O2 HMS Research Computing

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Two Factor Authentication (2FA)

2FA is required to access O2 from outside the HMS network

export DUO_PASSCODE=push

Add above line to /home/$USER/.bashrc file. You will get authentication requests on your phone DUO app when you login or copy to/from O2. Alternatively, you can set the DUO default at secure.med.harvard.edu, *My Settings & Devices* tab.

Access

ssh <ec>@o2.hms.harvard.edu to log into O2 from a Mac terminal (<ec> is your eCommons id, something like abc123).
ssh -XY <ec>@o2.hms.harvard.edu lets you run graphical programs
Use MobaXterm to log in from a Windows computer

Transfer Data

Use Filezilla (filezilla-project.org) program to copy files to/from O2. Mac users can also scp or sftp from a terminal window.
scp <ec>@transfer.rc.hms.harvard.edu:/file/on/O2 /local/path to download a file from O2 to a local machine.
scp local/file <ec>@transfer.rc.hms.harvard.edu:/path/to/O2 to upload a local file to O2
Log in to **transfer.rc.hms.harvard.edu** to copy to/from research.files

Display Graphics

X11 must be active on home machine to visualize/plot on O2
Mac computers: XQuartz (www.xquartz.org) is required
Windows computers: X11 is built-in to the MobaXterm program
Interactive jobs must include the "**--x11**" argument
Non-interactive jobs must include "**--x11=batch**" argument

Software

Software/tools are available as "modules" on O2

module load <tool_name>	load a module (lets you run a tool)
module unload <tool_name>	unload a module
module purge	unload *all* modules
module list	list currently loaded modules
module spider	search for a module
module avail	list available modules

Storage Spaces

/n/scratch3	write large and **temporary** files here
/home/<ec>	home folder for user "ec" (100 GB limit)*
/n/groups/ /n/data1 /n/data2	group folders with snapshots**
/n/no_backup2/	group folders without snapshots**
/n/shared_db	shared databases on O2

Notes: *home directory is public by default. **subject to RC approval

Partitions

Select a partition based on your job requirements

Partition	Job Type	Priority	Max Cores per job	Runtime	
				Max.	Min.
interactive	interactive	14	20	12 hours	N/A
short	Bash	12	20	12 hours	N/A
medium		6	20	5 days	12 hrs
long		4	20	30 days	5 days
mpi		12	640	5 days	N/A
priority		14	20	30 days	N/A
transfer		NA	4	5 days	N/A
gpu		NA	20	5 GPU hours	N/A
highmem		NA	16	5 days	N/A

mpi is exclusively for jobs running distributed-memory parallel programs; gpu allows access to GPU cards; highmem has a few computers with very large memory (RAM)

Interactive Jobs

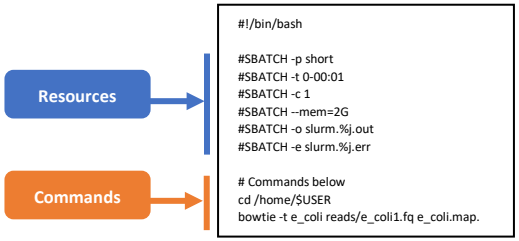
Interactive sessions reserve resources for you to run multiple commands interactively. Good for trying out a workflow.

srun --pty -p <partition > -t <time> --mem=<value> bash

--pty	required to initiate an interactive job
-p	submit to a specific partition (e.g., short)
-t	max time. Format DD-HH:MM, DD-HH, or MM:SS
--mem=	max memory required (--mem=1G reserves 1 GB)

Batch (Non-interactive) jobs

Batch jobs require "sbatch" script file describing requested resources (time, memory, etc.) and commands to run. Use a text editor to make a file with a name like e_bowtie.sbatch and contents like:.



#SBATCH -p	submit to a specific partition; required
#SBATCH -t	max time. Format DD-HH:MM, DD-HH, or MM:SS; required
#SBATCH --mem=	max memory (e.g., --mem=1G reserves 1 GB)
#SBATCH -c	# of cores (Default 1. Must match # cores/threads in command, like bowtie -p 4)
#SBATCH -o	write output to the specified file, where "%j" is replaced with the job allocation number
#SBATCH -e	write error messages to a different file
sbatch e_bowtie.sbatch	type on O2 command line to submit job. Job will wait ("pend") a while, then run commands from e_bowtie.sbatch on one of O2's compute nodes (not login node)

Job Priority

sshare -Uu <ec>	gives your current FairShare factor, which starts at 1 (high priority), decreases to 0 as you run more or larger jobs, gradually increases after jobs finish

Job Monitoring

O2squeue	table with jobs pending (in queue)
squeue -u <ec> -t <state>	only view jobs in specified state. States include PENDING, RUNNING, COMPLETED, etc.
squeue -u <ec> -p <partition>	only view jobs in partition(s)
scontrol show jobid <jobid>	detailed info for a given jobid
O2sacct	Job statistics: JobID, Partition, State, NodeList, Start, Timelimit, Elapsed CPUTime, TotalCPU, AllocTRES, MaxRSS (memory)
O2sacct -h	See how to use O2sacct to find specific jobs
scancel <jobid>	cancel job with the given jobid
scancel -t <state>	cancel all pending jobs

O2 Cluster Status

https://wiki.rc.hms.harvard.edu/display/O2/O2+Cluster+Status
The website shows all service outage for the O2 cluster, including planned maintenance, and unplanned events.

Storage Usage

quota	show your usage in home directory and group folders for which you're a member
/n/cluster/bin/scratch3_quota.sh	show your usage in the scratch3 directory (command must be run from a login node)
du --apparent-size -hs <dir>	show the size of a directory (<dir>)