



Transitioning from Peregrine to Eagle

HPC Operations

January 2019

Sections

System Access

Transferring Data From Peregrine

Running Jobs

Allocation Management

Q & A

Slide Conventions

- Verbatim command-line interaction:
 - “\$” precedes explicit typed input from the user.
 - “↵” represents hitting “enter” or “return” after input to execute it.
 - “...” denotes text output from execution was omitted for brevity.
 - “#” precedes comments, which only provide extra information.

```
$ ssh hpc_user@eagle.nrel.gov↵
```

...

```
Password+0TPToken: # Your input will be invisible
```

- Command-line executables in prose:
 - “The command **rsync** is very useful.”

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HPC Accounts

Access Eagle with the same credentials as Peregrine.

```
$ ssh hpc_user@eagle.hpc.nrel.gov ↵
```

...

```
Password:*****↵
```

```
$ ssh hpc_user@eagle.nrel.gov ↵
```

...

```
Password+OTPToken:*****↵
```



Eagle DNS Configuration

Internal		External (Requires OTP Token)	
<u>Login</u>	<u>DAV</u>	<u>Login</u>	<u>DAV</u>
eagle.hpc.nrel.gov	eagle-dav.hpc.nrel.gov	eagle.nrel.gov	eagle-dav.nrel.gov

Direct Hostnames	
<u>Login</u>	<u>DAV</u>
el1.hpc.nrel.gov	ed1.hpc.nrel.gov
el2.hpc.nrel.gov	ed2.hpc.nrel.gov
el3.hpc.nrel.gov	ed3.hpc.nrel.gov

RSA Keys

Copy keys generated for your username between systems to avoid password prompts when using secure protocols:

****Do NOT use ssh-keygen on HPC Systems**

```
$ ssh hpc_user@peregrine.hpc.nrel.gov  
...  
[hpc_user@login1 ~]$ ssh-copy-id eagle  
Password:*****  
...  
[hpc_user@login1 ~]$ ssh eagle # No password needed  
...  
[hpc_user@el1 ~]$ ssh-copy-id peregrine  
Password:*****
```

Graphical Interface

- Running desktop sessions on the DAV nodes works the same as it did on Peregrine using FastX. There is also a web interface available on the Eagle DAV nodes. Access with direct hostnames to DAV nodes ed[1-3].hpc.nrel.gov
- Please see this page for more detailed instructions:
<https://www.nrel.gov/hpc/eagle-software-fastx.html>



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Eagle Filesystem

- Eagle has modern storage hardware and will not share filesystems with Peregrine, except Mass Storage (`/mss`). Users need to copy files they want from Peregrine over.
- Eagle features a new `/shared-projects` mountpoint, allowing mutual access to users of differing projects. If interested, please send a request to HPC-Help@nrel.gov specifying a desired directory name, list of users who may access, and the user who will administrate the directory.

Transferring Small Batches (<10GB)

The commonly used network transfer commands **scp** and **rsync** are most practical in this case.

```
# Copy a small file from Peregrine to Eagle
$ scp /scratch/hpc_user/small.file eagle:~
```

The benefits of bandwidth parallelization in more sophisticated transfer technologies mentioned in the next slide are not noticeable at this scale.

Transferring Large Batches (>10GB)

- To transfer any amount of data over ~10GB between systems, we recommend using Globus.
- Globus uses GridFTP which is optimized for HPC infrastructure, streamlining massively-multifile transfers as well as Very Large File transfers.
- We've provided a separate document with expanded instructions on using Globus with this presentation.



File Manager

RECENTLY USED

- nrel#globus
- nrel#globus-mss
- nrel#eglobus1

PINNED BOOKMARKS

- eagle/~/
- peregrine/scratch

• Bookmark Manager

Activity

Endpoints

Publish

Collection

nrel



Cancel

nrel#globus-s3

nrel@globusid.org

NREL transfer to/from AWS S3

nrel#globus-mss

nrel@globusid.org

Transfer files to/from NREL Mass Storage System (MSS)

nrel#globus

nrel@globusid.org

Provides transfer ability from/to Peregrine /scratch

nrel#eglobus3

nrel@globusid.org

Transfer files to/from Eagle /scratch /projects /home

nrel#eglobus2

nrel@globusid.org

Transfer files to/from Eagle /scratch /projects /home server2

nrel#eglobus1

nrel@globusid.org

Transfer files to/from Eagle /scratch /projects server1



File Manager | Globus

https://app.globus.org/file-manager

globus

File Manager

Collection: nrel#globus

Path: /projects/csc000/msolari/

select all

Sort

Share

Transfer or Sync to...

New Folder

Rename

Delete Selected

Preview (limited)

Download (https)

Open (https)

Get Link

Start

Transfer & Sync Options

Start

RECENTLY USED

- nrel#globus
- nrel#globus-mss
- nrel#globus1

PINNED BOOKMARKS

- eagle/~/
- peregrine/scratch

Bookmark Manager

Activity

Endpoints

Publish

Groups

Console

File Manager

Bookmarks

Panel

Bookmark Manager

1 Transfer or Sync to...

2 nrel#globus1

3 select all

4 Start

The screenshot shows the Globus File Manager interface. On the left, there's a sidebar with links like 'RECENTLY USED' (nrel#globus, nrel#globus-mss, nrel#globus1), 'PINNED BOOKMARKS' (eagle/~/, peregrine/scratch), and 'Bookmark Manager'. The main area has 'File Manager' tabs at the top. In the center, there are two search bars: 'Collection' with 'nrel#globus' and 'Path' with '/projects/csc000/msolari/'. Below these are two buttons: 'select all' (circled in red) and 'Sort'. A list of files/folders is shown: 'project-data-to-move-to-eagle1' (10 B), 'project-data-to-move-to-eagle2' (10 B), 'project-data-to-move-to-eagle3' (10 B), and 'projectdata' (10 B). To the right of the list is a context menu with options: 'Share' (highlighted with a red box and circled in red), 'Transfer or Sync to...', 'New Folder', 'Rename', 'Delete Selected', 'Preview (limited)', 'Download (https)', 'Open (https)', and 'Get Link'. At the bottom are 'Transfer & Sync Options' and two large blue 'Start' buttons. Red numbers 1 through 4 are overlaid on the interface: 1 points to the 'Transfer or Sync to...' option in the context menu; 2 points to the 'nrel#globus1' entry in the collection search bar; 3 points to the 'select all' button; and 4 points to one of the 'Start' buttons at the bottom.

Globus Endpoints

These are the current NREL Globus Endpoints

- **nrel#globus** - This endpoint will give you access to any files you have on Peregrine:/scratch and /projects.
- **nrel#globus-s3** - This endpoint allows you to copy files to/from AWS S3 buckets.
- **nrel#globus-mss** - This endpoint allows you to copy files to/from NREL's Mass Storage System (MSS).
- **nrel#eglobus1; nrel#eglobus2; nrel#eglobus3.** These endpoints allow you to transfer files to/from Eagle's /scratch, /projects, and your Eagle /home directory

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Simple Linux Utility for Resource Management

- Eagle uses Slurm, as opposed to PBS on Peregrine.
- We will host workshops dedicated to Slurm usage. Please watch our training page, as well as for announcements:
<https://www.nrel.gov/hpc/training.html>
- We have drafted extensive and concise documentation about effective Slurm usage on Eagle:
<https://www.nrel.gov/hpc/eagle-running-jobs.html>

Noteworthy Job Submission Changes

A maximum job duration is now **required** on all Eagle job submissions. They will be rejected if not specified:

```
$ srun -A handle --pty $SHELL
error: Job submit/allocate failed: Time limit
specification required, but not provided
```

Some compute nodes now feature GPUs:

```
# 2 nodes with 2 GPUs per node, 4 total GPUs for 1 day
$ srun -t1-00 -N2 -A handle --gres=gpu:2 --pty $SHELL
```

Job Submission Recommendations

Slurm will pick the optimal partition (known as a “queue” on Peregrine) based your job’s characteristics. In opposition to standard Peregrine practice, we suggest that users **avoid specifying partitions** on their jobs with `-p` or `--partition`.

To access specific hardware, we strongly encourage requesting by feature instead of specifying the corresponding partition:

```
# Request 4 "bigmem" nodes for 30 minutes interactively
$ srun -t30 -N4 -A handle --mem=200000 --pty $SHELL
```

- <https://www.nrel.gov/hpc/eagle-job-partitions-scheduling.html>

Job Submission Recommendations cont.

For debugging purposes, there is a “*debug*” partition. Use it if you need to quickly test if your job will run on a compute node with **-p debug**.

```
$ srun -t30 -A handle -p debug --pty $SHELL ↵
```

Node Availability

To check the availability of what hardware features are in use, run `shownodes`. Similarly, you can run `sinfo` for more nuanced output.

\$ shownodes	partition	#	free	USED	reserved	completing	offline	down
	bigmem	m	0	46	0	0	0	0
	debug	d	10	1	0	0	0	0
	gpu	g	0	44	0	0	0	0
	standard	s	4	1967	7	4	10	17
	TOTALs		14	2058	7	4	10	17
	%S		0.7	97.5	0.3	0.2	0.5	0.8

Translating Your Job Scripts

- Eagle's Slurm configuration **will not respect PBS commands.**
- Many new job-queue features are now available, and it is worth your effort to reconsider the program-flow of your jobs. If you can accurately minimize the resource demands of your jobs, you can also minimize your queue wait times.
- We've provided a PBS-to-Slurm translation sheet with this presentation which is catered to our operating environment.

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Allocated NREL Hours

- Eagle is approximately 3× more performant than Peregrine. It will charge 3 of your project's "NREL Hours" for every 1 hour of time you occupy a compute node, unlike Peregrine which is 1-to-1.
- **The 3× cost will remain after Peregrine is shutoff.**
- Like on Peregrine, projects which exhaust their allotted hours will still be able to submit and run jobs **but they will be enqueued at minimum priority.**

Tracking Allocation Usage

alloc_tracker has been deprecated.

Please use **hours_report** instead.

```
[hpc_user@el1 ~]$ hours_report
Gathering data from database.....Done
...
User hpc_user has access to and used:
Allocation Handle      System      Hours Used Note
-----
handle                  Peregrine    125
handle                  Eagle       320
```

Advanced Tracking

`hours_report --showall`

- List each project, its PI, and its NREL hour usage.

`hours_report --showall --drillbyuser` (*default output*)

- List each project like above, but also show each member's contributing usage of allotted hours.

`hours_report --help`

- List usage instructions. `hours_report` is still in development and new features will be documented here.

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Discussions From Previous Sessions

- Eagle only supports XFCE for FastX desktop sessions currently. If you have a valid business need for an alternate desktop environment, please contact HPC-Help@nrel.gov
- For those unfamiliar with DAV nodes, DAV is “Data Analysis & Visualization” but this effectively means the node features a GPU for performant remote graphical application usage.
- Globus endpoint for AWS S3 buckets will require case-by-case configuration, please contact HPC-Help@nrel.gov if needed.
- For debugging purposes (i.e. get a node with minimal resources fast) use `--partition=debug` or only specify account and a short time.
- Jobs do not charge more NREL hours for specific hardware features, only `--qos=high` will charge more time than usual.

Discussions From Previous Sessions

- We are brainstorming solutions for those who won't strongly benefit from Eagle's extra clock-cycles and therefore won't warrant the 3-times cost when Peregrine is decommissioned. For now, please use Peregrine.
- To clarify when submitting jobs with minimal specifications to “decrease queue wait time”, this does not mean Slurm gives out the most performant nodes first—the opposite. Slurm will reserve more specialized nodes for jobs which specifically ask for them. The only time a node with a unique hardware feature would operate as a standard node is in the event that *all the standard nodes are in use*. This will maximize the amount of nodes with a job at any given time. It is still in your benefit to specify features rather than partitions, as Slurm will have a more precise awareness of available resources than you probably do and optimize accordingly.

Feedback is Appreciated!

If you have any suggestions to improve this presentation
we invite you to share with us at HPC-Help@nrel.gov

Thank You

www.nrel.gov

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