# Lab 03 – Introduction to Great Lakes

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NERS/ENGR 570 - Methods and Practice of Scientific Computing (F20)

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# Outline

- Accessing Great Lakes
- Environment and Modules
- Slurm job scheduler
- Back to git

# Learning Objectives: By the end of Today's Lab you should be able to

- (*Skill*) Login to Great Lakes and transfer files to and from Great Lakes
- (*Skill*) use environment modules
- (*Skill*) compose job scripts and submit jobs to the compute nodes

# Accessing Great Lakes

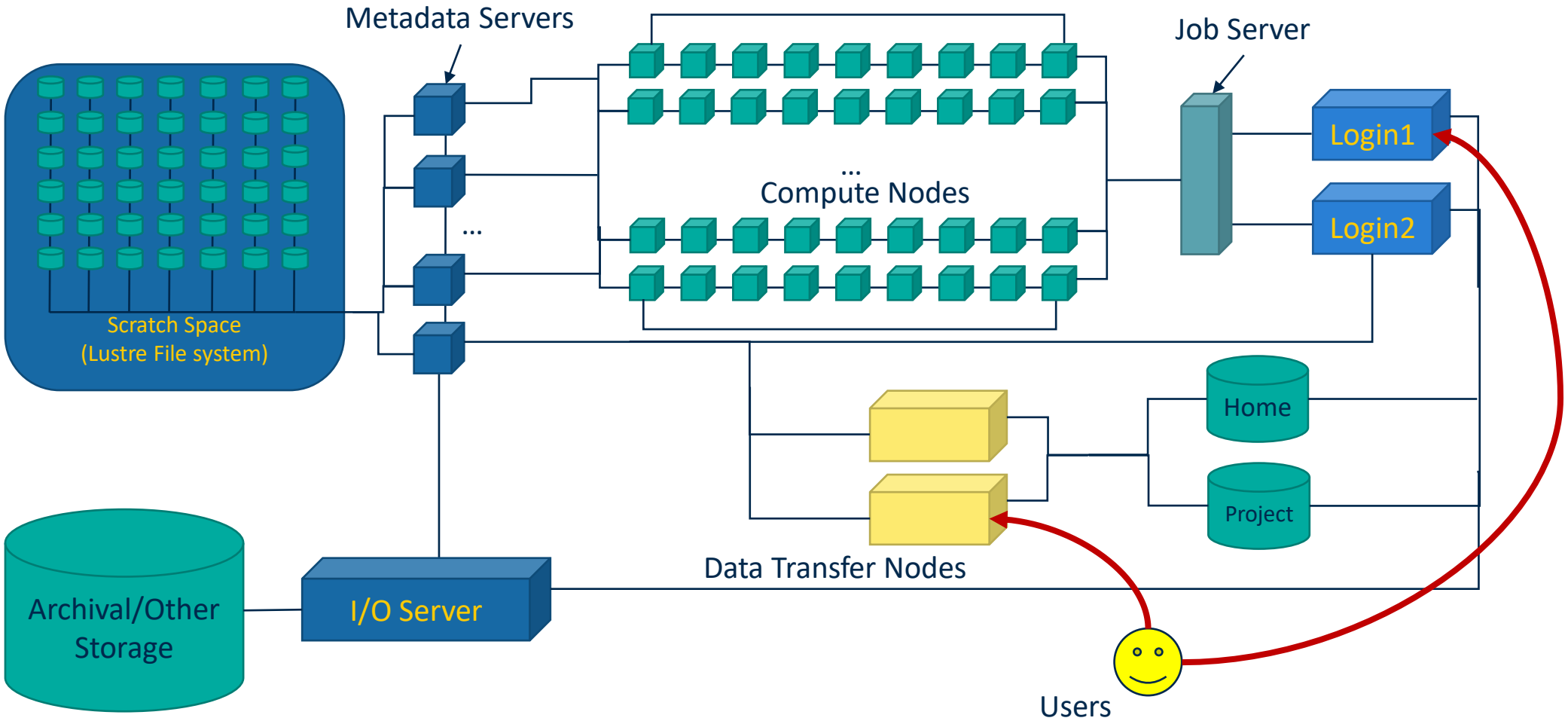
https://arc-ts.umich.edu/greatlakes/

ssh

sftp

https

# Great Lakes (or most HPC's)



# Environment and Modules

# Modules

**What are they?**

- Simple tool to manage the shell environment
- Enables installation of multiple versions of software tools
- Available on nearly all HPC clusters
- Confusingly there are two versions
  - environment-modules (old)
  - Lmod (new)

**Essential usage**

- What do I have loaded? `$ module list`
- What can I load? `$ module avail`
- What provides X? `$ module spider X`
- Load something `$ module load X`
- Unload something `$ module unload X`
- I screwed up. Start over. `$ module purge`

# “Packaging” or Saving Modules

- I just loaded like 10 modules, I want to save this setting
  - `$ module save <name>`
- Clear and reset it:
  - `$ module purge && module restore <name>`
- See what collections you’ve saved
  - `$ module savelist`

# Slurm Job Scheduler

Simple Linux Utility for Resource Management


# Examining the queue (squeue)

# Job Options

(RTFM: https://arc-ts.umich.edu/greatlakes/slurm-user-guide/)

- Essentials
  - Name `--jobname=`
  - Computational resources
    - What queue/account/project? `--account=`
    - What partition? `--partition=`
    - How much walltime? `--time=`
    - How many nodes? `--nodes=`
    - How many processors per node? `--ntasks-per-node=`
    - How much memory? `--mem=` or `--mem-per-cpu=`
    - Where to put job output? `--output=`
- Advanced
  - Mail options `--mail-user=` and `--mail-type=`
  - Environment `--export=`
  - Job dependencies `--dependency=`

# Running Interactive Jobs

- Basic command

```
$ srun --pty --account= [OPTIONS] /bin/bash;
```

# Job Scripts (They're shell scripts!)

```
#!/bin/bash

#SBATCH --jobname=
#SBATCH --account=
#SBATCH --partition=
# so on and so forth

Your commands here!
```

- Submit with `sbatch`
  - Can also use command line options
  - `$ sbatch myscript.slurm`

# Helpful Aliases

```
alias ll='ls-ahl'
alias which='alias | /usr/bin/which --tty-only --read-alias --show-dot --show-tilde'
alias ml='modle list'
alias ma='module avail'
alias sme='squeue -u $USER'
```

# Writing your own modules

- Modify MODULEPATH in .bashrc
  - `export MODULEPATH=$MODULEPATH:/gpfs/accounts/ners570f20_class_root/ners570f20_class/shared_data/modules`
  - `module load ners570-env`

Example Module File (old format)

```
#%Module

set msg "Sets environment variables and aliases for NERS570
Course"

proc ModulesHelp { } {
   puts stderr $msg
}

module-whatis $msg

set projdir
"/gpfs/accounts/ners570f20_class_root/ners570f20_class"
set accnt ners570f20_class
set user $::env(USER)

# Environment variables
setenv    PROJACCNT $accnt
setenv    PROJSHARE $projdir/shared_data
setenv    PROJHOME  $projdir/$user
setenv    PROJWORK  /scratch/$accnt\_root/$accnt/$user


# Aliases
set-alias     ll        {ls -ahl}
set-alias     ml        {module list}
set-alias     ma        {module avail}
set-alias     sme       {squeue -u \$USER}
set-alias     showq     {squeue -A \$PROJACCNT}
set-alias     watchme   {watch -n1 squeue -u \$USER}
set-alias     watchq    {watch -n1 squeue -A \$PROJACCNT}
```