

GW COLONIAL ONE



HPC Workshop 1

What we're covering:

- Logging in
- Navigating the shell
- Modules, environment variables and .profile
- Quotas
- Purges
- File transfer and management:
 - scp
 - Globus
 - Lustre vs NFS filesystems
 - Lustre striping & inodes
- Interactive SLURM Exercise

HPC Workshop - HPC @ GWU

Colonial One





HPC Workshop - HPC @ GWU

Current Specs:

- Dell C8220 cluster, 213 node
- 53x GPU nodes, 2x NVIDIA K20 GPUs
- 1x 2TB Node, Quad 12-Core 3.0GHz Xeon E7-8857v2 CPUs
- 159x CPU nodes, 2x 2.6GHz 8-core Xeon CPUs, 64/128/256GB of RAM

Totals:

- 3,228 (2,592) Intel Xeon CPU cores
- 264,576 NVIDIA CUDA cores
- over 27 TB of RAM
- Mellanox FDR Infiniband fabric
- Two primary filesystems
- 262 TB NFS fileserver for /home and /groups
- 262 TB Lustre filesystem for high-speed scratch
- 268 TB Dell Compellent for archival



HPC Workshop - HPC @ GWU

Colonial One:

- Serves over 600 users in over 135 research groups
- Runs 24/7, 365 days a year
- Processes > 2,000 jobs every day
- User demand is 91% of capacity
- Open to entire GW community
- 129 open proposals for funding reference Colonial One



HPC Workshop - HPC @ GWU

Jobs Run on Colonial One:

- Study structure of subatomic particles
- Large-scale molecular dynamics simulations
- Network analysis
- Drug design for cancer therapy
- Protein engineering for immune response against bacteria and viruses including HIV/AIDS
- fMRI analyses of injured brains
- Genomic sequencing
- Phylogenetic mapping of evolutionary traits
- Satellite imagery
- Population and census dynamics



HPC - Logging In

Requirements:

- SSH Client
- Colonial One account

Log into Colonial One:

ssh [username@login.colonialone.gwu.edu](#)

Use your NetID and password!



HPC - Navigating the shell

Pathname

- A path through the directory system
- *pwd* – shows current path
- Absolute vs. Relative path

/ - the forward slash

- Represents the very bottom (root) of the file system
- acts as a divider in between directories on the file system



HPC - Navigating the Shell

- `pwd`: Print Working Directory, shows you where you are
- `.` versus `..` : Your current directory versus the directory one level above
- The `~` character: Shortcut your home directory
- `ls`: list current path contents
- `ls -la`: list all details of the current path in long form
- `cd`: change directory
 - `cd /absolute/path`
 - `cd path/relative/to/where/I/am`



HPC - Modules

Modules load an environment so a program can run correctly.

Module commands:

- module list
- module avail
- module load
- module unload
- module spider



Environment variables

Environment variables are a set of dynamic named values that can affect the way running processes will behave on a computer. They are part of the environment in which a process runs.

Environment commands:

- `printenv`
- `printenv Variable_Name`
- `echo $Variable_Name`
- `export Variable_Name=Value`



HPC - Shell Configuration Files

- `.bashrc`: Runs when logging into a BASH session. Local to the BASH shell
 - You can enter the same commands inside `.bashrc_profile` as you can inside `.profile`
 - change your prompt: `export PS1='[\u@\h:\w]\$ '`
 - `[hurlburj@login4:~]$`
- Other shells have similar names: `.cshrc` (C shell), `.ksh` (Korn shell)



HPC - Quotas

Home and Group Quotas

- Soft quotas are in place now
- Home quota: /home/username - default 25GB
- Group quota: /groups/groupname - default 250GB
- Check quota: type "quotareport" at the shell

Colonial One is not meant for archival data. Please remove data from old jobs once you finish your project.



HPC - Purge

What data is purged?

- Home and Group shares are not purged
- The high speed lustre file system IS purged every month
- Lustre is to be used for scratch space while running jobs

When is data purged?

- At the beginning of every month



HPC - Purge Policy

Lustre Purge Policy Coming into Effect 3/1/2017

1. **Frequency:** A purge will be conducted on the first day of every month (starting on **3/1/2017**). In the past, purges have been scheduled based on how close lustre utilization was to capacity. In the updated procedure, a purge will be conducted irrespective of lustre utilization. Again, a purge will be conducted on the first of every month even if the 1st falls on a weekend or holiday.
2. **File Access Time:** All files whose access time is greater than 60 days will be subject to purging. NOTE: updating access times with the sole intent of circumventing purging of files may result in disciplinary action including account suspension.
3. **File Size:** Files will be subject to purging regardless of the size they occupy on disk.



HPC - File Transfer with SCP

SCP - Secure Copy

- Usage:
 - `scp from [...] to`
 - `scp <sourcefile> <destfile>`
 - `scp host:<sourcefile> <destfile>`
 - `scp user@host:<sourcefile> <destfile>`
- Syntax is like `cp`
 - `-r` flag to recursively copy directories
 - `man scp` for more options




HPC - File Transfer with Globus

Globus is the industry standard for transferring large amounts of science and engineering research data between datacenters and endpoints.

Key points are:

- Built on GridFTP technology.
- Data Transfers can be encrypted in flight (not encrypted by default).
- Transfer run in the background and can be interrupted and restarted, even if a file is partially transmitted.
- Free for individuals (institutes must pay to use the service).
- Globus is used literally everywhere by everyone transferring data in the HPC world. AWS, National Labs, National Supercomputing Centers, Universities, and even GWU!

HPC - File Transfer with Globus



The screenshot shows the Globus website homepage. At the top, there's a navigation bar with the Globus logo, a search bar, and links for Products, Pricing, Developers, Support, and Log In. The main visual is a large graphic with three orange arrows labeled 'share', 'transfer', and 'publish' forming a cycle around a blue box labeled 'RESEARCH DATA'. To the right of this graphic, the text 'Research data management simplified.' is displayed. Below the graphic, a large counter shows '205,549,720,689 MB TRANSFERRED'. The bottom section is divided into three columns: 'Researchers' (focus on research, not IT problems), 'Resource Providers' (Globus gives you more control over your data infrastructure), and 'We're Hiring!' (Looking for a unique challenge? Join our growing team). Each column has a 'LEARN MORE' link with a right arrow icon.

globus

Google™ Custom Search

Products ▾ Pricing Developers Support ▾ Log In

share transfer publish

RESEARCH DATA

Research data management simplified.

205,549,720,689 MB TRANSFERRED

Researchers

Focus on your research, not IT problems. We make it easy to move, manage, and share big data.

[LEARN MORE](#) ➤

Resource Providers

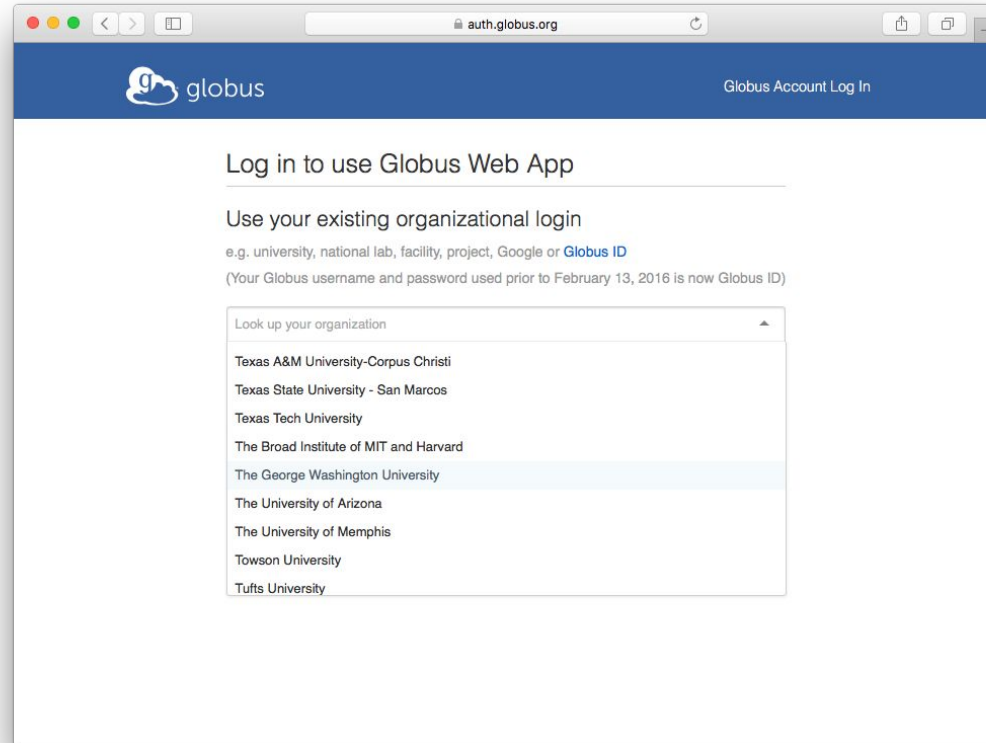
Globus gives you more control over your data infrastructure, while providing excellent ease-of-use for

We're Hiring!

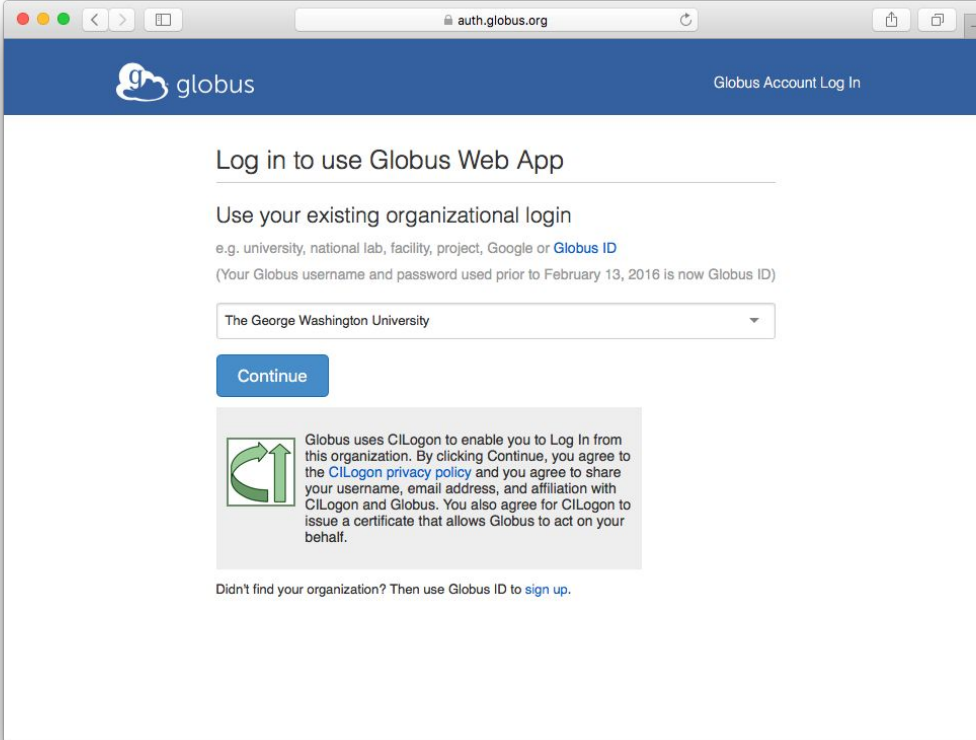
Looking for a unique challenge? Join our growing team and help us transform the way research is done.

[OPEN POSITIONS](#) ➤

HPC - File Transfer with Globus



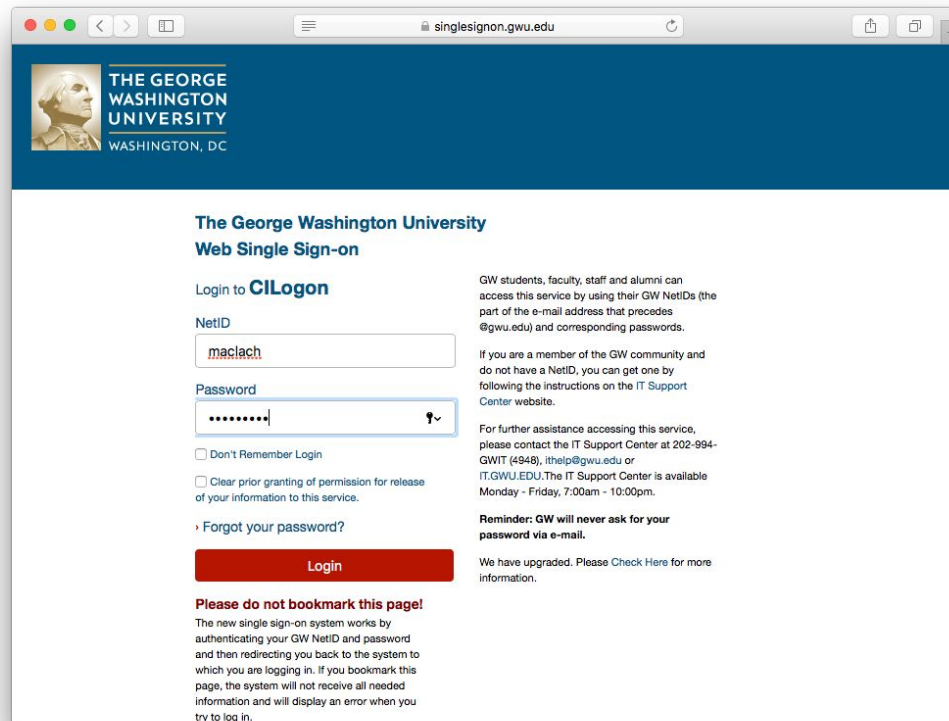
HPC - File Transfer with Globus



A screenshot of a web browser window showing the Globus Account Log In page. The browser's address bar displays 'auth.globus.org'. The page has a blue header with the Globus logo on the left and 'Globus Account Log In' on the right. The main content area is white and contains the following elements:

- A heading: 'Log in to use Globus Web App'.
- A sub-heading: 'Use your existing organizational login'.
- Example text: 'e.g. university, national lab, facility, project, Google or [Globus ID](#)'.
- Clarification text: '(Your Globus username and password used prior to February 13, 2016 is now Globus ID)'.
- A dropdown menu showing 'The George Washington University'.
- A blue 'Continue' button.
- A green circular arrow icon.
- A text block explaining the use of CILogon and the agreement to share information.
- A link for users who didn't find their organization: 'Didn't find your organization? Then use Globus ID to [sign up](#).'

HPC - File Transfer with Globus



The screenshot shows a web browser window with the address bar displaying "singlesignon.gwu.edu". The page header features the George Washington University logo and name. The main content area is titled "The George Washington University Web Single Sign-on". It includes a "Login to CILogon" section with fields for "NetID" (containing "maclach") and "Password" (masked with dots). Below these fields are checkboxes for "Don't Remember Login" and "Clear prior granting of permission for release of your information to this service.", and a link for "Forgot your password?". A red "Login" button is positioned below the form. To the right of the login form, there is explanatory text about NetIDs and a reminder that passwords are never asked for via email. At the bottom left, a warning states "Please do not bookmark this page!" with a brief explanation of the single sign-on system's requirements.

THE GEORGE WASHINGTON UNIVERSITY
WASHINGTON, DC

The George Washington University Web Single Sign-on

Login to **CILogon**

NetID

Password

☐ 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.

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.

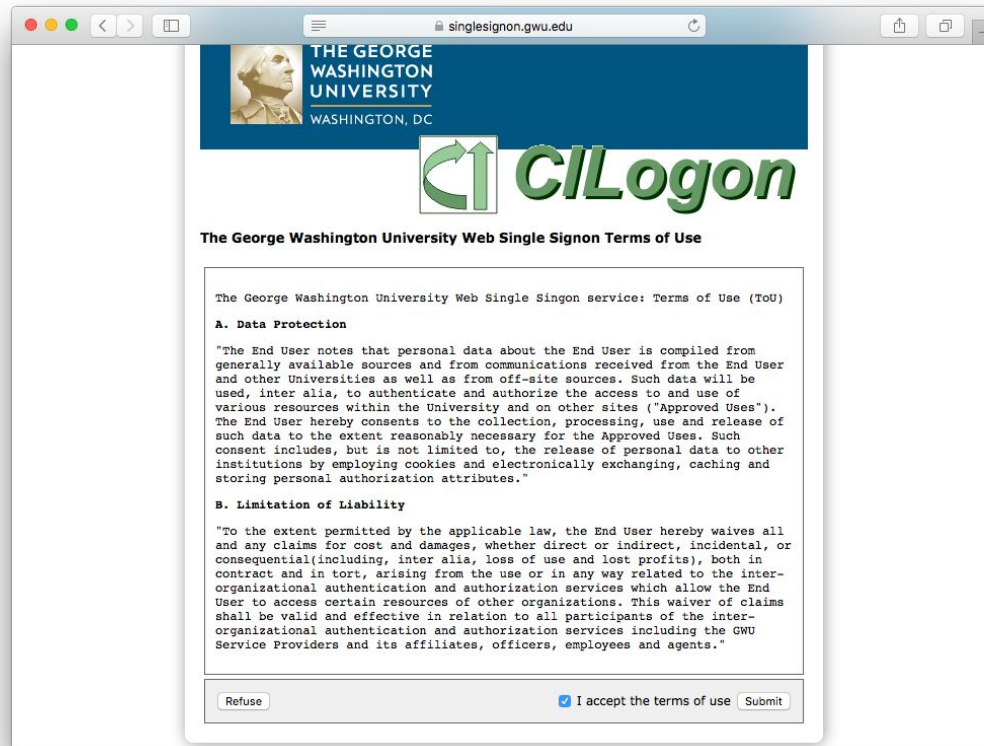
If you are a member of the GW community and do not have a NetID, you can get one by following the instructions on the IT Support Center website.

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.

HPC - File Transfer with Globus



The screenshot shows a web browser window with the address bar displaying "singlesignon.gwu.edu". The page header features the George Washington University logo and the "CILogon" logo. The main content is titled "The George Washington University Web Single Signon Terms of Use". It contains two sections: "A. Data Protection" and "B. Limitation of Liability". At the bottom, there are two buttons: "Refuse" and "Submit", with a checkbox labeled "I accept the terms of use" that is checked.

THE GEORGE WASHINGTON UNIVERSITY
WASHINGTON, DC

CILogon

The George Washington University Web Single Signon Terms of Use

The George Washington University Web Single Signon 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."

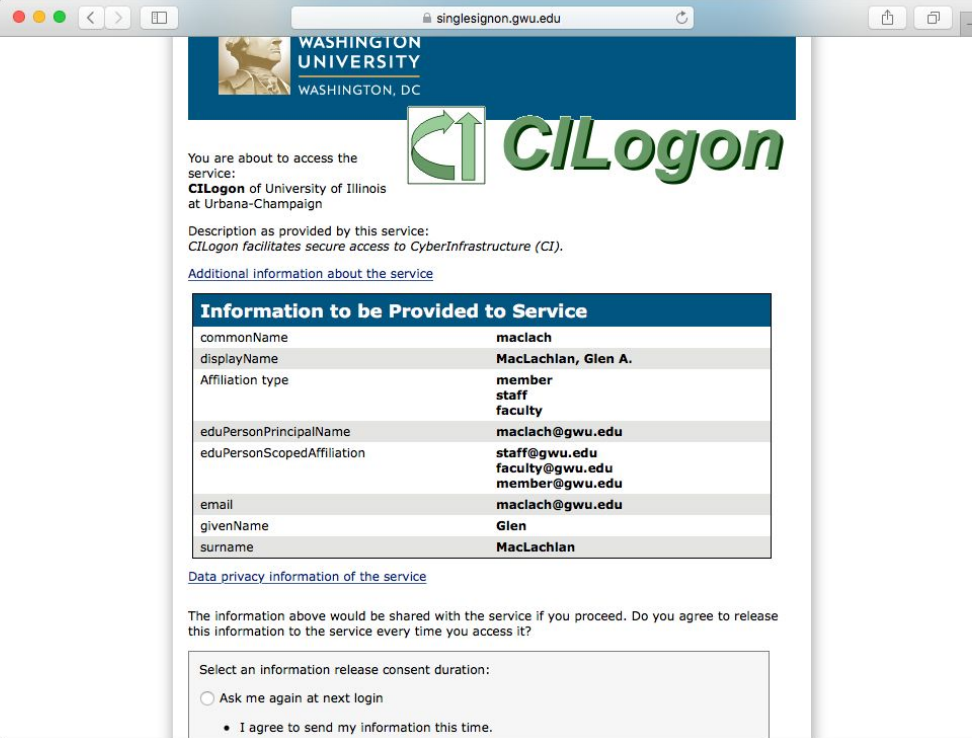
B. Limitation of Liability

"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."

☒ I accept the terms of use

HPC - File Transfer with Globus

WASHINGTON UNIVERSITY
WASHINGTON, DC



You are about to access the service:
CILogon of University of Illinois at Urbana-Champaign

Description as provided by this service:
CILogon facilitates secure access to CyberInfrastructure (CI).

[Additional information about the service](#)

Information to be Provided to Service	
commonName	maclach
displayName	MacLachlan, Glen A.
Affiliation type	member staff faculty
eduPersonPrincipalName	maclach@gwu.edu
eduPersonScopedAffiliation	staff@gwu.edu faculty@gwu.edu member@gwu.edu
email	maclach@gwu.edu
givenName	Glen
surname	MacLachlan

[Data privacy information of the service](#)

The information above would be shared with the service if you proceed. Do you agree to release this information to the service every time you access it?

Select an information release consent duration:

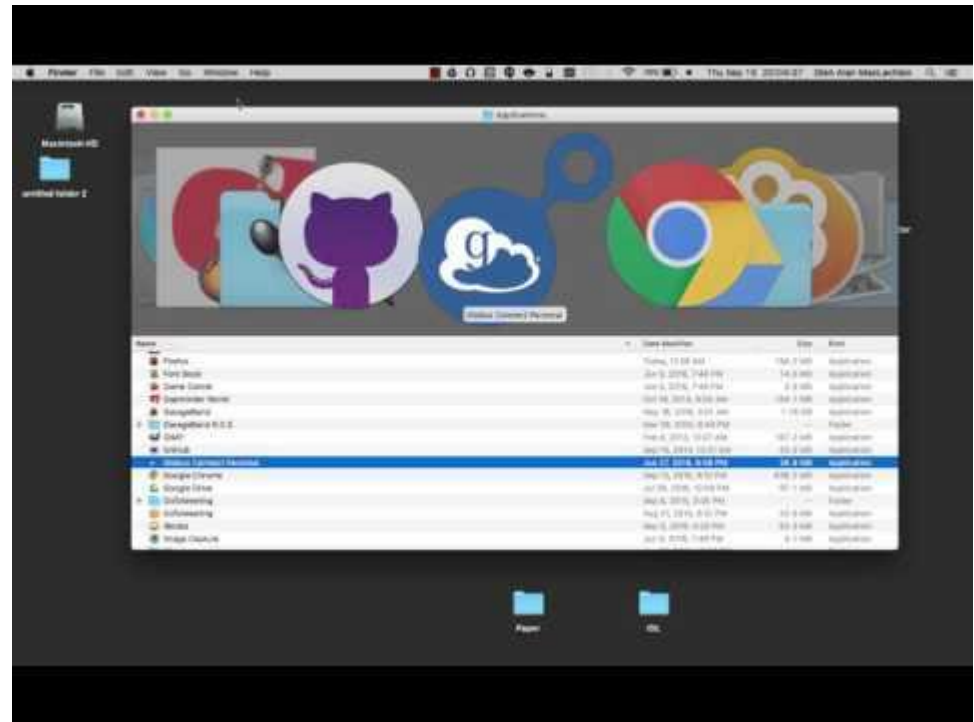
☐ Ask me again at next login

☒ I agree to send my information this time.

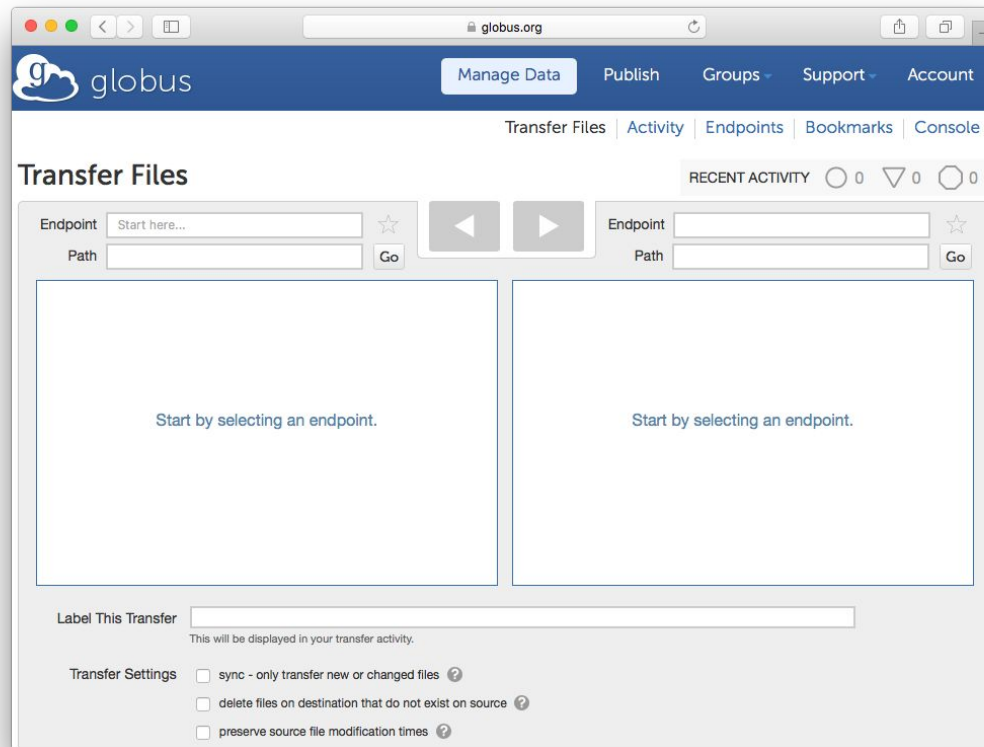
HPC - File Transfer with Globus

Setting up a personal endpoint...

1. Go to EndPoints
2. Add globus personal connect endpoint and name it
3. generate and copy set up key
4. Download installer and install.
5. Open app and paste setup key
6. Go back to webpage and find endpoint



HPC - File Transfer with Globus



The screenshot shows the Globus website interface in a web browser. The browser's address bar displays "globus.org". The website's header includes the Globus logo and navigation links: "Manage Data", "Publish", "Groups", "Support", and "Account". Below the header, a secondary navigation bar contains "Transfer Files", "Activity", "Endpoints", "Bookmarks", and "Console". The "Transfer Files" section is active, showing a "RECENT ACTIVITY" section with three circular icons and the number "0". The main content area is titled "Transfer Files" and features two identical panels. Each panel has an "Endpoint" input field with a placeholder "Start here...", a "Path" input field, and a "Go" button. Below the input fields, a large box contains the text "Start by selecting an endpoint." At the bottom of the interface, there is a "Label This Transfer" section with a text input field and a note "This will be displayed in your transfer activity." Below this, the "Transfer Settings" section includes three checkboxes: "sync - only transfer new or changed files", "delete files on destination that do not exist on source", and "preserve source file modification times". Each checkbox has a help icon (a question mark in a circle) next to it.

globus

Manage Data Publish Groups Support Account

Transfer Files Activity Endpoints Bookmarks Console

RECENT ACTIVITY 0 0 0

Transfer Files

Endpoint Start here... ☆

Path Go

Start by selecting an endpoint.

Endpoint ☆

Path Go

Start by selecting an endpoint.

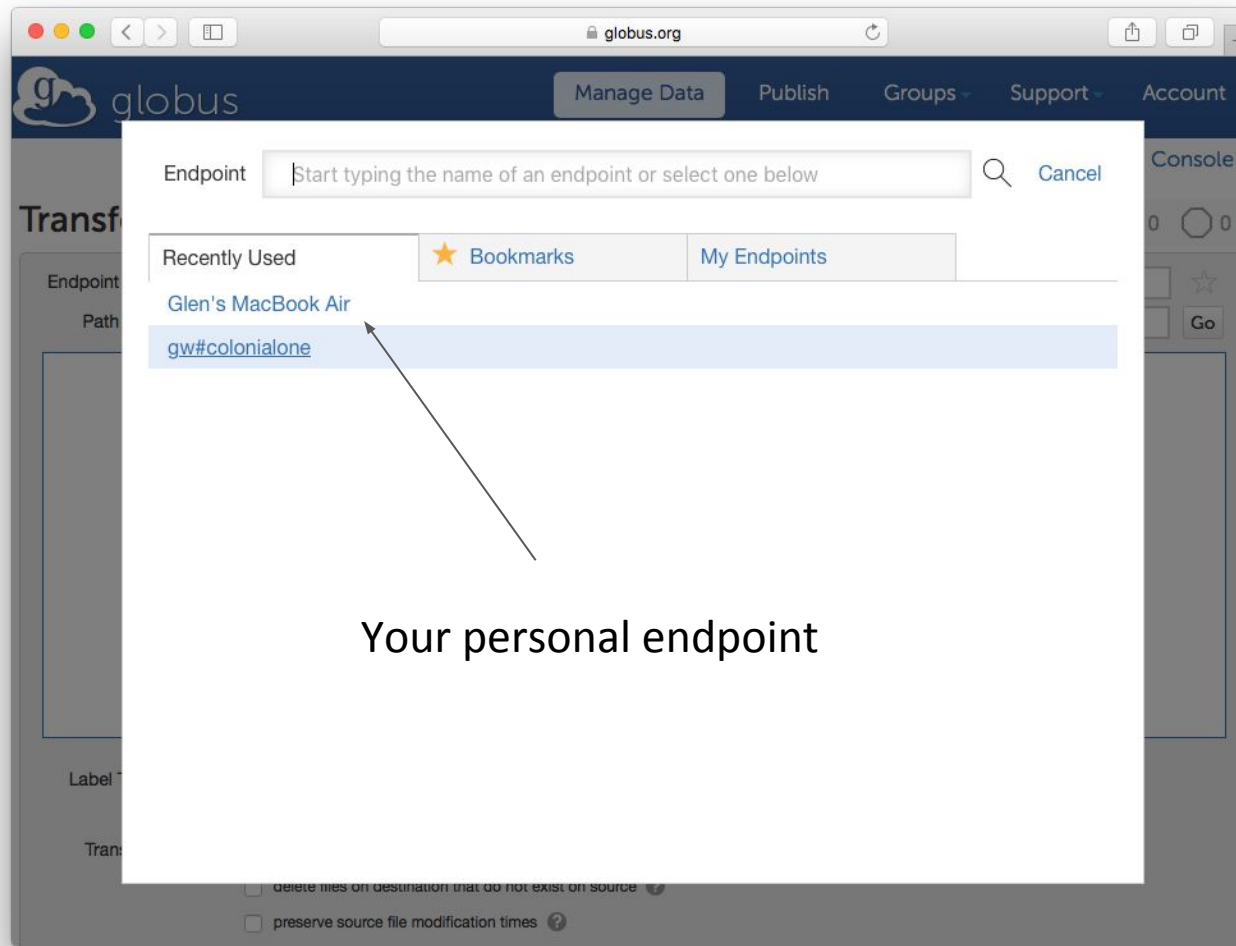
Label This Transfer

This will be displayed in your transfer activity.

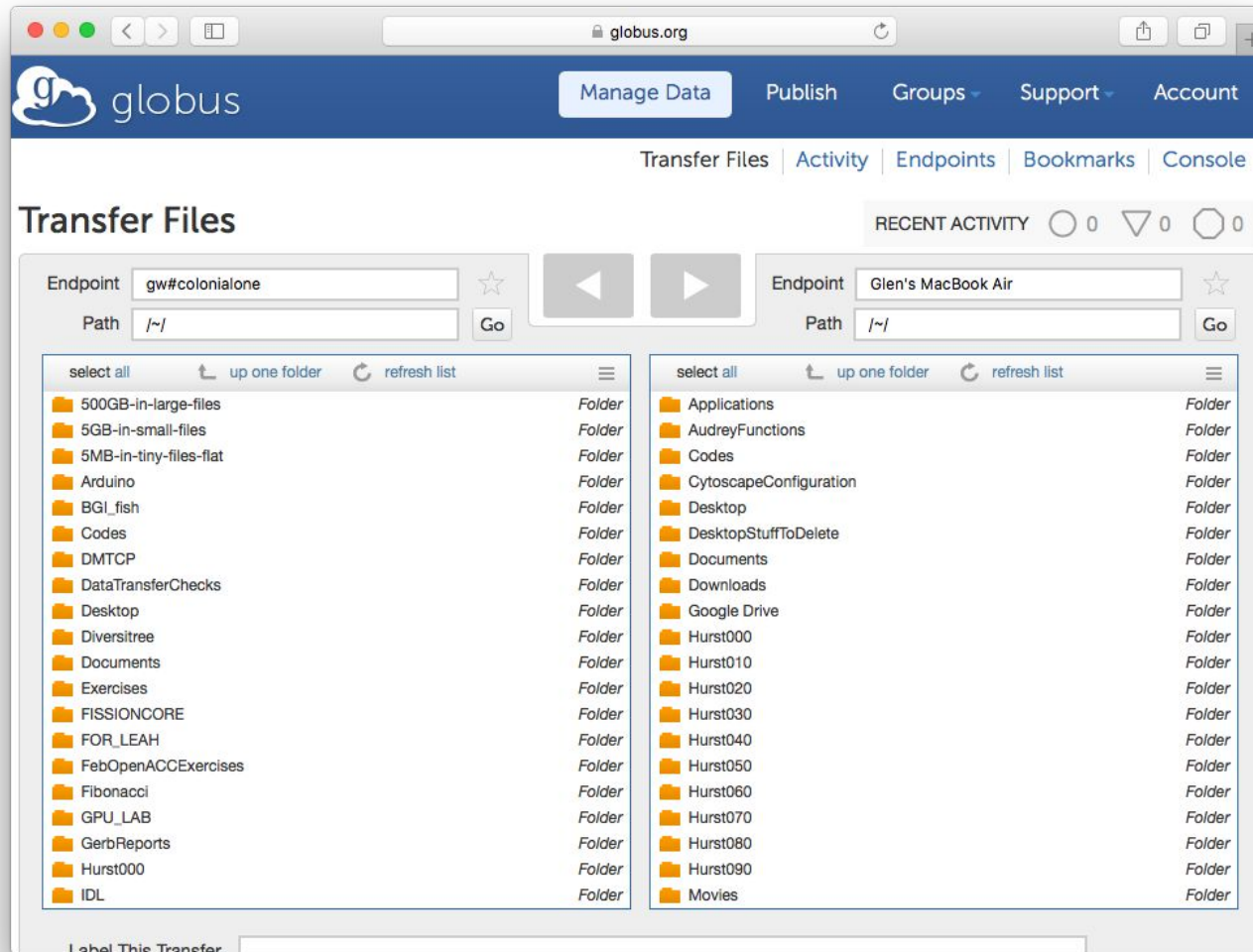
Transfer Settings

- ☐ sync - only transfer new or changed files ?
- ☐ delete files on destination that do not exist on source ?
- ☐ preserve source file modification times ?

HPC - File Transfer with Globus



HPC - File Transfer with Globus





HPC - Lustre and NFS

Lustre:

- Lustre is a free and open standard for creating a parallel high-speed file system
- It works by “striping” data over several different storage volumes.
- Lustre is a high speed storage system
- Lustre should be used for running jobs
- Is purged monthly

NFS:

- Network File System
- Hosts /home and /group directories
- NFS is slow compared to lustre
- Is not purged



HPC - Lustre

How to use Lustre:

- Using Lustre is one of the simplest things you can do on Colonial One or any cluster. You simply need to read or write to a lustre directory. Nothing else is required!

On Colonial One the lustre file system is found here:

- `cd /lustre/groups`

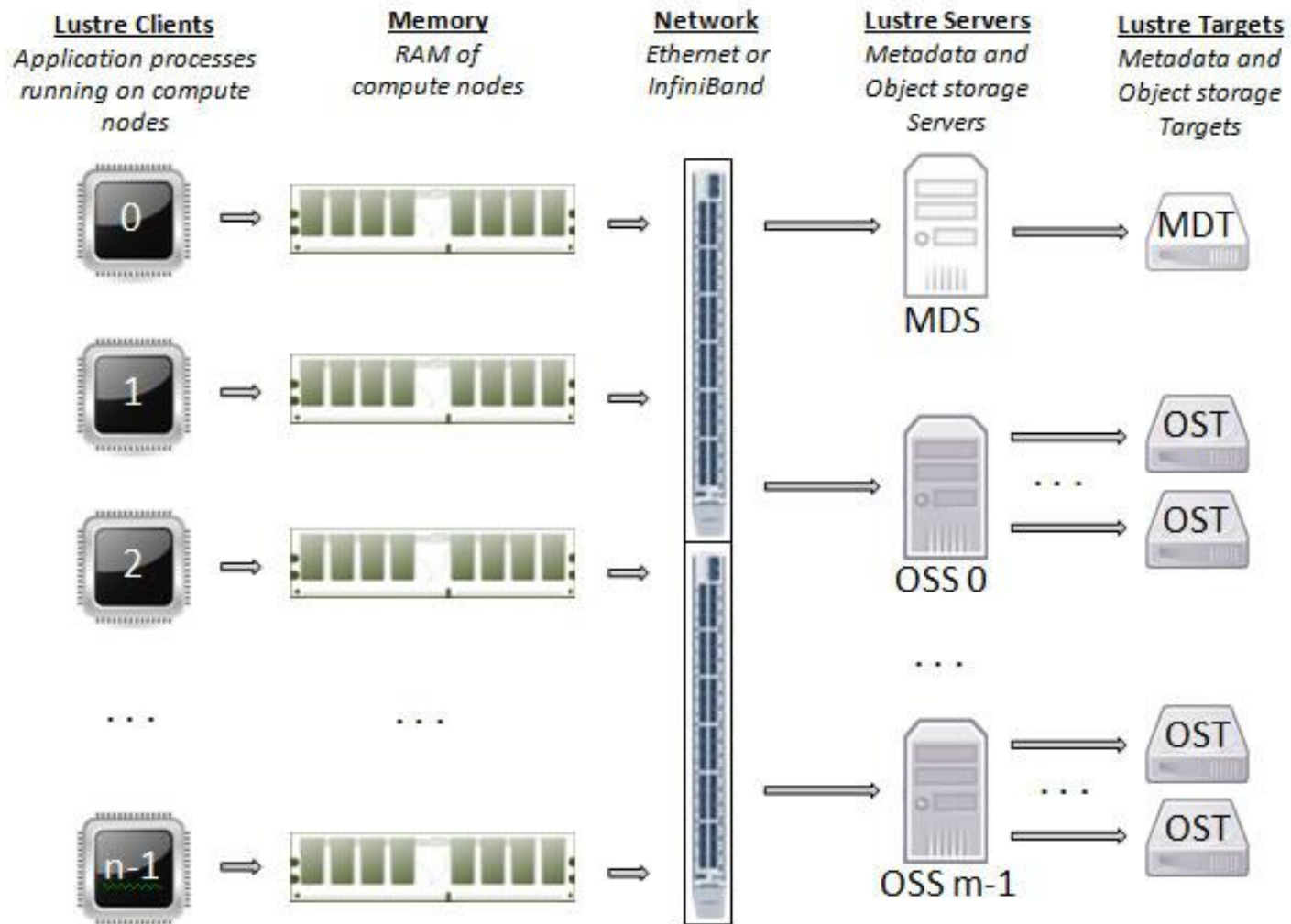


HPC - Lustre Overview

Lustre System Components

1. Object Storage Server (OSS) – The OSS handles requests for storing files on one or more local Object Storage Targets.
2. Object Storage Target (OST) -The OST stores file data as “stripes” of files. A single file may be striped across one or more OSTs. When a file is striped, pieces of the file are stored on more than one OST. The OSS provides information about where and how files are striped.
3. Metadata Server (MDS) – The MDS is the gateway node that provides access to the Metadata Target nodes, MDTs.
4. Metadata Target (MDT) – The MDT stores metadata such as file attributes like file size, ownership, permissions, access times.
5. Lustre Clients – The nodes that mount the lustre file system. The login and compute nodes on Colonial One are examples of lustre clients.

HPC - Lustre Overview





HPC - Lustre Striping

Files are split into “chunks” and stored on separate OSTs so they can be read (or written) in parallel and therefore increase I/O bandwidth.

For large files it makes sense to stripe over many OSTs (on Colonial One we have 12 OSTs). However, for small files better performance can be gained by disabling striping.

```
lfs getstripe <dir|filename>
```

```
lfs getstripe --verbose <dir|filename>
```

Stripe size: The size of the chunks in bytes

Stripe count: The number of OSTs to stripe across. -1 means use all OSTs in the filesystem.

Stripe offset: The index of the OST where the first stripe is to be placed. The default is -1, which results in random selection.



HPC - Lustre Striping

You can set stripe settings for either files or directories. If you set striping for a directory, all files in that directory inherit the directory's settings.

```
lfs setstripe <dir|filename>
```

```
lfs setstripe -S stripe_size -c stripe_count -o stripe_offset <dir|filename>
```

Setting “-c 1” disables striping!

You can pre-create files of zero length and then write to them later.

```
lfs setstripe -c 10 bigdir
```

```
tar cf bigdir.tar bigdir
```



HPC - Useful Lustre Commands

`lfs ls`

`lfs df -h`

`lfs df -i`

`lfs quota -h -v -u maclach`

`lfs osts <dir|filename>`

`lfs find /lustre/groups/phys6130_10 -mtime +30 -type f -print`

See `man lfs` for more examples!



HPC - Lustre Striping Exercise

Create a large file with dd using different stripe patterns and see how the timings vary with the number of OSTs. For example,

```
lfs setstripe -c 1 test_1;dd of=test_1 if=/dev/zero bs=1024k count=100000 iflag=count_bytes  
lfs setstripe -c 2 test_2;dd of=test_2 if=/dev/zero bs=1024k count=100000 iflag=count_bytes  
lfs setstripe -c 4 test_4;dd of=test_4 if=/dev/zero bs=1024k count=100000 iflag=count_bytes  
lfs setstripe -c 8 test_8;dd of=test_8 if=/dev/zero bs=1024k count=100000 iflag=count_bytes  
lfs setstripe -c 12 test_12;dd of=test_12 if=/dev/zero bs=1024k count=100000  
iflag=count_bytes
```



HPC - Job Scheduler

Colonial One uses SLURM to schedule and prioritize jobs on the cluster.

SLURM (Simple Linux Utility for Resource Management) is a software package for submitting, scheduling, and monitoring jobs on large compute clusters.

HPC - Interactive SLURM Exercise

```
601222 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601223 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601224 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601225 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601226 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601227 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601228 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601229 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601230 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601231 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601214 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601213 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601212 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601211 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601210 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601209 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601208 ivygpu-no eigensys wfreeman PD 0:00 4 (Resources)
601536 short bash naclach R 0:18 1 node134
601501 short /home/sv svc_hive R 2:51:24 1 node130
601510 short ckg mRNA ckgreen R 40:27 1 node133
601509 short bash lfbrooks R 1:01:26 1 node131
601090 short raxml_al clowen R 1:20:10:57 1 node150
601088 short raxml_40 clowen R 1:20:18:48 1 node150
601069 short raxml_30 clowen R 1:20:24:34 1 node150
[naclach@login4 ~]$ squeue -u naclach
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
601536 short bash naclach R 0:40 1 node134
[naclach@login4 ~]$ ssh node1
```



For More Information

Colonial One overview:

<http://it.gwu.edu/colonialone-high-performance-computing>

User documentation:

<http://colonialone.gwu.edu>

Or send us email:

Colonial One support - hpchelp@gwu.edu