CSAFE Computing Resources

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Chapter 1

Introduction

This book gives the reader step-by-step instructions for accessing and using several CSAFE computing resources. CSAFE has access to

- 1. Large Scale Storage (LSS)
- 2. CSAFE Rstudio Servers
- 3. The Pronto Job Scheduler

1.1 Large Scale Storage (LSS)

ResearchIT at Iowa State University provides Large Scale Storage (LSS) at low cost to research labs. CSAFE has purchased more than 30 terabytes of space on LSS. As of 2022-06-10 the following CSAFE project folders are on LSS:

- csafe-admin-vid
- csafe-firearms
- csafe-handwriting
- csafe-handwriting-irb
- \bullet csafe-mentisdb
- csafe-mobile
- csafe-shoeprints
- csafe-stego
- csafe-transcripts
- csafe-wvmediaimp

Chapter 3 explains how to connect to LSS.

1.2 CSAFE RStudio Servers

CSAFE has access to two RStudio Servers. To the user, the experience is almost exactly the same as using RStudio on a personal computer. The main benefit of running RStudio on the server is that the server has more RAM and more cores than most personal computers.

Chapter 4 explains how to use the Rstudio servers.

1.3 The Pronto Job Scheduler

ResearchIT at ISU manages a whole host of high performance servers to which CSAFE has purchased access. Instead of accessing one of these servers individually, users submit their jobs (scripts) to the Pronto Job Scheduler which assigns the jobs to the most appropriate servers.

Chapter 5 explains how to run R scripts on the Pronto Job Scheduler. Python, MATLAB, and other programming languages can be run on Pronto, but this book only covers R.

1.4 Do I use the CSAFE Rstudio Server or Pronto?

When deciding whether to use an RStudio server or Pronto, you might want to consider the following benefits and drawbacks of each.

RStudio Server

- \bullet benefits
 - It runs the RStudio graphical user interface so the user experience is quite similar to working in Rstudio on a personal computer.
- drawbacks
 - Each server has less than 20 cores
 - It is a shared user machine which means that if a lot of people are using the server, your jobs might run slower.

Pronto

- benefits
 - It has dozens of servers with hundreds of cores each

- It manages the resources for users so you don't have to worry about slowing down other peoples jobs

\bullet drawbacks

- It doesn't have a graphical user interface so users interact with Pronto through the command line
- Users submit their jobs to Pronto using something called a SLURM script, which is quite a different workflow compared running scripts in Rstudio

Chapter 2

Getting Started

If you are working from off campus you need to use ISU's virtual private network (VPN) to connect to any of the computing resources covered in this guide. You also need to set up SSH keys. Section ??(off-campus) explains how to install and use the ISU VPN and SSH keys. If you will only be working on campus, you may skip this section.

This chapter also includes a Quick Start Guide (Section ??(quick-start)) for people who are already comfortable with virtual private networks and command line prompts.

The last section in this chapter explains how people are granted access to the computing resources covered in this guide.

2.1 Quick Start Guide

2.1.1 Connect to Large Scale Storage

- 1. If you are an undergraduate student, use your CSAFE email net-id and password in the following steps.
- 2. If you are off campus, download the ISU virtual private from https://vpn. iastate.edu and log-in using your ISU net-id and password.
- 3. On Windows open File Explorer and in the top textbox type
 - \\las.iastate.edu\research if you are on campus or
 - \\las-dfs-01.las.iastate.edu\lss if you are off campus.
- 4. On Mac click Go > Connect to Server and type
 - smb://iastate/lss/research if you are on campus or
 - smb://las-dfs-01.las.iastate.edu if you are off campus.

- 5. Enter your net-id and password.
- 6. Open the research folder and go to your CSAFE project folder.

2.1.2 Connect to CSAFE Rstudio Server

- 1. If you are an undergraduate student, use your CSAFE email net-id and password in the following steps.
- 2. If you are off campus, download the ISU virtual private from https://vpn. iastate.edu and log-in using your ISU net-id and password.
- 3. Go to the website https://reiss.csafe.iastate.edu/ or https://locard.csafe.iastate.edu/.
- 4. Enter your net-id and password.

2.1.3 Connect to the Pronto Job Scheduler

- 1. If you are an undergraduate student, use your CSAFE email net-id and password in the following steps.
- 2. If you are off campus, download the ISU virtual private from https://vpn. iastate.edu and log-in using your ISU net-id and password.
- 3. On Windows open the PowerShell. On Mac open the Terminal.
- 4. Type ssh your-netid@pronto.las.iastate.edu
- 5. Enter your net-id and password.

2.2 Working Off Campus

If you are on campus, you may skip this section. If you are off campus, you will need to

- 1. Download and sign in to a virtual private network (see 2.2.1)
- 2. Generate SSH keys (see 2.2.2)

2.2.1 Install the ISU Virtual Private Network (VPN)

Iowa State University uses Cisco AnyConnect as their virtual private network (VPN) software. You will need to install it on your computer.

- 1. Go to https://vpn.iastate.edu
- 2. Select Primary as the GROUP and click Login



3. Sign in with your ISU net-id and password

IOWA ST	ATE UNIVERSITY
	Sign In
Username	
Password	
Remember me	
Rememberine	Sign In

4. The site should detect your computer's operating system and give you the option to download the VPN for your operating system.



- 5. Click Download ### Sign In to the ISU VPN {#signin-vpn}
- 6. Open Cisco AnyConnect
- 7. Type vpn.iastate.edu and click Connect



8. Sign in with your ISU net-id and password



2.2.2 Generate SSH keys

ResearchIT gives instructions for setting up SSH keys at https://researchit.las.iastate.edu/how-generate-ssh-keys. Setting up my SSH keys took lots of trial and error. If you run into problems or get stuck, email researchit@iastate.edu.

Chapter 3

Large Scale Storage (LSS)

The Large Scale Storage (LSS) is a research file storage service at ISU. CSAFE has purchased storage space on LSS for a handful of CSAFE projects, such as firearms and handwriting, to store project data.

 *** Add discussion of folder privileges and their impact on storing IRB data on the server

Windows

- 1. If you are **off campus**, log-in to the ISU VPN
- 2. Open file explorer
- 3. If you are **off campus** type \\las-dfs-01.las.iastate.edu\lss in the top textbox. If you are **on campus** you only need to type \\las.iastate.edu\lss
- 4. Enter your ISU net-id and password
- 5. Open the research folder
- 6. Open folder for your CSAFE project

Mac

- 1. If you are off campus, log-in to the ISU VPN
- 2. Select Go > Connect to Server



- 3. If you are **off campus** type smb://las-dfs-01.las.iastate.edu in the text box. If you are **on campus** type smb://las.iastate.edu Click the + sign if you would like your computer to remember the server
- 4. Click Connect
- 5. Enter your net-id and password
- 6. Open the LSS folder
- 7. Open the research folder
- 8. Open folder for your CSAFE project

Chapter 4

The CSAFE RStudio Servers

CSAFE has two RStudio Servers that are operated by CSSM:

- 1. https://reiss.csafe.iastate.edu/
- 2. https://locard.csafe.iastate.edu/

4.1 Connect to an RStudio Server

- 1. If you are off campus, connect to the ISU \overline{VPN}
- 2. Go to the website https://reiss.csafe.iastate.edu/ or https://locard.csafe.iastate.edu/
- 3. Log in with your ISU net-id and password. If you are an undergraduate student, use your CSAFE net-id.

4.2 Working with Directories and File Paths

^{***} Email cssm_it@iastate.edu for help

^{***} Explain how to change your working directory to one of the CSAFE project folders on the server *** Explain how file paths need to be formatted for files in one of the CSAFE projects on the server

4.3 Trouble Shooting

*** Explain: try clearing cookies if you are unable to log-in

Chapter 5

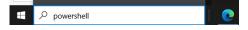
Pronto

5.1 Connecting to the Pronto job scheduler

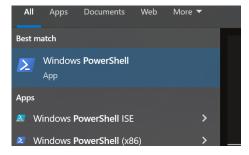
You connect to the pronto job scheduler through the PowerShell on Windows or the Terminal on Mac.

Windows

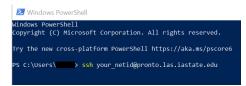
1. Type powershell in the Windows Search Bar next to the Start Menu



2. Click Windows PowerShell in the list to open the PowerShell



3. Type ssh your_netid@pronto.las.iastate.edu



- 4. Type your net-id password
- 5. You should now see

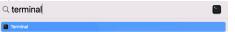
```
[your_netid@pronto ~]$
```

Mac

1. Do a spotlight search by clicking on the magnifying glass in the upper right corner of the screen



2. Type terminal and click Terminal in the list



4. Type your net-id password

5.2 Connecting to the Pronto data transfer node

You need to transfer your data to Pronto using the Pronto data transfer node (ProntoDTN). CSAFE has a folder for CSAFE users on ProntoDTN. The file path is prontodtn.las.iastate.edu > work > LAS > csafe-lab. Create a folder for yourself in the csafe-lab folder. Most users use their net-id as the folder name, but I think you can name it anything you want.

The work directory is not backed-up so don't use this folder for long term storage.

Each user also has a home folder. These folders have limited storage so researchIT recommends only placing small files in the home folder. I find it easier to store everything in my work folder and not use my home folder at all.

Windows

- 1. Open file explorer
- 2. Type \\prontodtn.las.iastate.edu in the top textbox



3. Open the work folder

- 4. Open the LAS folder
- 5. Open the csafe-lab folder
- 6. Create a new folder with your net-id as the name

Mac



2. Type smb://prontodtn.las.iastate.edu in the text box. Click the + sign if you would like your computer to remember the server.



- 3. Click Connect
- 4. Enter your net-id and password
- 5. Select Work and click OK.
- 6. Open the LAS folder
- 7. Open the csafe-lab folder
- 8. Create a new folder with your net-id as the name

5.2.1Transfering data from ProntoDTN to LSS

5.2.2 Transfering large amounts of data using Globus

If you have large amounts of data to transfer, researchIT recommends that you use Globus Connect Personal. Go to https://researchit.las.iastate.edu/how-transfer-files-pronto-globus to download Globus.

Instructions for transferring data with Globus are here: https://docs.globus.org/how-to/get-started/.

5.3 Running an R script on Pronto

There are two ways to run a script on Pronto:

- 1. in an interactive session
- 2. as a batch job

If I understand correctly, an interactive session is intended for troubleshooting your code. ResearchIT says, "Once you've got your program running in an interactive session please switch to an sbatch script if possible." [https://researchit.las.iastate.edu/pronto?msclkid=3263c889c17811ec81e13068586d8872]

Pronto uses the Simple Linux Utility for Resource Management (Slurm) to allocate resources (computer nodes and clusters) to users [https://en.wikipedia.org/wiki/Slurm_Workload_Manager]. In order to run your script as a batch job, you need to write a Slurm file that includes information about your job and the resources your would like to request.

5.4 Interactive Sessions

5.4.1 Example: Start an interactive session

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. In the Pronto terminal, type

```
$ srun --nodes 1 --tasks 4 --partition interactive --time 01:00:00 --pty bash
```

This starts an interactive session.

4. Load the module for R version 4.0.4. This version of R requires that a specific version of gcc be loaded first.

```
$ module load gcc/10.2.0-zuvaafu
$ module load r/4.0.4-py3-4khjixy
```

5. Tell Pronto to install R packages in your csafe-lab work folder. (This is considered the best practice by ResearchIT https://researchit.las.iastate.edu/how-run-r-pronto?msclkid=865a487bc65e11ecbfd7e59a7ab1dc47.)

```
$ export R_LIBS_USER=/work/LAS/your-lab/yournetid/Rlibs
$ mkdir -p $R_LIBS_USER
```

6. Start the R interpreter

```
$ R
```

5.4.2 Example: Install a package from CRAN

1. Start an interactive R session (see 5.4.1)

```
2. > install.packages("dplyr",lib="/work/LAS/csafe-lab/your_netid/Rlibs", repos="https://mirror
```

5.4.3 Example: Install a package from Github

Occasionally, you might want to install a package that isn't available on CRAN but is available on GitHub. This example shows how to do that on Pronto.

- 1. Start an interactive R session (see 5.4.1)
- 2. If you haven't already, you need to install the devtools package

```
> install.packages("devtools",lib="/work/LAS/csafe-lab/your_netid/Rlibs", repos="https://mir
```

- 3. Every GitHub repository url has the format https://github.com/GithubUsernam/GithubRepo. Use the GithubUsername/GithubRepo in the install_github function.
 - > devtools::install_github("GithubUsername/GithubRepo")

5.5 Batch Jobs

5.5.1 Example: A basic R script

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work >
 LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

```
a = 5
print(a)
```

Save the script as basic.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node
#SBATCH --crpus-per-task=1 # ask for 1 cpu
#SBATCH --mem=1G # asks for 1 GB of RAM

#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2

# everything below this line is optional
#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console out
#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message
module load r
cd /work/LAS/csafe-lab/your_netid
R --save < basic.R</pre>
```

Save the file as basic.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix basic.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

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```
$ sbatch /work/LAS/csafe-lab/your_netid/basic.txt
```

This will add your job to the queue. The script is so short, your job will probably run immediately.

9. Two new files - job_<job#>_err.txt and job_<job#>_out.txt - should appear in your csafe-lab work folder. If basic.R ran successfully, the job_<job#>_out file should contain

```
> a = 5
> print(a)
[1] 5
>
```

and job_<job#>_err.txt should be blank. If the error file isn't blank, troubleshoot the error(s). If you get stuck, email researchit@iastate.edu.

5.5.2 Example: Save a dataframe to a CSV file

In this example, I will show you how to save a dataframe to a csv file.

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work > LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

```
# draw 10 samples from normal distribution
data = rnorm(10)

# put in a dataframe
df = data.frame(x=data)

# save dataframe
write.csv(df, "data.csv")
```

Save the script as dataframe.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node

#SBATCH --cpus-per-task=1 # ask for 1 cpu

#SBATCH --mem=1G # asks for 1 GB of RAM

#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2

# everything below this line is optional

#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console ow

#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message

module load r

cd /work/LAS/csafe-lab/your_netid

R --save < dataframe.R
```

Save the file as dataframe.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix dataframe.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/dataframe.txt
```

This will add your job to the queue. The script is so short, your job will probably run immediately.

9. The dataframe should be saved in a file data.csv in your csafe-lab work folder. There should be two other new files — data.csv, job_<job#>_err.txt and job_<job#>_out.txt — in your csafe-lab work folder as well. If the error file isn't blank, troubleshoot the error(s). If you get stuck, email researchit@iastate.edu.

5.5.3 Example: Load data from a CSV file

In this example, we will load the csv file data.csv that we saved in Example 5.5.2.

1. If you are off campus, connect to the ISU VPN (see ??)

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- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work > LAS > csafe-lab > your_netid (see 5.2)
- 4. Double-check that the file data.csv is still in your csafe-lab work folder. If you deleted it, follow the steps in example 5.5.2 to recreate it.
- 5. Create a new R script with the following lines of code:

```
df = read.csv("data.csv")
head(df)
```

Save the script as load.R and copy it to you csafe-lab work folder.

6. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node
#SBATCH --cpus-per-task=1 # ask for 1 cpu
#SBATCH --mem=1G # asks for 1 GB of RAM
#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2 seconds.

# everything below this line is optional
#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console output
#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error messages

module load r
cd /work/LAS/csafe-lab/your_netid
R --save < load.R</pre>
```

Save the file as load.txt.

- 7. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix load.txt to change the line breaks to UNIX format.
- 8. Copy the text file to your csafe-lab work folder.
- 9. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/load.txt
```

This will add your job to the queue. The script is so short, your job will probably run immediately.

10. Open the file job_<job#>_out.txt in your csafe-lab work folder and make sure that the first six lines of the dataframe were printed.

5.5.4 Example: Install R packages

Just like in Rstudio on your local machine, you will need to install any R packages that you want use. In this example, we will install futile.logger, doParallel, doRNG, and tidyverse so that we can use these packages in future examples.

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work >
 LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

The line starting with lib= tells Pronto to install the R packages in your csafe-lab work folder. The line starting with repos= tells Pronto which CRAN mirror to use. ResearchIT says that these two lines should always be used [https://researchit.las.iastate.edu/how-run-r-pronto]. Save the script as install_packages.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node

#SBATCH --crus-per-task=1 # ask for 1 cpu

#SBATCH --mem=1G # asks for 1 GB of RAM

#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2

# everything below this line is optional

#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console out

#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message
```

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```
export R_LIBS_USER=/work/LAS/csafe-lab/your_netid/Rlibs
mkdir -p $R_LIBS_USER

module load r
cd /work/LAS/csafe-lab/your_netid
R --save < install_packages.R</pre>
```

Save the file as install_packages.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix install_packages.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/install_packages.txt
```

This will add your job to the queue. Just like on your local machine, it might take several minutes to install the packages.

9. There should be two other new files - data.csv, job_<job#>_err.txt and job_<job#>_out.txt - in your csafe-lab work folder.

5.5.5 Example: Run code in parallel

The main benefit of Pronto is that it can run code in parallel. In this example, I will show you how to run a for loop in parallel using the doParallel library. R has other packages for parallel computing, but ResearchIT uses doParallel in their how-to [https://researchit.las.iastate.edu/how-run-r-pronto] so that's what I will use here.

If you completed Example 5.5.4 the doParallel package will already be installed. If you need to install the doParallel package see Examples 5.4.2 or 5.5.4 for instructions.

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work > LAS > csafe-lab > your_netid (see 5.2)

4. Create a new R script with the following lines of code:

```
library(doParallel)

nCores = as.integer(Sys.getenv("SLURM_CPUS_PER_TASK"))
myCluster = parallel::makeCluster(nCores)
doParallel::registerDoParallel(myCluster)

results = foreach(i=1:10) %dopar% {
   rnorm(1000)}
saveRDS(results, "parallel_results.rds")
```

Save the script as parallel.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node
#SBATCH --cpus-per-task=10 # ask for 10 cpu
#SBATCH --mem=1G # asks for 1 GB of RAM
#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2
# everything below this line is optional
#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console ow
#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message
export R_LIBS_USER=/work/LAS/csafe-lab/your_netid/Rlibs
module load r
cd /work/LAS/csafe-lab/your_netid
R --save < parallel.R</pre>
```

Save the file as parallel.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix parallel.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/parallel.txt
```

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9. The results of the parallel loop should be saved in parallel.txt in your csafe-lab work folder.

5.5.6 Example: Set the seed for the random number generator

If you run Example 5.5.5 multiple times, the numbers sampled from the normal distribution will likely be different each time. If you want to make the sample reproducible (produce the same sample each time), set the seed for the random number generator. The most common way to set a seed is with the set.seed() function. This function does not work with "dopar" from the doParallel package, but it does work with "dorng".

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work >
 LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

```
library(doParallel)
library(doRNG)

nCores = as.integer(Sys.getenv("SLURM_CPUS_PER_TASK"))
myCluster = parallel::makeCluster(nCores)
doParallel::registerDoParallel(myCluster)

starting_seed = 300

set.seed(starting_seed)
r1 = foreach(i=1:4) %dorng%{ runif(1) }

set.seed(starting_seed)
r2 = foreach(i=1:4) %dorng%{ runif(1) }
identical(r1, r2)
```

Save the script as seed.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node

#SBATCH --cpus-per-task=10 # ask for 10 cpu

#SBATCH --mem=1G # asks for 1 GB of RAM

#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2

# everything below this line is optional

#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console ou #SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message

export R_LIBS_USER=/work/LAS/csafe-lab/your_netid/Rlibs

module load r

cd /work/LAS/csafe-lab/your_netid
```

Save the file as seed.txt.

R --save < seed.R

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix seed.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/seed.txt
```

9. Open the job_<job#>_out.txt file to make sure that the result of identical(r1, r2) is TRUE.

5.5.7 Example: Use functions from dplyr and magrittr in parallel

The previous parallel examples used the base R functions rnorm and runif. If we want to use functions from packages that we install, we need to pass the package names to the %dorng% operator. We will learn how to do this in this example.

If you haven't already installed the tidyverse package, follow the steps in Example 4 to install the tidyverse or install dplyr and magrittr separately.

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- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work > LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

```
library(doParallel)
library(doRNG)
library(magrittr)
library(dplyr)
nCores = as.integer(Sys.getenv("SLURM_CPUS_PER_TASK"))
myCluster = parallel::makeCluster(nCores)
doParallel::registerDoParallel(myCluster)
set.seed(100)
r1 = foreach(i=1:10, .packages=c("dplyr", "magrittr")) %dorng%{
 cluster_centers = df %>% slice_sample(n=40)
set.seed(100)
r2 = foreach(i=1:10, .packages=c("dplyr", "magrittr")) %dorng%{
  cluster_centers = df %>% slice_sample(n=40)
set.seed(200)
r3 = foreach(i=1:10, .packages=c("dplyr", "magrittr")) %dorng%{
 cluster_centers = df %>% slice_sample(n=40)
}
identical(r1, r2)
identical(r1, r3)
```

Save the script as magrittr.R. Copy the script to your csafe-lab work folder

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node

#SBATCH --cpus-per-task=10 # ask for 10 cpu

#SBATCH --mem=1G # asks for 1 GB of RAM

#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2 seconds.
```

```
# everything below this line is optional
#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console ou
#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message
export R_LIBS_USER=/work/LAS/csafe-lab/your_netid/Rlibs

module load r
cd /work/LAS/csafe-lab/your_netid
R --save < magrittr.R</pre>
```

Save the file as magrittr.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix magrittr.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/magrittr.txt
```

9. Open the job_<job#>_out.txt file to make sure that the result of identical(r1, r2) is TRUE and identical(r1, r3) is FALSE.

5.5.8 Example: Use a user-defined function to save results inside a parallel loop

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work >
 LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

```
library(doParallel)
library(doRNG)
source("parallel_save.R")

nCores = as.integer(Sys.getenv("SLURM_CPUS_PER_TASK"))
```

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```
myCluster = parallel::makeCluster(nCores)
doParallel::registerDoParallel(myCluster)

starting_seed = 300

set.seed(starting_seed)
r1 = foreach(i=1:10) %dorng% {
    save_sample(n=10000, filename=paste0("sample_",i,".rds"))
}
```

Save the script as run_parallel_save.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node
#SBATCH --cpus-per-task=10
#SBATCH --mem=2G
#SBATCH --time=00:15:00

# everything below this line is optional
#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console output
#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error messages

export R_LIBS_USER=/work/LAS/csafe-lab/your_netid/Rlibs

module load r
cd /work/LAS/csafe-lab/your_netid
R --save < run_parallel_save.R</pre>
```

Save the file as parallel_save.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix parallel_save.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/parallel_save.txt
```

9. There should be ten rds files names sample_1.rds, sample_2.rds, etc. in your csafe-lab folder.

5.5.9 Example: Create a log file

In this example we will create a simple log file using the futile.logger package.

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Open your csafe-lab work folder prontodtn.las.iastate.edu > work >
 LAS > csafe-lab > your_netid (see 5.2)
- 4. Create a new R script with the following lines of code:

```
library(futile.logger)
futile.logger::flog.appender(appender.file("log_file.txt"), name='log')
futile.logger::flog.info("start script...", name='log')
a = 5
futile.logger::flog.info("variable a = %d", a, name='log')
```

Save the script as log.R. Copy the script to your csafe-lab work folder.

5. Create a text file for Slurm with the following text:

```
#!/bin/bash

#SBATCH --nodes=1 # request one node

#SBATCH --cpus-per-task=10 # ask for 10 cpu

#SBATCH --mem=1G # asks for 1 GB of RAM

#SBATCH --time=00:30:02 # ask that the job be allowed to run for 30 minutes and 2

# everything below this line is optional

#SBATCH --output=/work/LAS/csafe-lab/your_netid/job_%J_out.txt # store console ow

#SBATCH --error=/work/LAS/csafe-lab/your_netid/job_%J_err.txt # store error message

export R_LIBS_USER=/work/LAS/csafe-lab/your_netid/Rlibs

module load r

cd /work/LAS/csafe-lab/your_netid

R --save < log.R
```

Save the file as log.txt.

- 6. (Windows Only) If you are using Windows, your text file will likely have DOS line breaks instead of UNIX line breaks which will cause an error when the file is run on Pronto. Open Terminal in RStudio, use cd folder/containing/text_file to change directories to the folder containing your text file, and type dos2unix log.txt to change the line breaks to UNIX format.
- 7. Copy the text file to your csafe-lab work folder.
- 8. In the command line prompt where you are connected to Pronto, type

```
$ sbatch /work/LAS/csafe-lab/your_netid/log.txt
```

9. A log file called <code>log_file.txt</code> should appear in your csafe-lab work folder. The contents of the log should look like

```
INFO [2022-05-04 10:42:37] start script...
INFO [2022-05-04 10:42:37] variable a = 5
```

5.6 Pronto Commands

5.6.1 List loaded modules

1. In an interactive session, type

```
$ module list
```

5.6.2 Purge all loaded modules

1. In an interactive session, type

```
$ module purge
```

5.6.3 View your job(s) in the Pronto queue

1. In pronto terminal (not in an interactive session), type

```
$ squeue -u your-netid
```

5.6.4 Cancel a job

1. In pronto terminal (not in an interactive session), type

```
$ scancel jobid
```

where jobid is the six-digit number for the job you want to cancel.

5.7 Install the handwriter package

CSAFE created an R package for statistical handwriting analysis called handwriter. The handwriter package requires a number of other R packages, some of which caused errors when I tried to install handwriter in an interactive session on Pronto following the instructions in 5.4.2. ResearchIT helped me figure out how to install the problem packages and ultimately install handwriter. This section records the step-by-step details of how I was able to install handwriter. My hope is that you will also be able to successfully install handwriter if you follow these steps. If you run into problems, email researchit@iastate.edu.

- 1. If you are off campus, connect to the ISU VPN (see ??)
- 2. Sign-in to Pronto (see 5).
- 3. Some of the packages used by handwriter are only available on Pronto for R 4.0.4. Start the R 4.0.4 interpreter in an interactive session on Pronto.

```
$ srun --nodes 1 --tasks 4 --partition interactive --time 01:00:00 --pty bash
$ module purge
$ module load gcc/10.2.0-zuvaafu
$ module load r/4.0.4-py3-4khjixy
$ R
```

4. Try to install the handwriter package

```
> install.packages("handwriter",lib="/work/LAS/csafe-lab/your_netid/Rlibs", repos
```

I received error messages stating that the packages igraph, randomForest, and magick could not be installed. I had to install these packages separately.

5. Install igraph

```
> install.packages("igraph",lib="/work/LAS/csafe-lab/your_netid/Rlibs", repos="https://mirro
```

- 6. Then randomForest
 - > install.packages("https://cran.r-project.org/src/contrib/Archive/randomForest/randomForest
- 7. Install magick

```
> install.packages("magick",
configure.vars=c("INCLUDE_DIR='. -D_GLIBCXX_USE_CXX11_ABI=0 -fopenmp -DMAGICKCORE_HDRI_ENABL
lib="/work/LAS/csafe-lab/your_netid/Rlibs",
repos="https://mirror.las.iastate.edu/CRAN")
```

5.8 Trouble-Shooting

5.8.1 Line breaks error

If you are using Windows and you try to run a text file created on Windows on Pronto, you will likely get the following error:

```
sbatch: error: Batch script contains DOS line breaks (\\r\\n) sbatch: error: instead of expected UNIX line breaks (\\n).
```

One way to fix the problem is to - Open Rstudio - Go to Tools > Terminal > New Terminal - Changes the directory to the folder containing basic.txt by typing 'cd /documents/my/folder' without the quotes and hitting enter. - Type 'dos2unix basic.txt' without the quotes and hit enter.