

STATS 810 class 13:
Introduction to parallel statistical computing in R on
greatlakes

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Outline

- 1 Logging in to greatlakes
- 2 Moving files on and off greatlakes
- 3 Working with batch jobs
- 4 R modules on greatlakes
- 5 A test for foreach
- 6 Editing text files on greatlakes
- 7 Other ways to run R on greatlakes

Requirements

We follow [Section 1.2](#) of the [greatlakes user guide](#). As preliminaries, you need:

- A Slurm account. You should already have a primary account, `stats_dept1`, and a smaller backup account for if you exhaust your resources, `stats_dept2`.
- A greatlakes cluster login account. If you have not yet filled in the form at <https://arc-ts.umich.edu/greatlakes/user-guide/> then do so.
- A umich internet address. Use the umich VPN if you are not on campus.

Connecting to greatlakes with macOS or Linux

- 1 Open a Terminal window (recall that, on a Mac, this can be done using Control-Spacebar and typing Terminal) and type

```
ssh username@greatlakes.arc-ts.umich.edu
```

where `username` is your username.

- 2 Login with your Kerberos level-1 password, and Duo two-factor authentication.

This creates a remote terminal shell on greatlakes.

Connecting to greatlakes with Windows

This is essentially the same as for macOS, except you may need to install a program that provides a terminal window.

- 1 Follow instructions to install PuTTY at <https://documentation.its.umich.edu/node/350>
- 2 Launch PuTTY and enter `greatlakes.arc-ts.umich.edu` as the host name, then click open. If you receive a “PuTTY Security Alert” pop-up, this is completely normal, click the “Yes” option. This will tell PuTTY to trust the host the next time you want to connect to it. From there, a terminal window will open; you will be required to enter your UMich unqname and then your Kerberos level-1 password in order to log in. Please note that as you type your password, nothing you type will appear on the screen; this is completely normal. Press “Enter/Return” key once you are done typing your password.
- 3 Complete the request for Duo two-factor authentication.

This creates a remote terminal shell on greatlakes.

Moving files on and off greatlakes: scp

On Mac or Linux, you can use `scp` which has similar syntax to `cp`. To copy `myfile` on your laptop to a subdirectory `mydir` of your home directory on greatlakes:

```
scp myfile uniqlname@greatlakes-xfer.arc-ts.umich.edu:mydir
```

To copy an entire directory, use the `-r` flag for recursive copy:

```
scp -r mydir uniqlname@greatlakes-xfer.arc-ts.umich.edu:
```

These commands can also be reversed to copy files from greatlakes to your machine. The following copies `mydir` back to the current working directory:

```
scp -r uniqlname@greatlakes-xfer.arc-ts.umich.edu:mydir .
```

You will need to authenticate via Duo to complete the file transfer. On Mac or Windows, [FileZilla](#) provides a file system user interface.

Cluster batch workflow

- 1 You create a batch script and submit it as a job
- 2 Your job is scheduled, and it enters the queue
- 3 When its turn arrives, your job will execute the batch script
- 4 Your script has access to all applications and data
- 5 When your script completes, anything it sent to standard output and error are saved in files stored in your submission directory
- 6 You can ask that email be sent to you when your jobs starts, ends, or fails
- 7 You can check on the status of your job at any time, or delete it if it's not doing what you want
- 8 A short time after your job completes, it disappears

Useful batch commands

Submit a job

```
sbatch sample.sbat
```

Query job status

```
squeue -j jobid  
squeue -u unickname
```

Delete a job

```
scancel jobid
```

Check a job script and estimate its start time

```
sbatch --test-only sample.sbat
```


More Slurm commands to try

```
sacct -u user
```

show recent job history

```
seff jobid
```

show cpu utilization for jobid

R modules on greatlakes

Software on greatlakes is packaged in modules which must be loaded

```
module load R
```

Other versions of R are available:

```
module avail R
```

We see that R4.2.0 is currently the default. For simple multicore computing, sending jobs to multiple cores on a single node, the default R module is appropriate. Other versions of R have been built and tested in other parallel environments, for example the `Rmpi` module runs R with `mpi`. R packages can be installed using `install.packages` within R, run at a terminal on the login node. Your home directory files (and therefore these packages) are accessible on all nodes of the cluster.

Set up test for foreach

- The `gl` subdirectory of the 810f23 git repository has a file `test.sbat` which submits a batch job running the parallel `foreach` test in `test.R`.
- A basic Linux exercise is to set up a directory on greatlakes with these files, at which point you can run

```
sbatch test.sbat
```

to submit the job.

- You can transfer the files from your laptop via `scp`, or by copy-paste, but it may be simplest to clone the class git repository into your greatlakes account,

```
git clone https://github.com/ionides/810f23.git
```

Editing text files on greatlakes

- Inspect the text file `test.sbat`, for example by

```
more test.sbat
```

Is it fairly self-explanatory?

- One thing that needs changing is to set your email address for alerts about jobs beginning and ending.
- To make these edits on greatlakes, you need a text editor.
- It is convenient to use a text editor that runs in a terminal. Options include

```
vi test.sbat  
emacs -nw test.sbat  
nano test.sbat
```

- It is useful to have some familiarity with each of these editors.

Comparing results

- You are now ready to run a batch job

```
sbatch test.sbat
```

- From inspecting the code in `test.R`, we see that the results are saved in `test.csv`
- Compare the run times with the results from running this code on your laptop, as done in homework 11.
- Also, try running the code in `test2.R` by

```
sbatch test2.sbat
```

What do you learn from comparing the outputs in `test2.csv` with `test.csv` on greatlakes and your laptop?

Other ways to run R on greatlakes

- It is sometimes useful to start an interactive session on greatlakes, particularly for debugging. This is done from the terminal as follows:

```
module load R
srun --nodes=1 --account=stats_dept1 --ntasks-per-node=8 \
  --pty /bin/bash
```

- You can then run R in the terminal by typing

```
R
```

- This R session will have access to the cores you have requested.
- Here, we require `nodes=1` unless we use `Rmpi` since `library(doParallel)` alone cannot work with cores across different machines.
- You can also run [web-based Rstudio](#). However, your task here is to run batch jobs, which remain the basic tool for intensive statistical computing.

Acknowledgments

- This lesson is prepared for STATS 810, Fall 2023.
- It builds on previous versions of STATS 810, the [Great Lakes User Guide](#) and [notes by Charles Antonelli and John Thiels](#).
- Compiled on November 27, 2023.