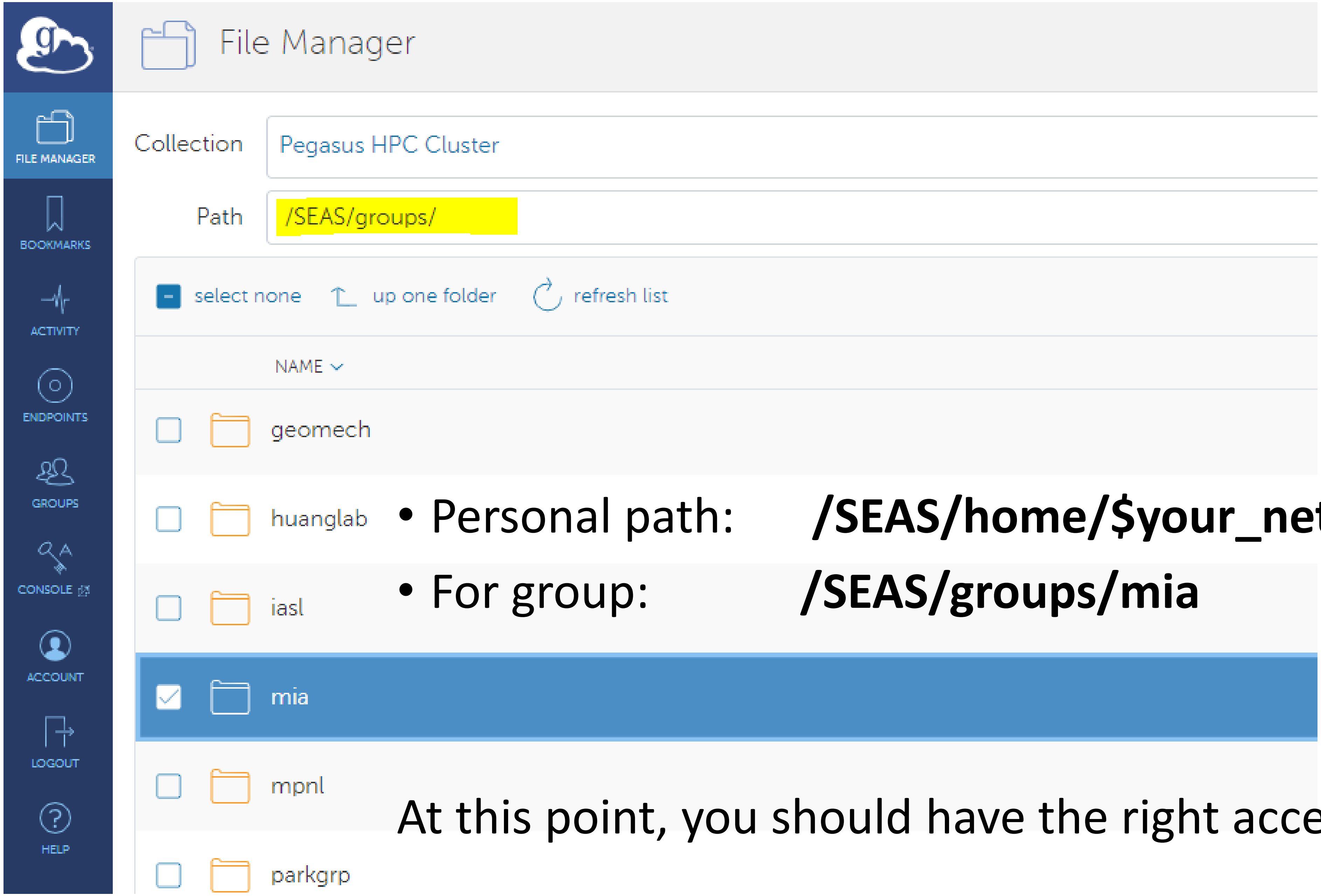
Path: /

☐ select all | up one folder | refresh list

NAME

- CCAS
- CHILDRENS
- GWSPH
- home
- lustre
- SEAS
- SMHS

Folders



File Manager

Collection: Pegasus HPC Cluster

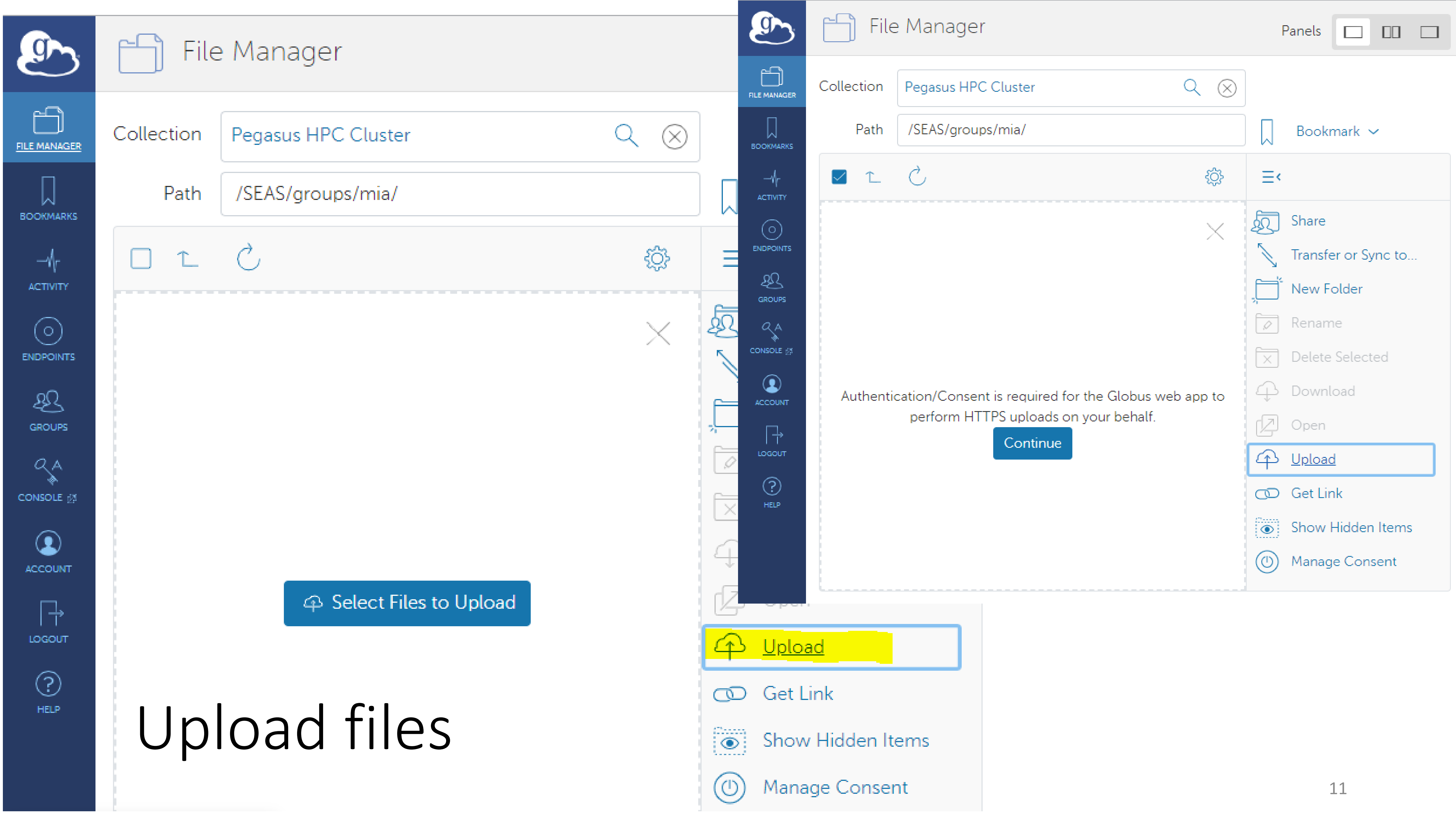
Path: /SEAS/groups/

- ☐ geomech
- ☐ huanglab
- ☐ iasl
- ☑ mia
- ☐ mpnl
- ☐ parkgrp

- Personal path: **/SEAS/home/$your_netID$**
- For group: **/SEAS/groups/mia**

At this point, you should have the right access (HPC account)

Upload files

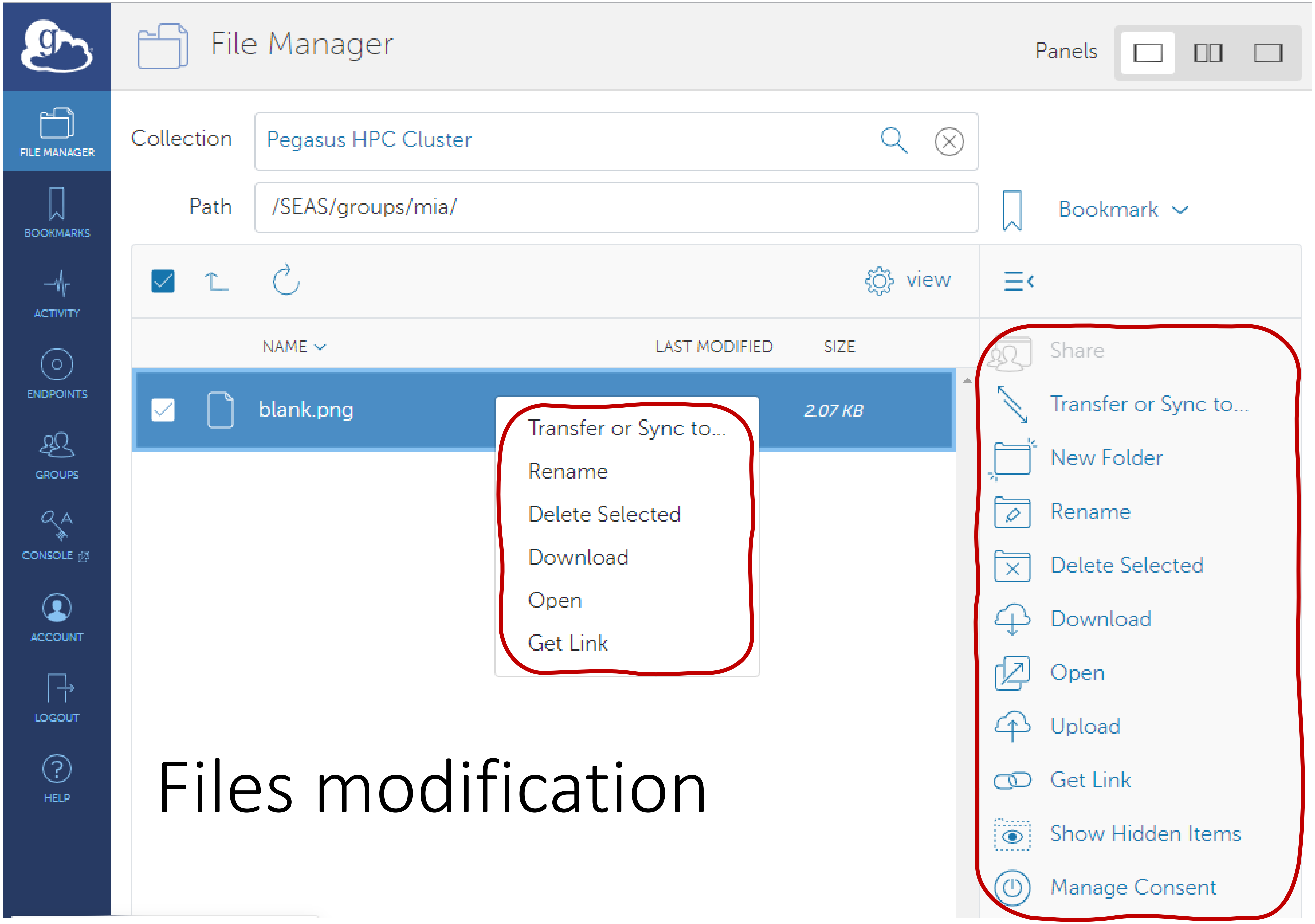


Collection: Pegasus HPC Cluster

Path: /SEAS/groups/mia/

Authentication/Consent is required for the Globus web app to perform HTTPS uploads on your behalf.

Files modification

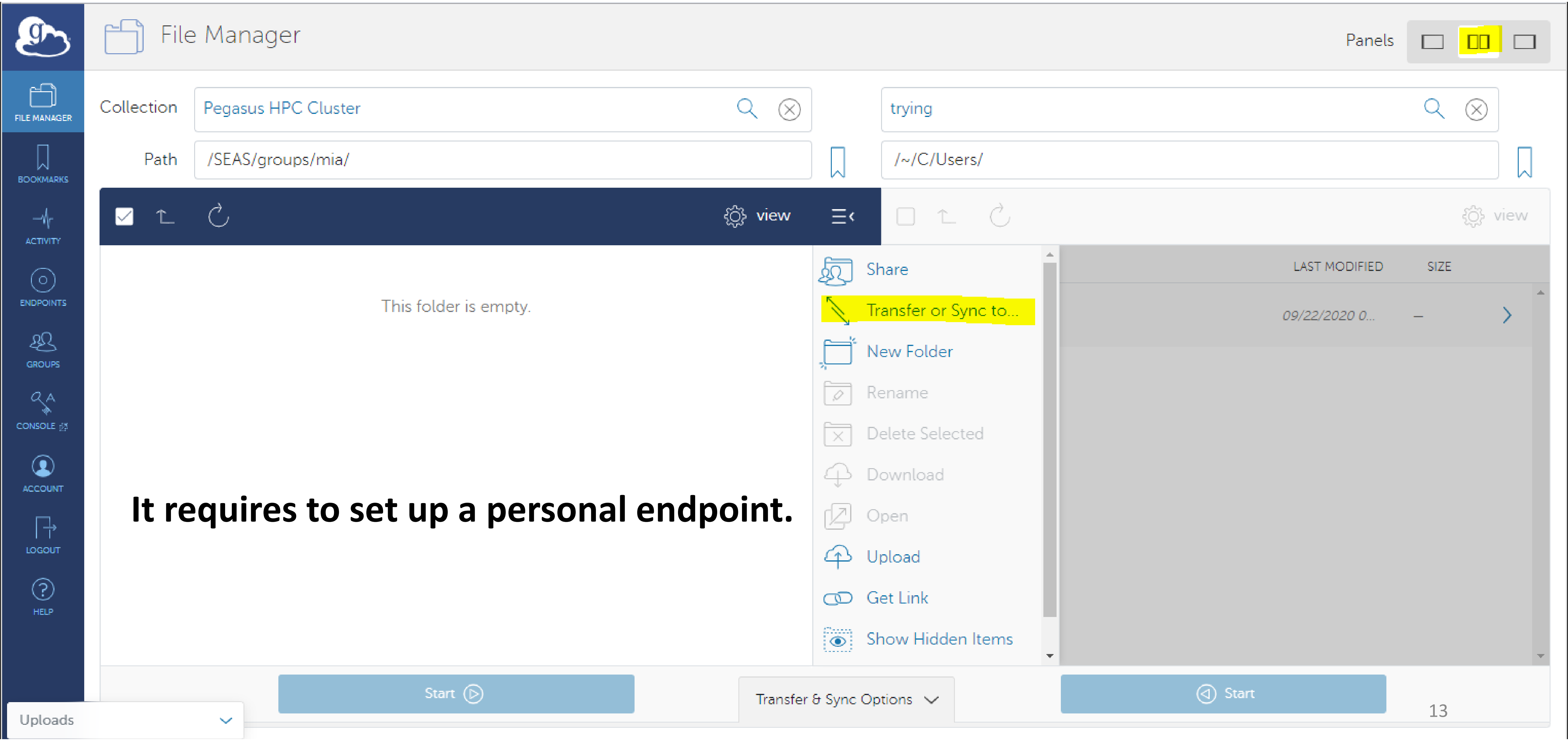


Collection: Pegasus HPC Cluster

Path: /SEAS/groups/mia/

NAME	LAST MODIFIED	SIZE
☑ blank.png		2.07 KB

Or… using the “Sync model”



Collection: Pegasus HPC Cluster

Path: /SEAS/groups/mia/

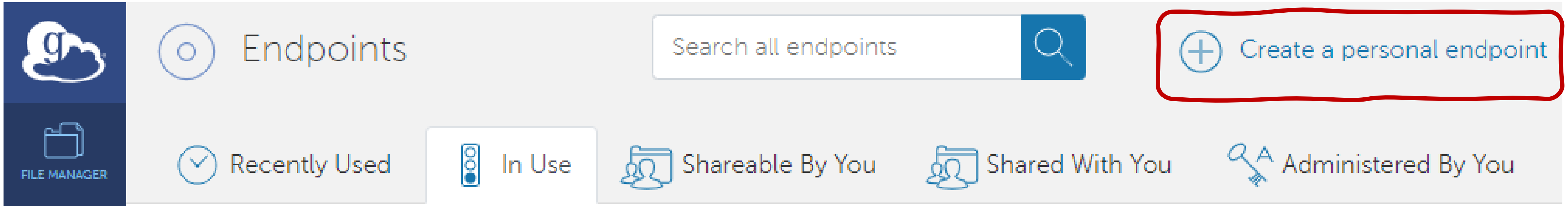
Collection: trying

Path: /~/C/Users/

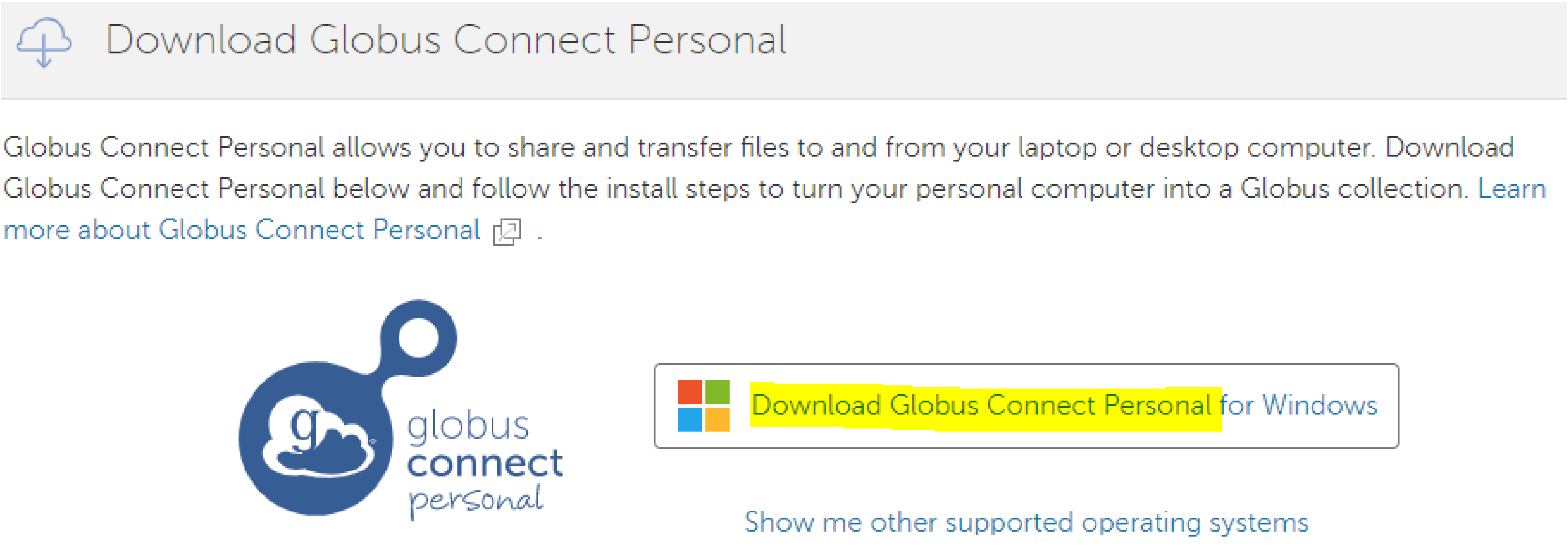
This folder is empty.

09/22/2020 0... –

It requires to set up a personal endpoint.



Create a personal endpoint



Globus Connect Personal allows you to share and transfer files to and from your laptop or desktop computer. Download Globus Connect Personal below and follow the install steps to turn your personal computer into a Globus collection. Learn more about Globus Connect Personal .

Download, install and set the server app to create a personal endpoint…

✓ Introduce to the new HPC: PEGASUS
✓ How to get an account
✓ How to upload files
Next How to log in the HPC system
To run jobs by SLURM

Review 1

- Request for an account
  - Research group name “**mia**”
- Endpoint name “**Pegasus HPC Cluster**”
- Path
  - Personal path: **/SEAS/home/$your_netID$**
  - For group: **/SEAS/groups/mia**

VPN Access

It needs GW network environment.

- Off-campus access (at home): requires GW's VPN.

  https://seascf.seas.gwu.edu/vpn-access

  (1) Download the **Cisco AnyConnect VPN Client**

  (2) Connect to "**go.vpn.gwu.edu**"

  (3) Use NetID and password to connect

- On-campus access: *skip this step*.

VPN:

Ready to connect.

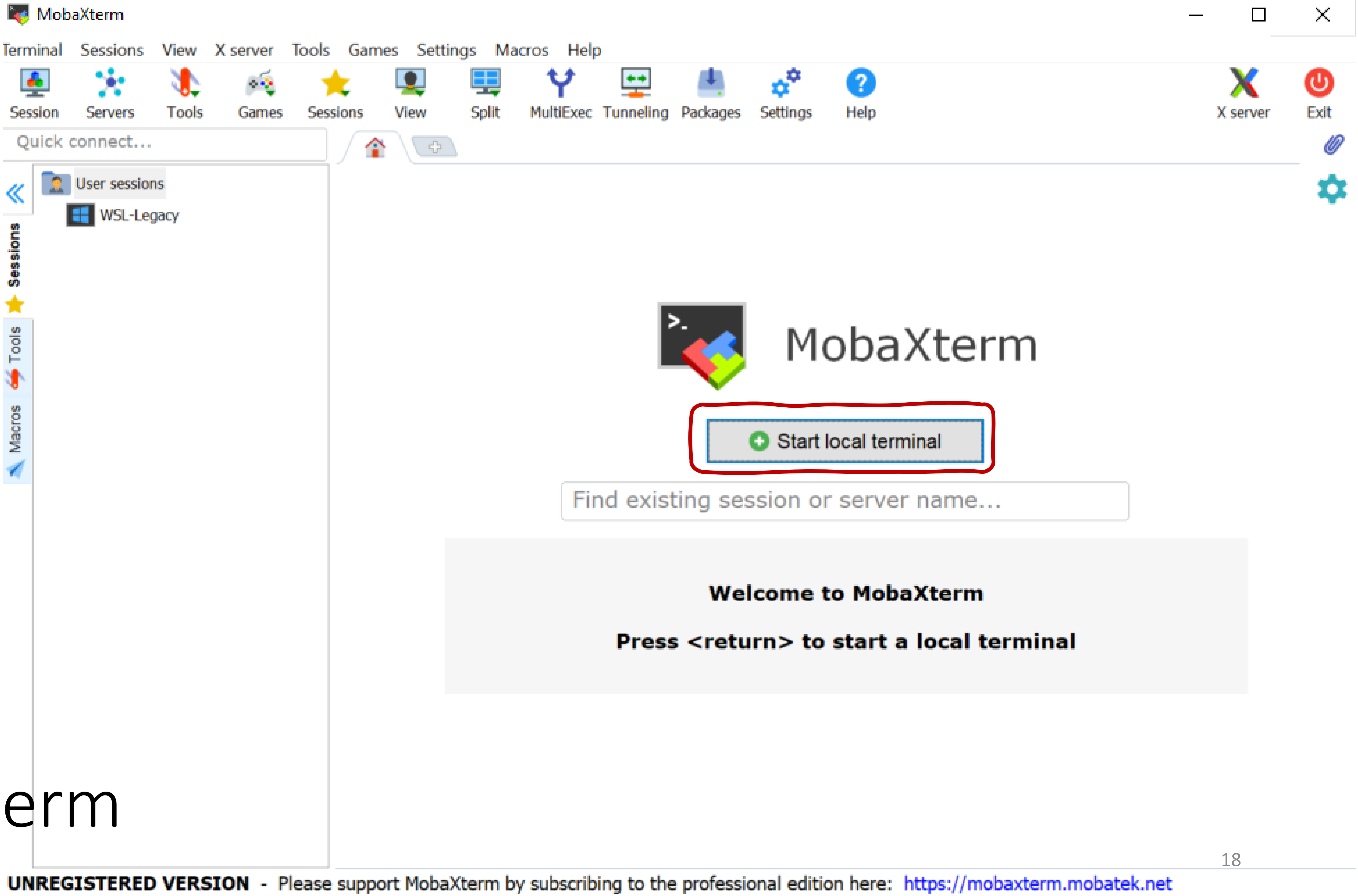
go.vpn.gwu.edu

SSH client

GW HPC system requires the **SSH** connection.

“SSH (Secure Shell) is a cryptographic network protocol for operating network services securely over an unsecured network.”

- MobaXterm https://mobaxterm.mobatek.net/
- PuTTY https://www.putty.org/
- …

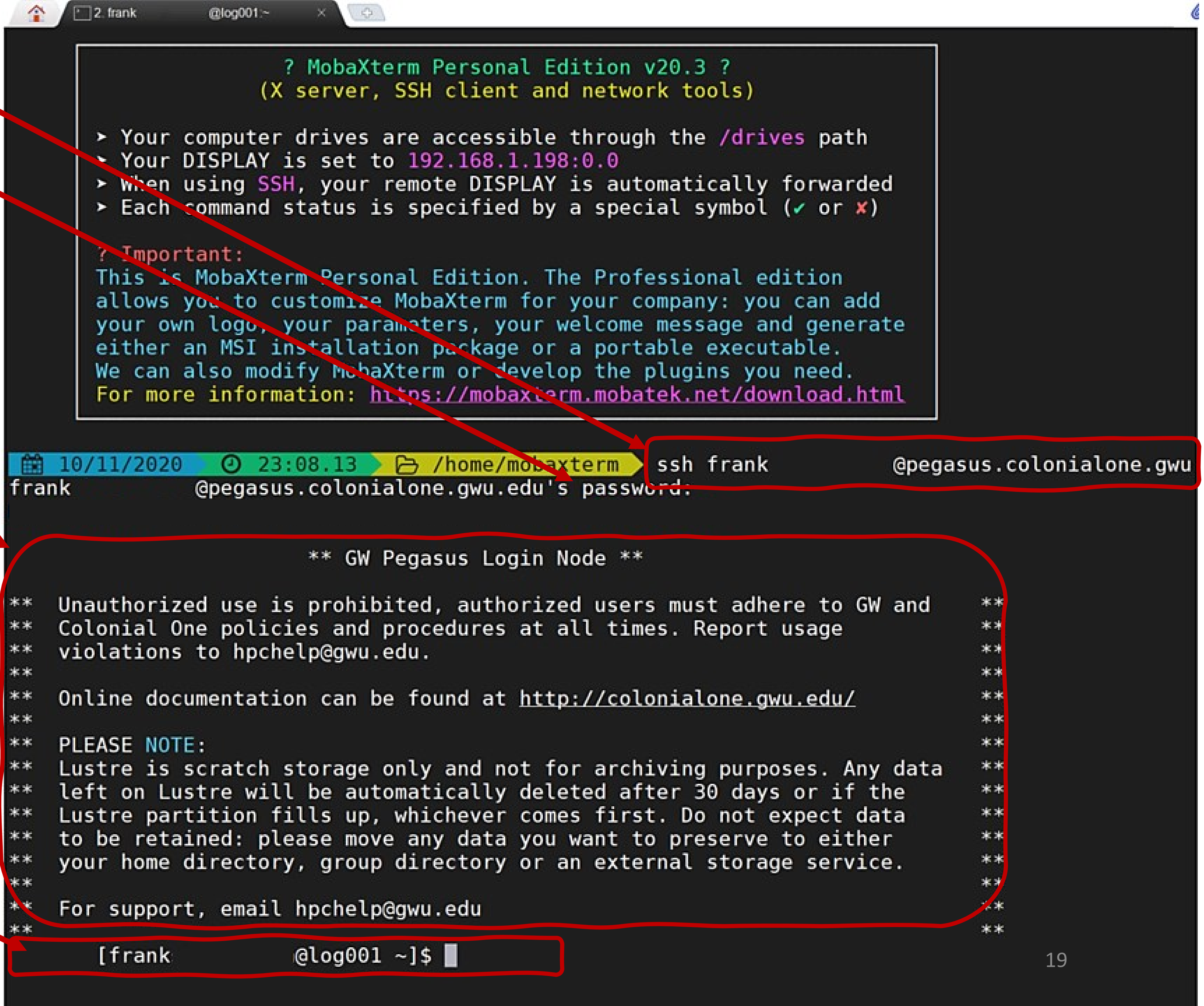


Welcome to MobaXterm

Press <return> to start a local terminal

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net

MobaXterm



ssh NetID@pegasus.colonialone.gwu

Password of NetID

Welcome info

Running jobs on the login nodes is prohibited

Command line

Login is successful when see this.

```
                 ? MobaXterm Personal Edition v20.3 ?
               (X server, SSH client and network tools)

 ➤ Your computer drives are accessible through the /drives path
 ➤ Your DISPLAY is set to 192.168.1.198:0.0
 ➤ When using SSH, your remote DISPLAY is automatically forwarded
 ➤ Each command status is specified by a special symbol (✓ or ✗)

 ? Important:
 This is MobaXterm Personal Edition. The Professional edition
 allows you to customize MobaXterm for your company: you can add
 your own logo, your parameters, your welcome message and generate
 either an MSI installation package or a portable executable.
 We can also modify MobaXterm or develop the plugins you need.
 For more information: https://mobaxterm.mobatek.net/download.html

 10/11/2020   23:08.13   /home/mobaxterm   ssh frank          @pegasus.colonialone.gwu
frank          @pegasus.colonialone.gwu.edu's password:

                        ** GW Pegasus Login Node **

**   Unauthorized use is prohibited, authorized users must adhere to GW and   **
**   Colonial One policies and procedures at all times. Report usage         **
**   violations to hpchelp@gwu.edu.                                          **
**                                                                           **
**   Online documentation can be found at http://colonialone.gwu.edu/        **
**                                                                           **
**   PLEASE NOTE:                                                            **
**   Lustre is scratch storage only and not for archiving purposes. Any data **
**   left on Lustre will be automatically deleted after 30 days or if the    **
**   Lustre partition fills up, whichever comes first. Do not expect data    **
**   to be retained: please move any data you want to preserve to either     **
**   your home directory, group directory or an external storage service.    **
**                                                                           **
**   For support, email hpchelp@gwu.edu                                      **
**                                                                           **
      [frank          @log001 ~]$ █
```

Linux commends

- Current directory: **pwd**

```
$ pwd
/SEAS/groups/mia
```

- Go to user’s main directory: **cd ~**
- Go to root: **cd /**
- Parent directory: **cd ..**
- Go to a directory: **cd /xxx/xxxx/xx**

Review 2

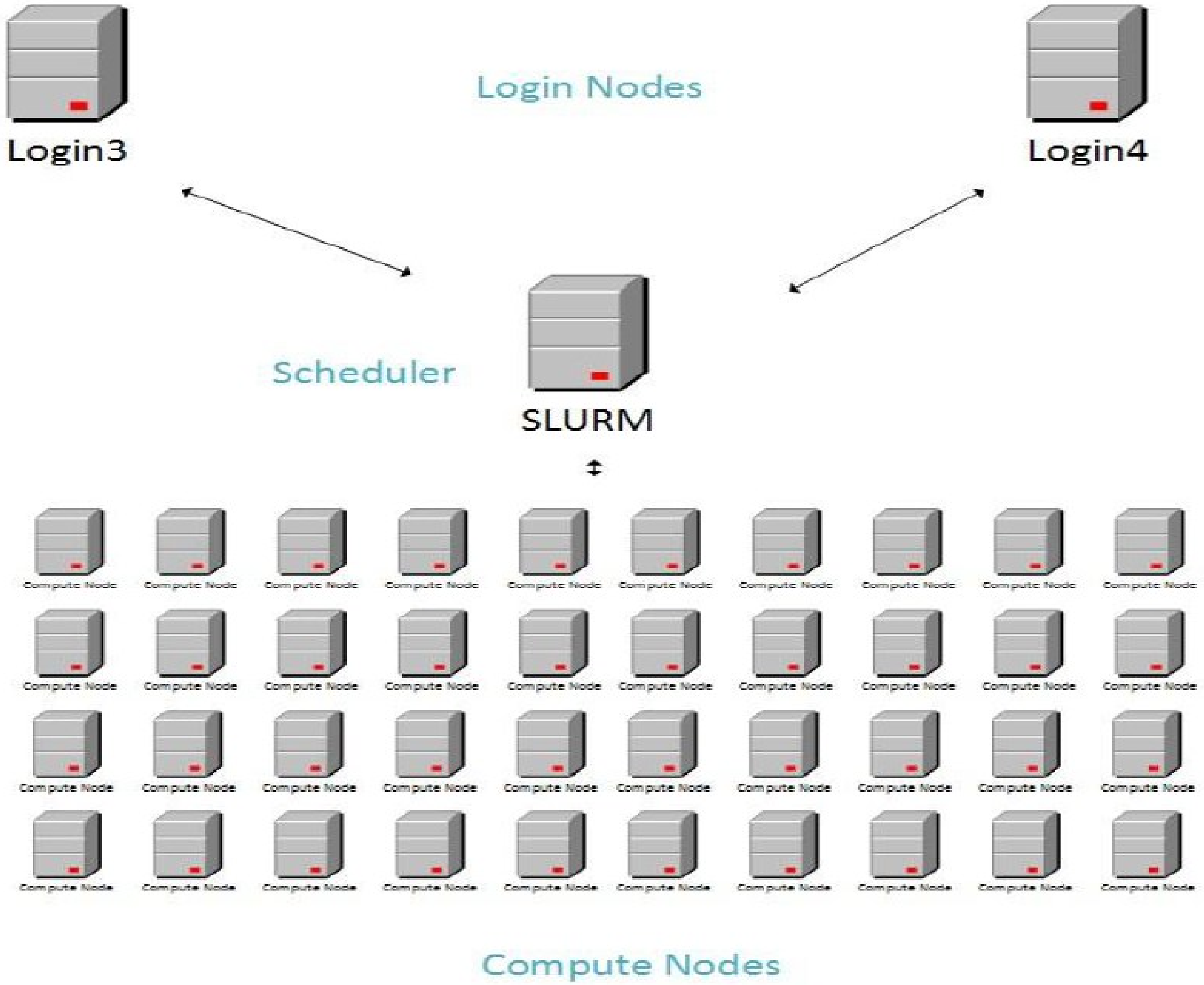
✓ Introduce to the new HPC: PEGASUS
✓ How to get an account
✓ How to upload files
✓ How to log in the HPC system
Next To run jobs by SLURM

- VPN connection to “**go.vpn.gwu.edu**” (off-campus)
- SSH client (like “MobaXterm”)
  - **ssh** *NetID*@**pegasus.colonialone.gwu**

Do not run jobs on the login nodes.

Do use the SLURM system.

SLURM is a cluster management and job scheduling system for Linux clusters.

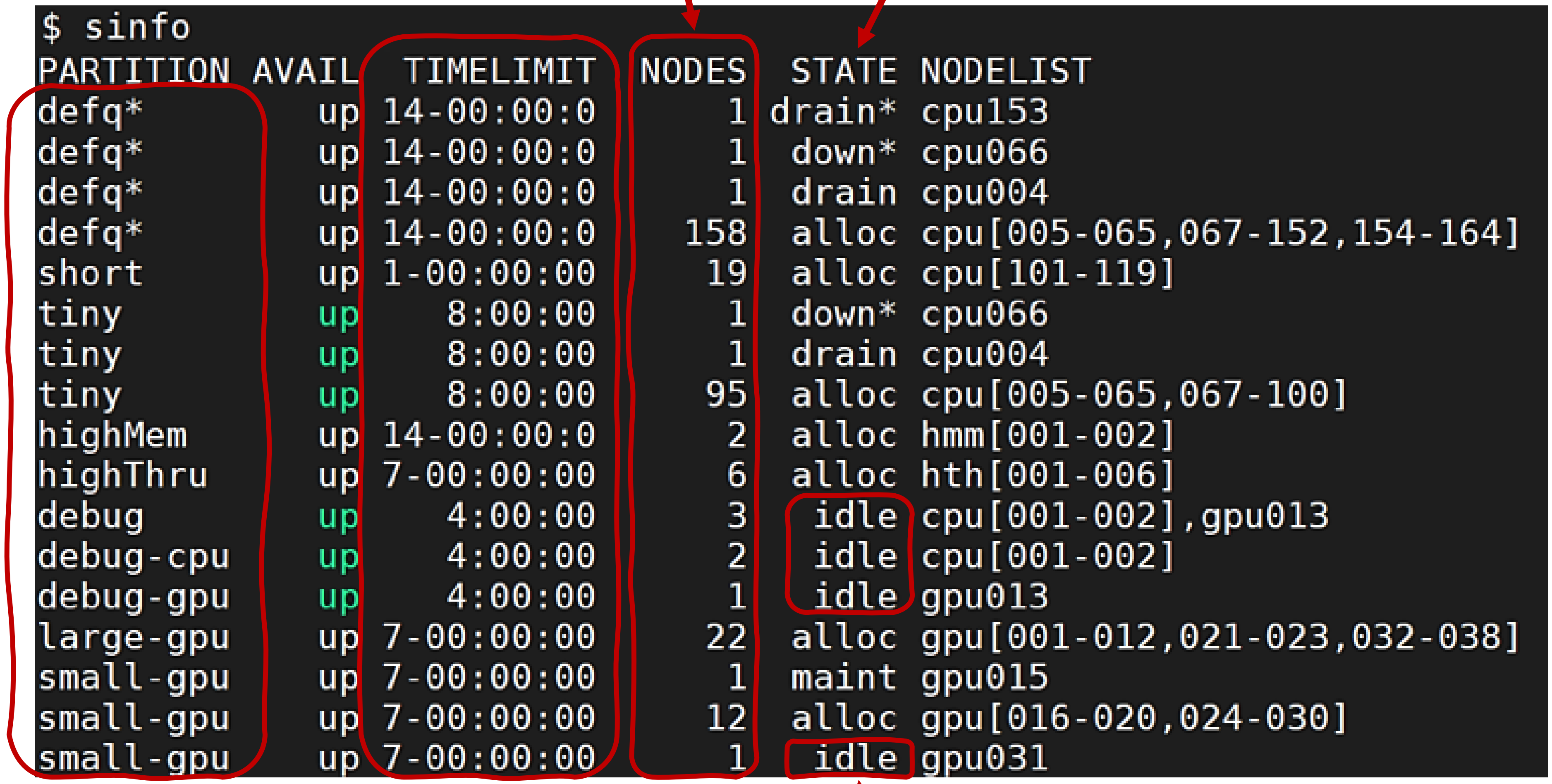


sinfo command

Number of nodes

Node state

Types of nodes



```
$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
defq*        up 14-00:00:0      1 drain* cpu153
defq*        up 14-00:00:0      1  down* cpu066
defq*        up 14-00:00:0      1  drain cpu004
defq*        up 14-00:00:0    158  alloc cpu[005-065,067-152,154-164]
short        up 1-00:00:00     19  alloc cpu[101-119]
tiny         up    8:00:00      1  down* cpu066
tiny         up    8:00:00      1  drain cpu004
tiny         up    8:00:00     95  alloc cpu[005-065,067-100]
highMem      up 14-00:00:0      2  alloc hmm[001-002]
highThru     up 7-00:00:00      6  alloc hth[001-006]
debug        up    4:00:00      3   idle cpu[001-002],gpu013
debug-cpu    up    4:00:00      2   idle cpu[001-002]
debug-gpu    up    4:00:00      1   idle gpu013
large-gpu    up 7-00:00:00     22  alloc gpu[001-012,021-023,032-038]
small-gpu    up 7-00:00:00      1  maint gpu015
small-gpu    up 7-00:00:00     12  alloc gpu[016-020,024-030]
small-gpu    up 7-00:00:00      1   idle gpu031
```

Time limit for running
day – h : m : s

“idle” is ready to use

Node type (Non-GPU)

- **defq*** – default compute nodes, CPU only
- **highThru** – Nodes in this category have **high CPU frequency nodes with a low core count**. These nodes are used for single threaded jobs that cannot take advantage of multiple cores.
- **highMem** – Nodes in this category have **large memory (3TB)** and are for jobs that require more memory intensive jobs.
- **short** – Designed for **quicker** turnaround of shorter running jobs (1 day).
- **tiny** – Designed for **even quicker** turnaround of shorter running jobs (8 hrs).
- **debug-cpu** – See more details later

Node type (GPU)

- **small-gpu** – Each has **two** NVIDIA Tesla V100 SXM2 16GB GPUs.
- **large-gpu** – Each has **four** NVIDIA Tesla V100 SXM2 16GB GPUs with NVLink enabled.
- **debug-gpu** – See more details later

Debug partition

The debug partition is intended for running **interactive jobs, or for short-duration test cases** (e.g., making sure your job scripts work correctly), and is not intended for general use.

The hardware is the same as the cpu/gpu partition nodes, but time limit is **4 hours**.

- **debug-cpu**
- **debug-gpu**

You must specify a time limit for your job.

Workflow

1. Upload data and code files ✓
2. Create a SLURM script to assign the job
3. Run the script
4. Outputs will be saved
5. Receive states and notifications by Email / or check by commands

A Python example

Find the primes in [2,100].

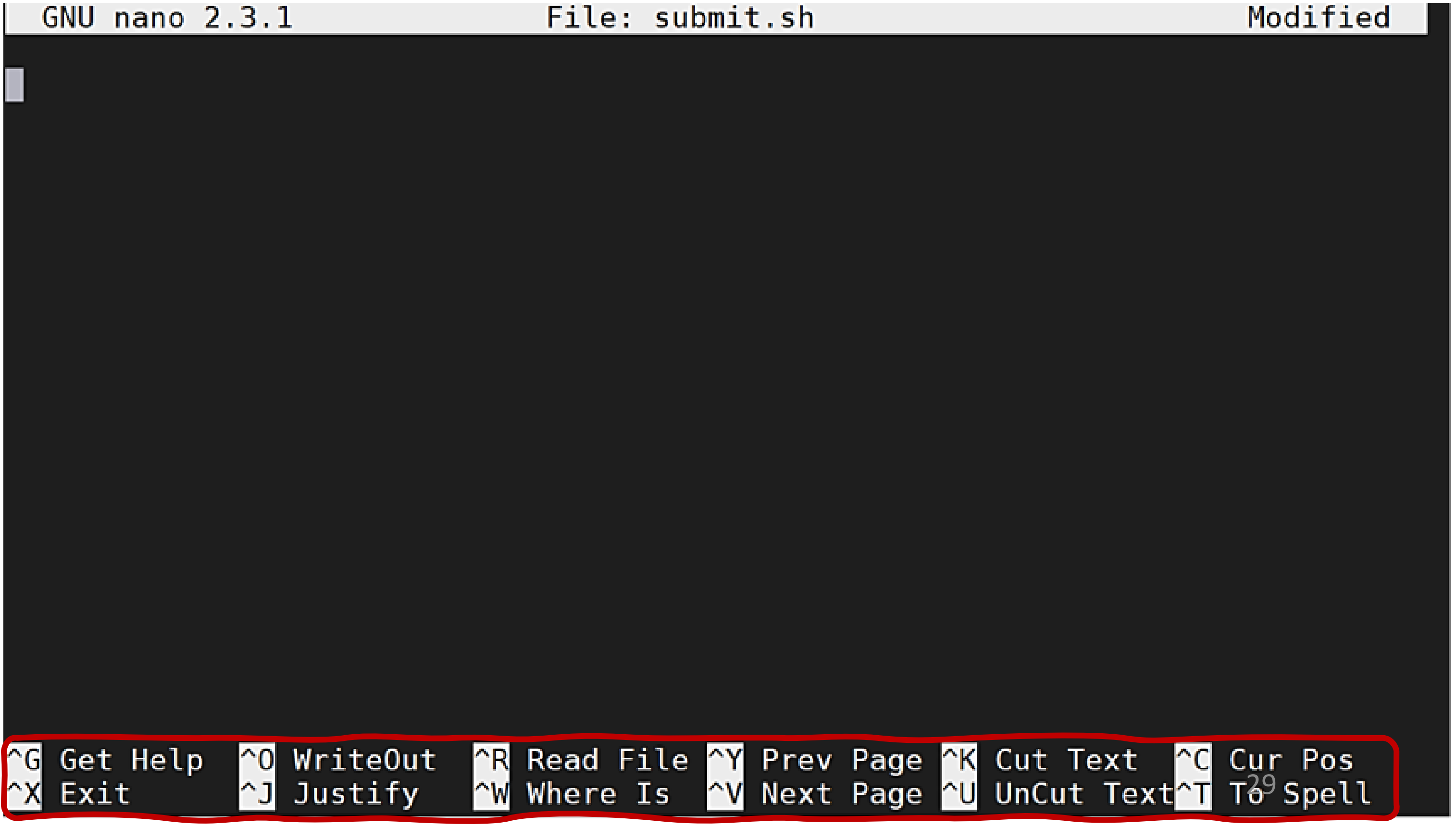
Code file name: **prime.py**; no data file.

```python
if __name__ == '__main__':
    for num in range(2, 101):
        prime = True
        for i in range(2, num):
            if (num % i == 0):
                prime = False
        if prime:
            print(num)
```

SLURM script

Create a SLURM script, named **submit.sh**
Recommend to use the **nano** editor.

```
$ nano submit.sh
```



```
  GNU nano 2.3.1              File: submit.sh                        Modified

^G Get Help  ^O WriteOut  ^R Read File ^Y Prev Page ^K Cut Text  ^C Cur Pos
^X Exit      ^J Justify   ^W Where Is  ^V Next Page ^U UnCut Text^T To Spell
```

operations

```
error: Batch script contains DOS line breaks (\r\n)
error: instead of expected UNIX line breaks (\n)
```

Use other editors in Win may occur errors.

SLURM script for Python

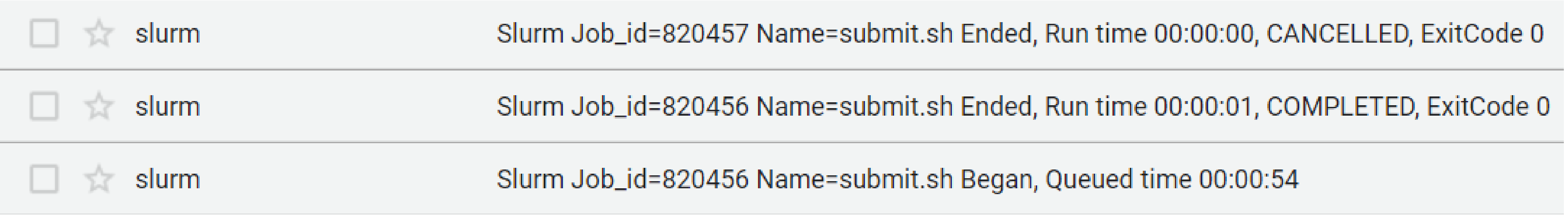
submit.sh

`#!/bin/sh`	
`#SBATCH --time 1:00`	← To limit running time; format: day – h : m : s
`#SBATCH -o testing%j.out`	File for outputs; “%j” is task number
`#SBATCH -e testing%j.err`	File for error/warning report
`#SBATCH -p defq`	Point the node
`#SBATCH --mail-user=user@email.com`	Email address for receiving states
`#SBATCH --mail-type=ALL`	Email type
`module load python/2.7.16`	Load modules for running code
`python /SEAS/home/$user_name$/prime.py`	Run code

Submit job -- sbatch

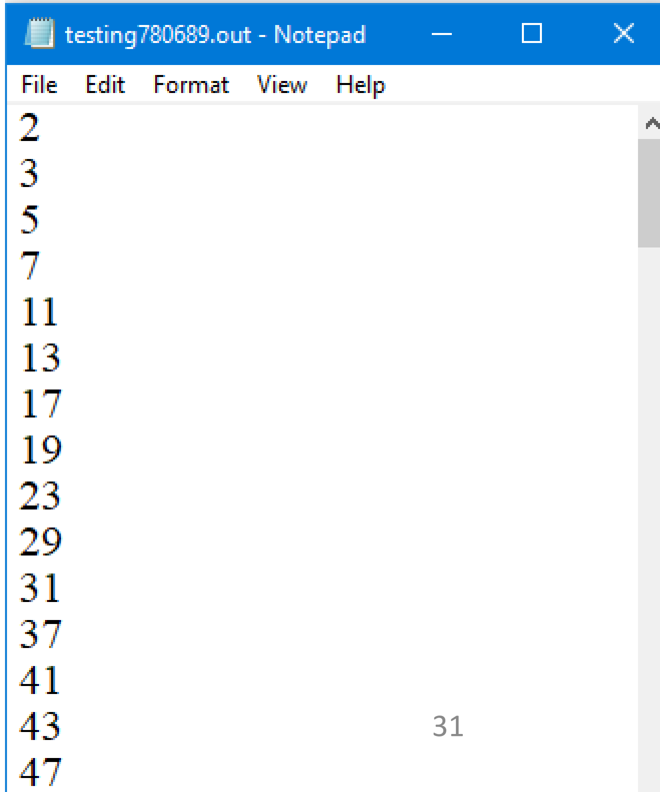
```
$ sbatch submit.sh
Submitted batch job xxxxxxx
```

If your job starts to run, the job is done or other **status changes**, you will get an email:



☐	☆	slurm	Slurm Job_id=820457 Name=submit.sh Ended, Run time 00:00:00, CANCELLED, ExitCode 0
☐	☆	slurm	Slurm Job_id=820456 Name=submit.sh Ended, Run time 00:00:01, COMPLETED, ExitCode 0
☐	☆	slurm	Slurm Job_id=820456 Name=submit.sh Began, Queued time 00:00:54

Running (printed) results are in the **testingxxxxxxx.out** file.
Error/warning reports are in the **testingxxxxxxx.err** file.
Open by *nano* or *Notepad* in Win.



```
2
3
5
7
11
13
17
19
23
29
31
37
41
43
47
```

Job status

If the job is in queue, to check job’s status:

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

```
 JOBID PARTITION      NAME     USER ST       TIME  NODES NODELIST(REASON)
820457      defq submit.s    frank PD       0:00      1 (Resources)
```

Statuses:

CA = CANCELLED

CD = COMPLETED

CG = COMPLETING

F = FAILED

NF = NODE_FAIL

PD = PENDING

R = RUNNING

S = SUSPENDED

TO = TIMEOUT

Estimate when a job will start:

```
$ squeue -u <username> --start
```

Cancel job:

```
$ scancel <jobid>
```

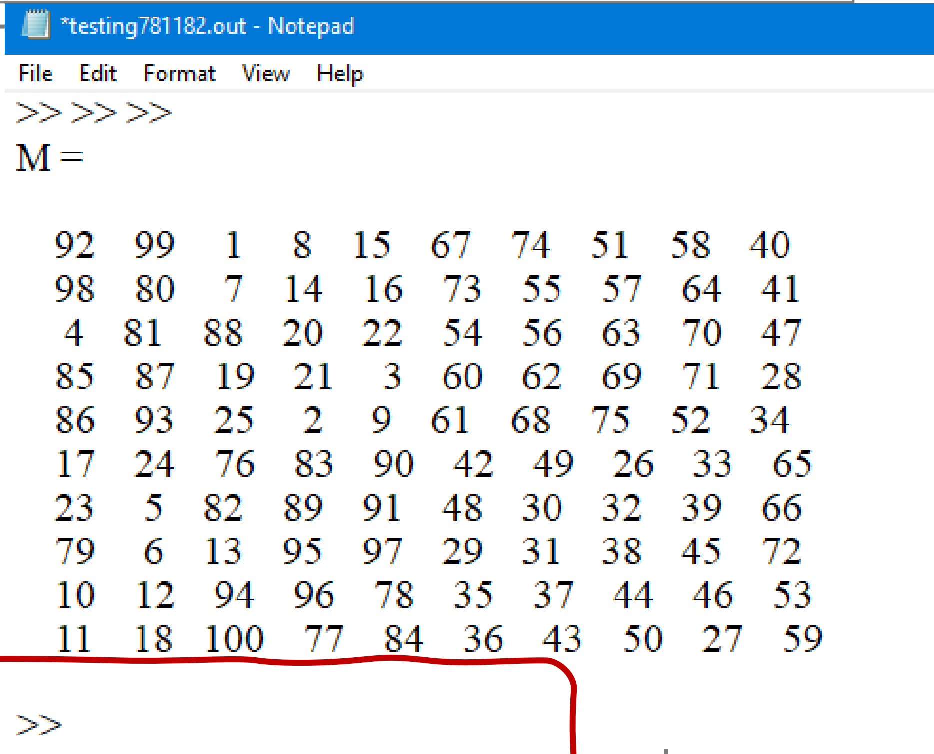
A Matlab example

Code file name: **matlab_simple.m**

```
% Creates a 10x10 Magic square
  M = magic(10);
  disp(M)
  exit
```

Submit_mat.sh

```
#!/bin/sh
#SBATCH --time 1:00
#SBATCH -o testing%j.out
#SBATCH -e testing%j.err
#SBATCH -p defq
#SBATCH --mail-user=user@email.com
#SBATCH --mail-type=ALL

module load matlab/2018b
matlab -nodisplay < /SEAS/home/$user_name$/matlab_simple.m
```



```
>> >> >>
M =

    92    99     1     8    15    67    74    51    58    40
    98    80     7    14    16    73    55    57    64    41
     4    81    88    20    22    54    56    63    70    47
    85    87    19    21     3    60    62    69    71    28
    86    93    25     2     9    61    68    75    52    34
    17    24    76    83    90    42    49    26    33    65
    23     5    82    89    91    48    30    32    39    66
    79     6    13    95    97    29    31    38    45    72
    10    12    94    96    78    35    37    44    46    53
    11    18   100    77    84    36    43    50    27    59

>>
```

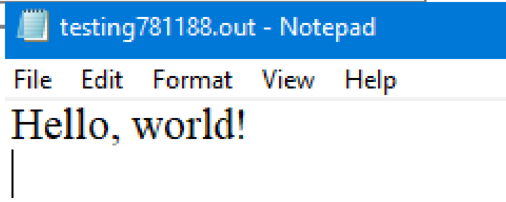
A C example

Code file name: **c_sample.c**

```c
#include <stdio.h>
int main (void)
{
  printf ("Hello, world!\n");
  return 0;
}
```

submit_c.sh

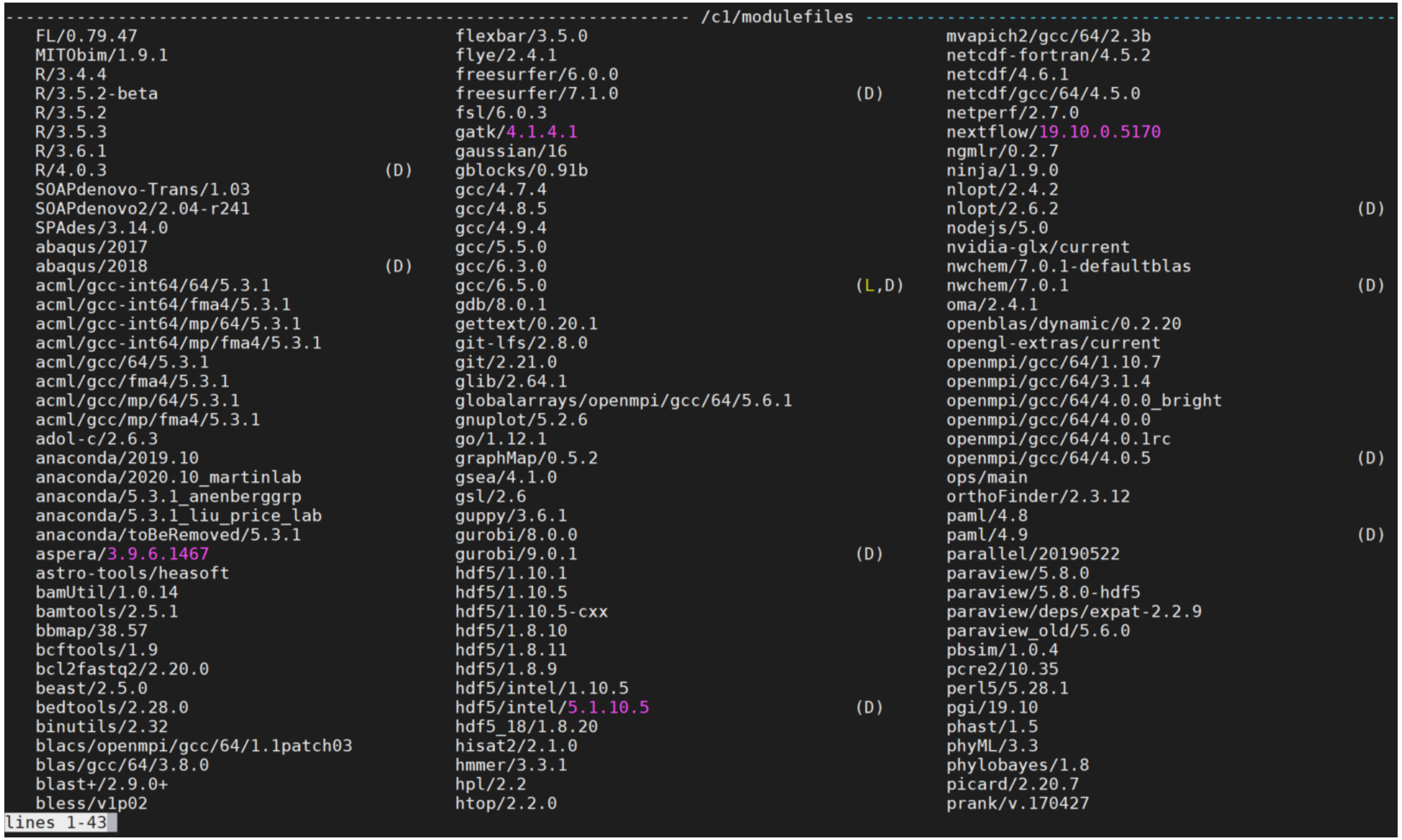
```
#!/bin/sh
#SBATCH --time 1:00
#SBATCH -o testing%j.out
#SBATCH -e testing%j.err
#SBATCH -p defq
#SBATCH --mail-user=user@email.com
#SBATCH --mail-type=ALL

module load gcc/6.5.0
gcc -Wall /SEAS/home/$user_name$/c_sample.c -o c_sample
```



```
Hello, world!
```

Modules

In your user directory, you can download and install your own modules.



```
------------------------------------------------------------------- /c1/modulefiles -----------------------------------------------------
   FL/0.79.47                               flexbar/3.5.0                                   mvapich2/gcc/64/2.3b
   MITObim/1.9.1                            flye/2.4.1                                      netcdf-fortran/4.5.2
   R/3.4.4                                  freesurfer/6.0.0                                netcdf/4.6.1
   R/3.5.2-beta                             freesurfer/7.1.0                       (D)      netcdf/gcc/64/4.5.0
   R/3.5.2                                  fsl/6.0.3                                       netperf/2.7.0
   R/3.5.3                                  gatk/4.1.4.1                                    nextflow/19.10.0.5170
   R/3.6.1                                  gaussian/16                                     ngmlr/0.2.7
   R/4.0.3                           (D)    gblocks/0.91b                                   ninja/1.9.0
   SOAPdenovo-Trans/1.03                    gcc/4.7.4                                       nlopt/2.4.2
   SOAPdenovo2/2.04-r241                    gcc/4.8.5                                       nlopt/2.6.2                             (D)
   SPAdes/3.14.0                            gcc/4.9.4                                       nodejs/5.0
   abaqus/2017                              gcc/5.5.0                                       nvidia-glx/current
   abaqus/2018                       (D)    gcc/6.3.0                                       nwchem/7.0.1-defaultblas
   acml/gcc-int64/64/5.3.1                  gcc/6.5.0                              (L,D)    nwchem/7.0.1                            (D)
   acml/gcc-int64/fma4/5.3.1                gdb/8.0.1                                       oma/2.4.1
   acml/gcc-int64/mp/64/5.3.1               gettext/0.20.1                                  openblas/dynamic/0.2.20
   acml/gcc-int64/mp/fma4/5.3.1             git-lfs/2.8.0                                   opengl-extras/current
   acml/gcc/64/5.3.1                        git/2.21.0                                      openmpi/gcc/64/1.10.7
   acml/gcc/fma4/5.3.1                      glib/2.64.1                                     openmpi/gcc/64/3.1.4
   acml/gcc/mp/64/5.3.1                     globalarrays/openmpi/gcc/64/5.6.1               openmpi/gcc/64/4.0.0_bright
   acml/gcc/mp/fma4/5.3.1                   gnuplot/5.2.6                                   openmpi/gcc/64/4.0.0
   adol-c/2.6.3                             go/1.12.1                                       openmpi/gcc/64/4.0.1rc
   anaconda/2019.10                         graphMap/0.5.2                                  openmpi/gcc/64/4.0.5                    (D)
   anaconda/2020.10_martinlab               gsea/4.1.0                                      ops/main
   anaconda/5.3.1_anenberggrp               gsl/2.6                                         orthoFinder/2.3.12
   anaconda/5.3.1_liu_price_lab             guppy/3.6.1                                     paml/4.8
   anaconda/toBeRemoved/5.3.1               gurobi/8.0.0                                    paml/4.9                                (D)
   aspera/3.9.6.1467                        gurobi/9.0.1                           (D)      parallel/20190522
   astro-tools/heasoft                      hdf5/1.10.1                                     paraview/5.8.0
   bamUtil/1.0.14                           hdf5/1.10.5                                     paraview/5.8.0-hdf5
   bamtools/2.5.1                           hdf5/1.10.5-cxx                                 paraview/deps/expat-2.2.9
   bbmap/38.57                              hdf5/1.8.10                                     paraview_old/5.6.0
   bcftools/1.9                             hdf5/1.8.11                                     pbsim/1.0.4
   bcl2fastq2/2.20.0                        hdf5/1.8.9                                      pcre2/10.35
   beast/2.5.0                              hdf5/intel/1.10.5                               perl5/5.28.1
   bedtools/2.28.0                          hdf5/intel/5.1.10.5                    (D)      pgi/19.10
   binutils/2.32                            hdf5_18/1.8.20                                  phast/1.5
   blacs/openmpi/gcc/64/1.1patch03          hisat2/2.1.0                                    phyML/3.3
   blas/gcc/64/3.8.0                        hmmer/3.3.1                                     phylobayes/1.8
   blast+/2.9.0+                            hpl/2.2                                         picard/2.20.7
   bless/v1p02                              htop/2.2.0                                      prank/v.170427
lines 1-43
```

Environments for codes to run.

Module commands:

• module avail	show all available modules (installed)
• module load	load a module
• module unload	
• module list	show currently loaded modules

https://colonialone.gwu.edu/available-modules/

Helpful resources

- **GWU HPC documents**:

  Highly recommend

  https://colonialone.gwu.edu/about/presentations/
- GWU HPC support email: hpchelp@gwu.edu ← For help
- SLURM system user guide:

  https://slurm.schedmd.com/
- The Linux command line for beginner:

  https://ubuntu.com/tutorials/command-line-for-beginners#1-overview

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