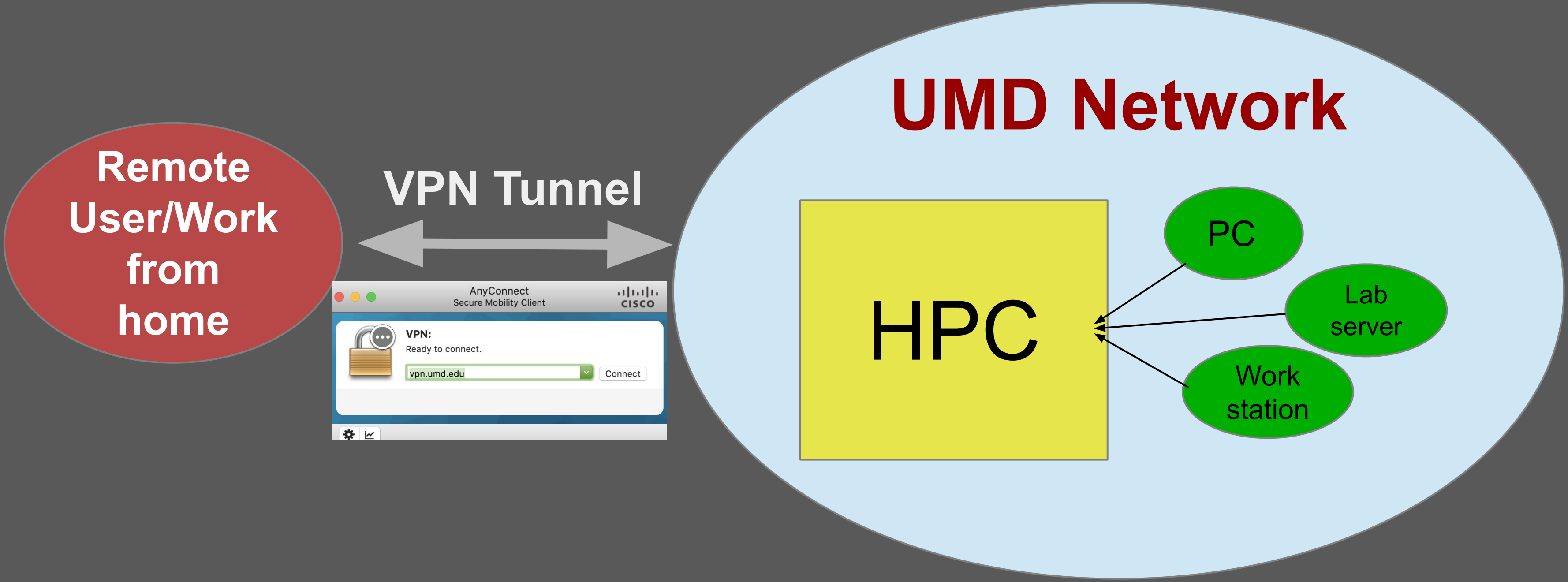
```
DingoMach:~ junaid$
```

Getting Started: Shelling into a server & copying files

Outline

- Access UMD network from home
- Launching the terminal/command prompt
- Connecting to your HPC
- Copying files to/from HPC
- Introducing SLURM job scheduling software

Accessing your HPC: get on UMD Network through VPN



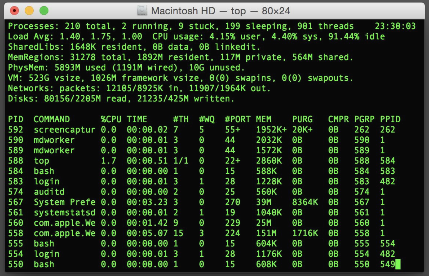
Accessing UMD Network

Virtual Private Network (VPN) allows you to work from off campus

- Secure connection from your computer at home to UMD network, with all the access you would expect from actually being on-site!

https://terpware.umd.edu/Windows/title/1840

https://it.umd.edu/spotlight/connections/what-vpn



```
Processes: 210 total, 2 running, 9 stuck, 199 sleeping, 901 threads    23:30:03
Load Avg: 1.40, 1.75, 1.00  CPU usage: 4.15% user, 4.40% sys, 91.44% idle
SharedLibs: 1648K resident, 0B data, 0B linkedit.
MemRegions: 31278 total, 1892M resident, 117M private, 564M shared.
PhysMem: 5893M used (1191M wired), 10G unused.
VM: 523G vsize, 1026M framework vsize, 0(0) swapins, 0(0) swapouts.
Networks: packets: 12105/8925K in, 11907/1964K out.
Disks: 80156/2205M read, 21235/425M written.

PID  COMMAND      %CPU TIME     #TH  #WQ  #PORT MEM    PURG   CMPR PGRP PPID
592  screencaptur 0.0  00:00.02 7    5    55+   1952K+ 20K+   0B   262  262
590  mdworker     0.0  00:00.01 3    0    44    2032K  0B     0B   590  1
589  mdworker     0.0  00:00.01 3    0    44    1572K  0B     0B   589  1
588  top          1.7  00:00.51 1/1  0    22+   2860K  0B     0B   588  584
584  bash         0.0  00:00.00 1    0    15    588K   0B     0B   584  583
583  login        0.0  00:00.01 3    1    28    1228K  0B     0B   583  482
574  auditd       0.0  00:00.00 2    0    25    560K   0B     0B   574  1
567  System Prefe 0.0  00:03.23 3    0    270   39M    8364K  0B   567  1
561  systemstatsd 0.0  00:00.01 2    1    19    1040K  0B     0B   561  1
560  com.apple.We 0.0  00:01.42 9    0    229   25M    0B     0B   560  1
558  com.apple.We 0.0  00:05.07 15   3    224   151M   1716K  0B   558  1
555  bash         0.0  00:00.00 1    0    15    604K   0B     0B   555  554
554  login        0.0  00:00.01 3    1    28    1176K  0B     0B   554  482
550  bash         0.0  00:00.00 1    0    15    608K   0B     0B   550  549
```

Accessing your HPC: Using the terminal

Terminal AKA Command line is a non-graphical interface to use your computer

- Mac has Terminal pre-installed in Utilities folder in Applications
- Windows has Command Prompt or CMD, but requires some set up to connect to HPC
  - Can use PowerShell or 3rd party App MobaXterm
  - https://mobaxterm.mobatek.net/
- Linux has Terminal pre-installed

Getting started: connecting to your server

Once you have an account, you can connect to your HPC or “shell in” through the terminal using the following syntax:

```
ssh <user name>@<server address>
```

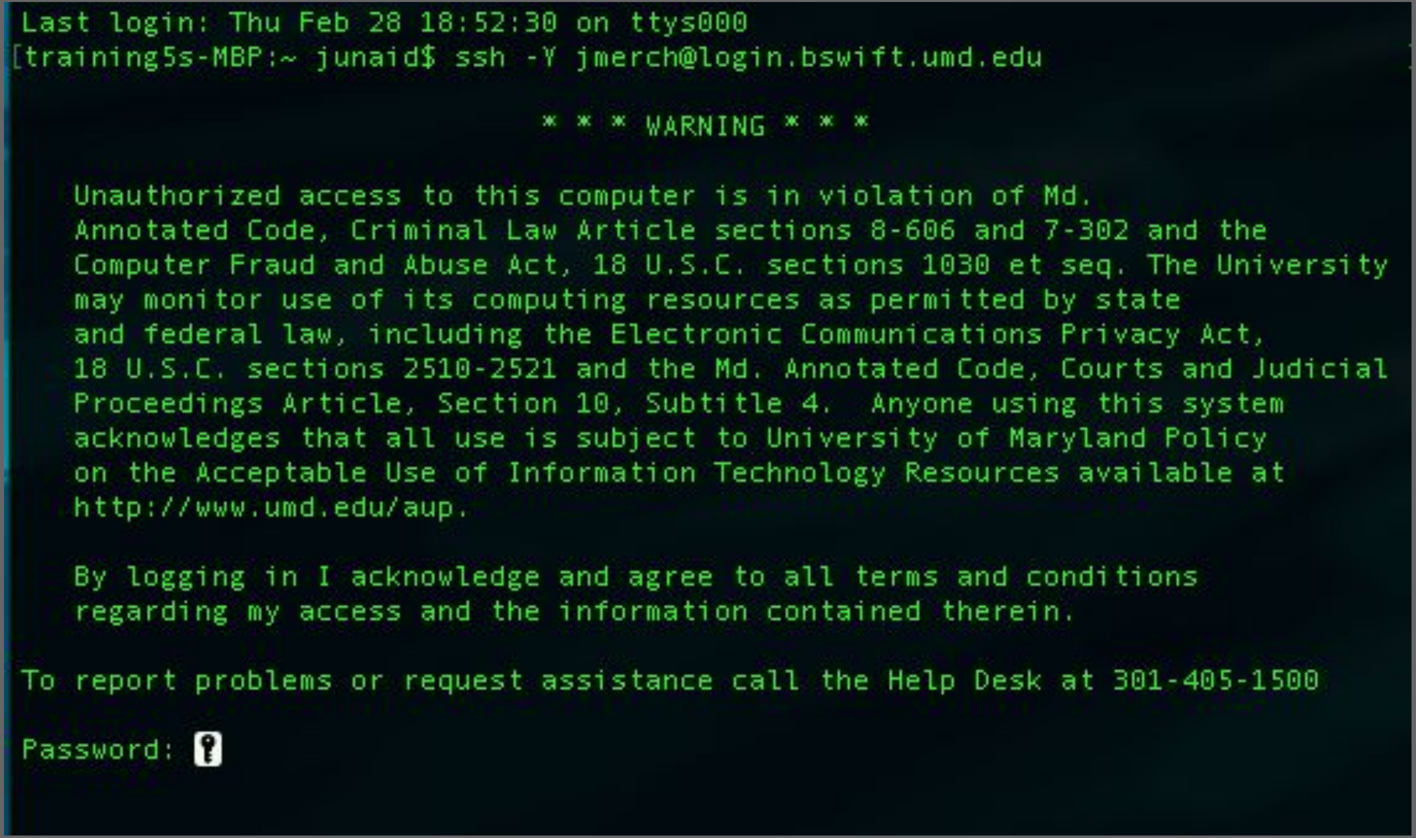
```
ssh jmerch@login.bswift.umd.edu
```

Enter your password when prompted (you won’t see the cursor move!!)

Now you’re on the head node of the HPC, where you can run basic commands, explore the directory structure, and submit jobs

<u>Do NOT run big jobs on the head node</u>

Getting started: connecting to your server



```
Last login: Thu Feb 28 18:52:30 on ttys000
[training5s-MBP:~ junaid$ ssh -Y jmerch@login.bswift.umd.edu

                              * * * WARNING * * *

   Unauthorized access to this computer is in violation of Md.
   Annotated Code, Criminal Law Article sections 8-606 and 7-302 and the
   Computer Fraud and Abuse Act, 18 U.S.C. sections 1030 et seq. The University
   may monitor use of its computing resources as permitted by state
   and federal law, including the Electronic Communications Privacy Act,
   18 U.S.C. sections 2510-2521 and the Md. Annotated Code, Courts and Judicial
   Proceedings Article, Section 10, Subtitle 4.  Anyone using this system
   acknowledges that all use is subject to University of Maryland Policy
   on the Acceptable Use of Information Technology Resources available at
   http://www.umd.edu/aup.

   By logging in I acknowledge and agree to all terms and conditions
   regarding my access and the information contained therein.

To report problems or request assistance call the Help Desk at 301-405-1500

Password:
```

Getting started: copying files to HPC

Here are some ways to move data between your local computer and server:

scp – secure copy; copy files to/from the HPC server.

From local to HPC:

```
scp /local/path/file.ext <user name>@<server address>:/path/to/folder
```

```
scp /Users/junaid/IHeartHpc.txt jmerch@login.bswift.umd.edu:/data/dir
```

From HPC to local:

```
scp <user name>@<server address>:/path/to/file /local/path/directory
```

```
scp jmerch@login.bswift.umd.edu:/data/Results.txt /Users/junaid/Desktop
```

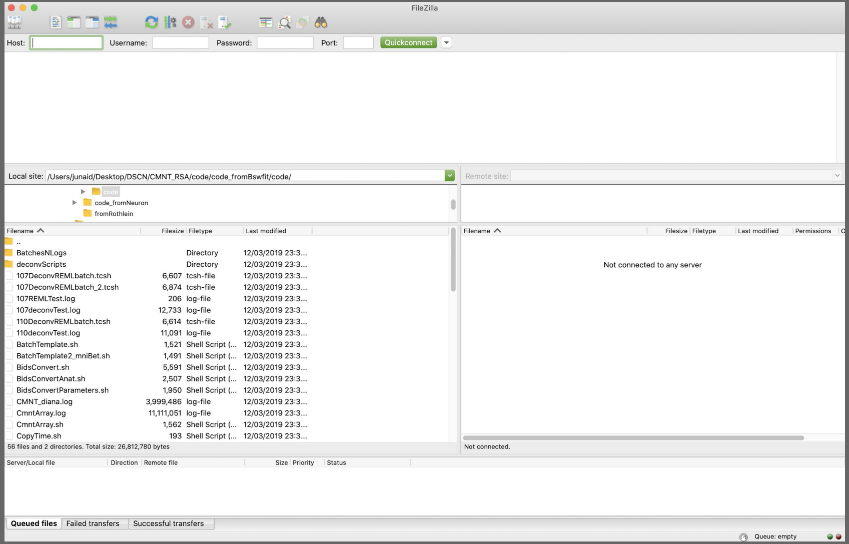
To copy entire directories, you can use the -r option after the scp command

More info: https://linuxize.com/post/how-to-use-scp-command-to-securely-transfer-files/

Getting started: copying files to/from HPC

You can use FileZilla for a graphical interface transfer:
https://filezilla-project.org/

I've occasionally gotten corrupted files using FileZilla.



Local site: /Users/junaid/Desktop/DSCN/CMNT_RSA/code/code_fromBswfit/code/

Remote site:

```
▶ code
▶ code_fromNeuron
  fromRothlein
```

Filename	Filesize	Filetype	Last modified
..			
BatchesNLogs		Directory	12/03/2019 23:3...
deconvScripts		Directory	12/03/2019 23:3...
107DeconvREMLbatch.tcsh	6,607	tcsh-file	12/03/2019 23:3...
107DeconvREMLbatch_2.tcsh	6,874	tcsh-file	12/03/2019 23:3...
107REMLTest.log	206	log-file	12/03/2019 23:3...
107deconvTest.log	12,733	log-file	12/03/2019 23:3...
110DeconvREMLbatch.tcsh	6,614	tcsh-file	12/03/2019 23:3...
110deconvTest.log	11,091	log-file	12/03/2019 23:3...
BatchTemplate.sh	1,521	Shell Script (...	12/03/2019 23:3...
BatchTemplate2_mniBet.sh	1,491	Shell Script (...	12/03/2019 23:3...
BidsConvert.sh	5,591	Shell Script (...	12/03/2019 23:3...
BidsConvertAnat.sh	2,507	Shell Script (...	12/03/2019 23:3...
BidsConvertParameters.sh	1,950	Shell Script (...	12/03/2019 23:3...
CMNT_diana.log	3,999,486	log-file	12/03/2019 23:3...
CmntArray.log	11,111,051	log-file	12/03/2019 23:3...
CmntArray.sh	1,562	Shell Script (...	12/03/2019 23:3...
CopyTime.sh	193	Shell Script (...	12/03/2019 23:3...

56 files and 2 directories. Total size: 26,812,780 bytes

Filename	Filesize	Filetype	Last modified	Permissions

Not connected to any server

Not connected.

Server/Local file	Direction	Remote file	Size	Priority	Status

slurm
workload manager

SLURM

Simple Linux Utility for Resource Management (SLURM)

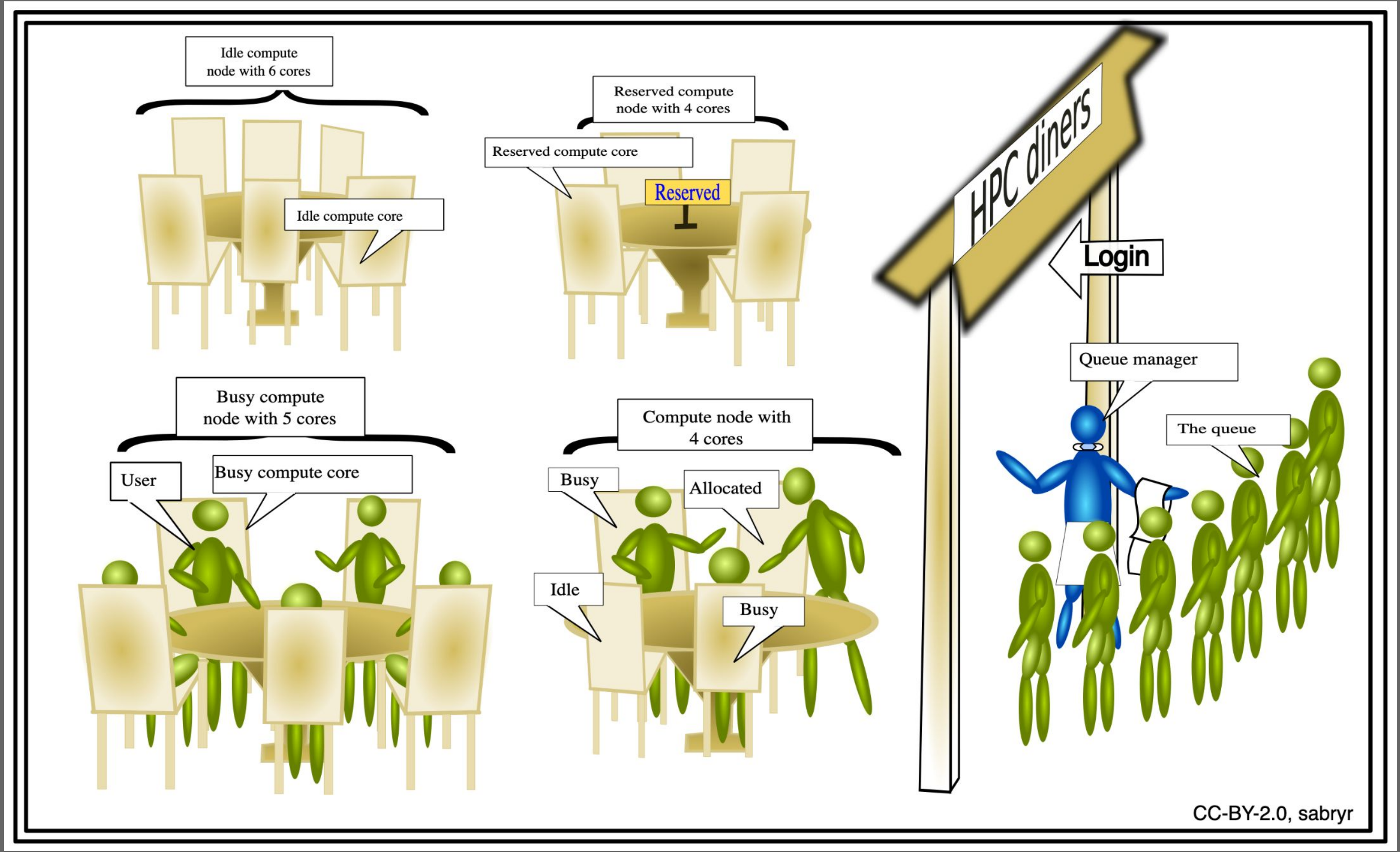
Workload manager, job scheduler, & queuing system for running processes on an HPC

Figures out what specifications you need, finds the available node that meets the requirements, and allocates your job to that node!

Runs multiple jobs in parallel at once.

Use in conjunction with the job script you want to run

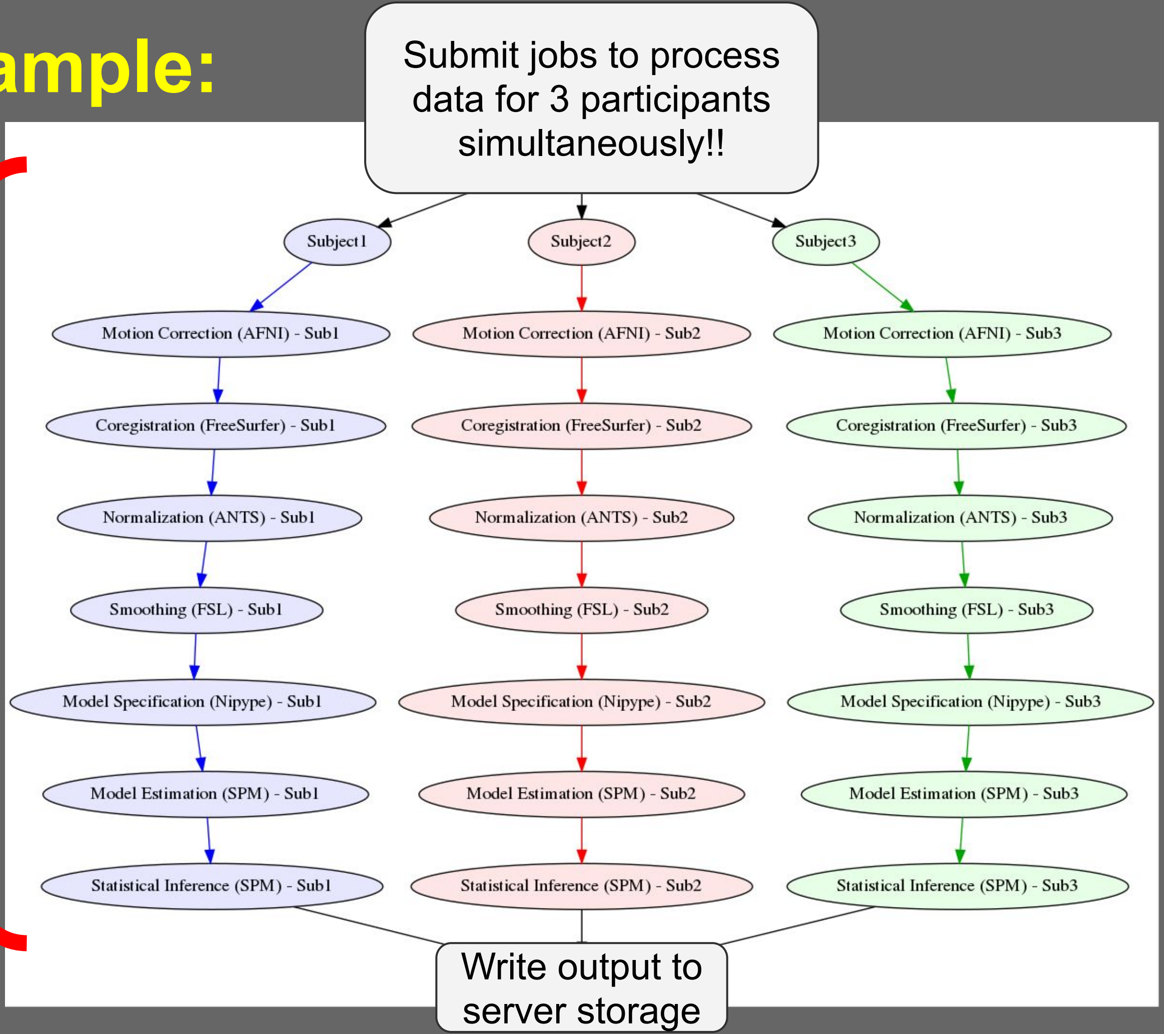
https://slurm.schedmd.com/quickstart.html



https://sabryr.github.io/hpc-intro/13-scheduler/index.html

Neuroimaging Example:

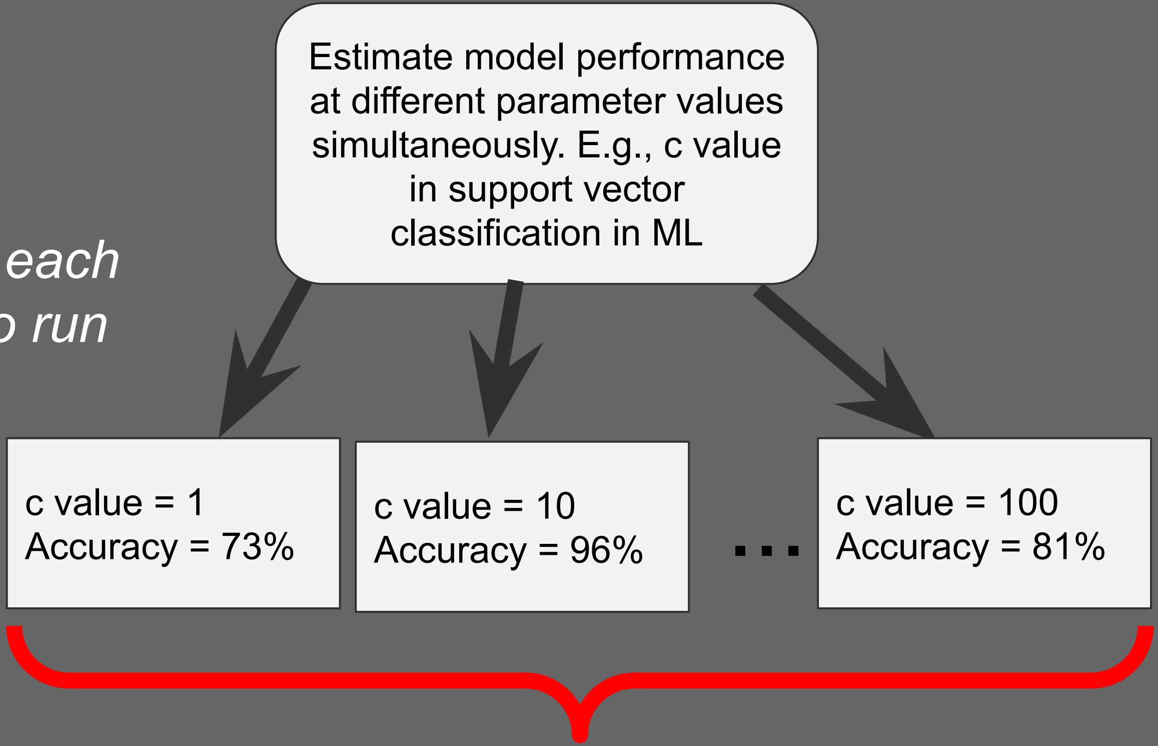
The data processing pipeline for each participant can be a series of data analysis steps



Submit jobs to process data for 3 participants simultaneously!!
Subject1
Subject2
Subject3
Motion Correction (AFNI) - Sub1
Motion Correction (AFNI) - Sub2
Motion Correction (AFNI) - Sub3
Coregistration (FreeSurfer) - Sub1
Coregistration (FreeSurfer) - Sub2
Coregistration (FreeSurfer) - Sub3
Normalization (ANTS) - Sub1
Normalization (ANTS) - Sub2
Normalization (ANTS) - Sub3
Smoothing (FSL) - Sub1
Smoothing (FSL) - Sub2
Smoothing (FSL) - Sub3
Model Specification (Nipype) - Sub1
Model Specification (Nipype) - Sub2
Model Specification (Nipype) - Sub3
Model Estimation (SPM) - Sub1
Model Estimation (SPM) - Sub2
Model Estimation (SPM) - Sub3
Statistical Inference (SPM) - Sub1
Statistical Inference (SPM) - Sub2
Statistical Inference (SPM) - Sub3
Write output to server storage

Parameter Tuning Example

Remember that each has to be able to run independently!



Estimate model performance at different parameter values simultaneously. E.g., c value in support vector classification in ML

c value = 1
Accuracy = 73%

c value = 10
Accuracy = 96%

. . .

c value = 100
Accuracy = 81%

After running the model at all values of parameter, you can compare to choose optimal value

SLURM Commands: sbatch

sbatch – probably the <u>most important</u> thing in this entire presentation

Allows you to submit a job to the appropriate node

Use with job script for whatever sort of process you want to run

Things you absolutely MUST specify when using sbatch to submit a job:

- # of Nodes
- Amount of RAM
- Time to process the job

You can specify a lot of other things: https://slurm.schedmd.com/sbatch.html

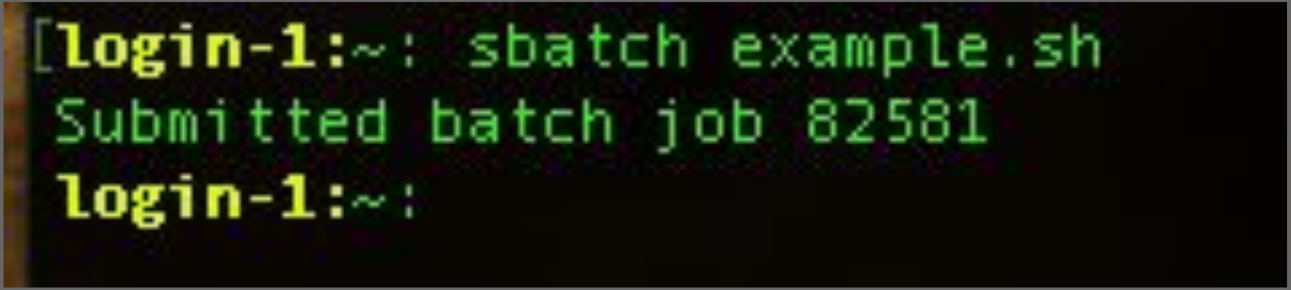
SLURM Commands: sbatch

sbatch https://slurm.schedmd.com/sbatch.html

Usage: `sbatch [options] <job script>`

For example: `sbatch RunSimulation.sh`

This will give you a job number that you can check in on later



```
[login-1:~: sbatch example.sh
 Submitted batch job 82581
 login-1:~:
```

Any questions so far?

Things are about rev up really quickly in the next presentation...

Presentation 5:
How to write & submit code for HPC w/examples in MATLAB & R

Outline

- Basic approach of writing code for HPC
- SLURM options
- A MATLAB example with introduction to wrappers
- An example of an R script (translates to Python)

Write stand-alone scripts

The easiest way to implement code on a HPC is to write stand alone code in whatever programming language you like and create a “wrapper” script for it

A wrapper script is basically a way to tell the shell to launch a computing node, and run whatever script you have set it to run

The wrapper function contains syntax/options that are specific to the job submission software you are using, i.e., SLURM

And gives instructions that are specific to the programming language you are using

Important considerations

The script that you write (in whatever programming language) has to be able to be run non-interactively.

- You should be able to run it without having to do anything once you start.
- It can take an input, but once it has started, you cannot interact with it

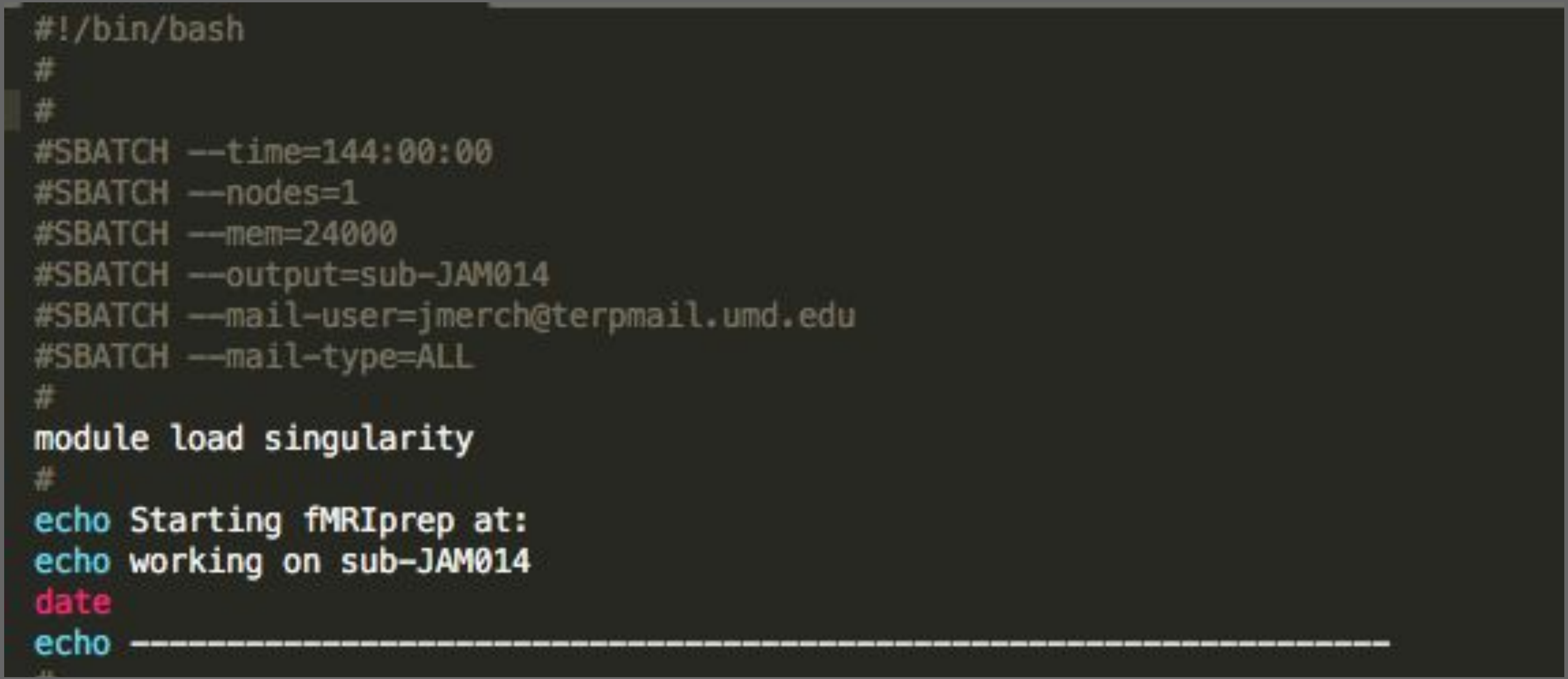
No graphical interfaces/GUIs and you cannot generate figures!

- When you submit a job, it is running on a node with no graphics potential

Solution/output of your code either needs to printed to screen or save to file

SLURM Job Scripts

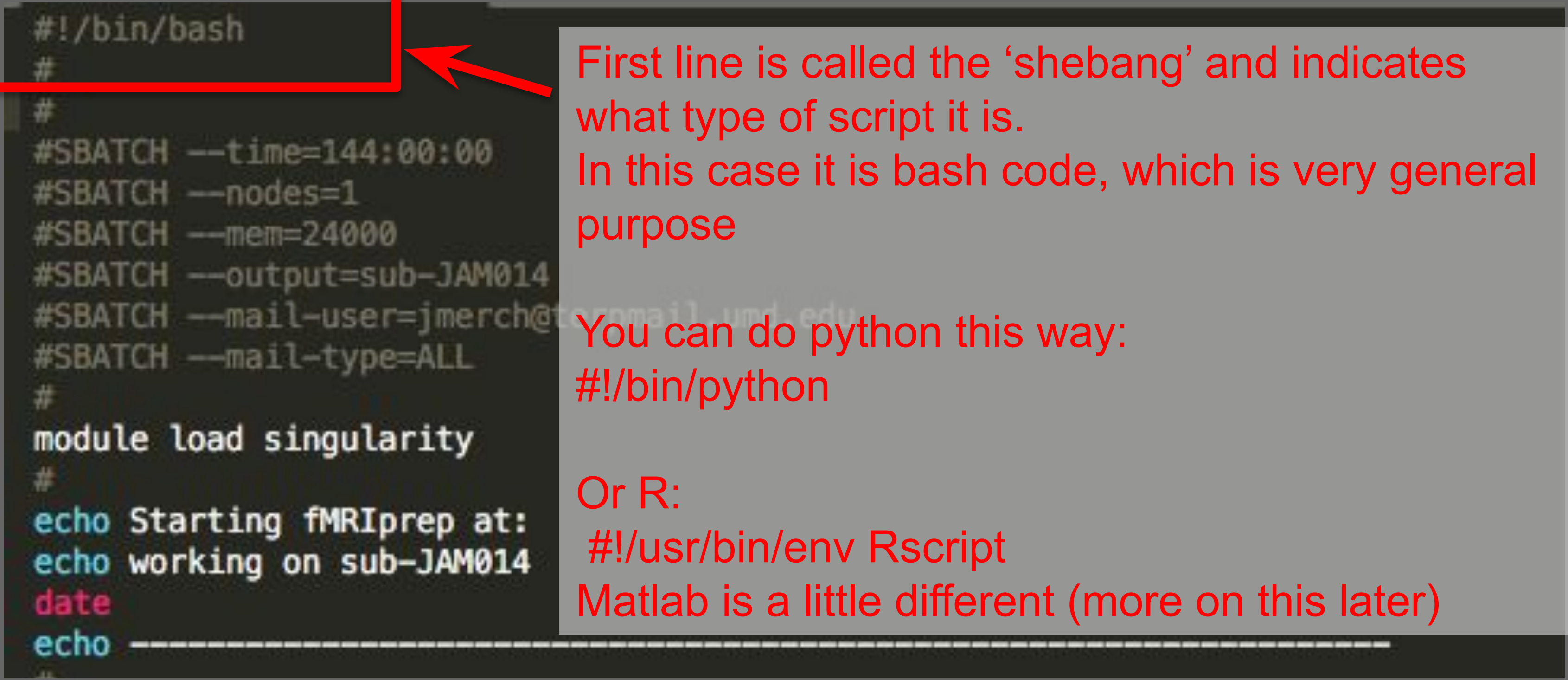
Before going too much further, we should look inside a job script



```
#!/bin/bash
#
#
#SBATCH --time=144:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
module load singularity
#
echo Starting fMRIprep at:
echo working on sub-JAM014
date
echo ------------------------------------------------------------------
```

SLURM Job Scripts

Before going too much further, we should look inside a job script



```
#!/bin/bash
#
#
#SBATCH --time=144:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
module load singularity
#
echo Starting fMRIprep at:
echo working on sub-JAM014
date
echo -------------------------------------------------------------------
```

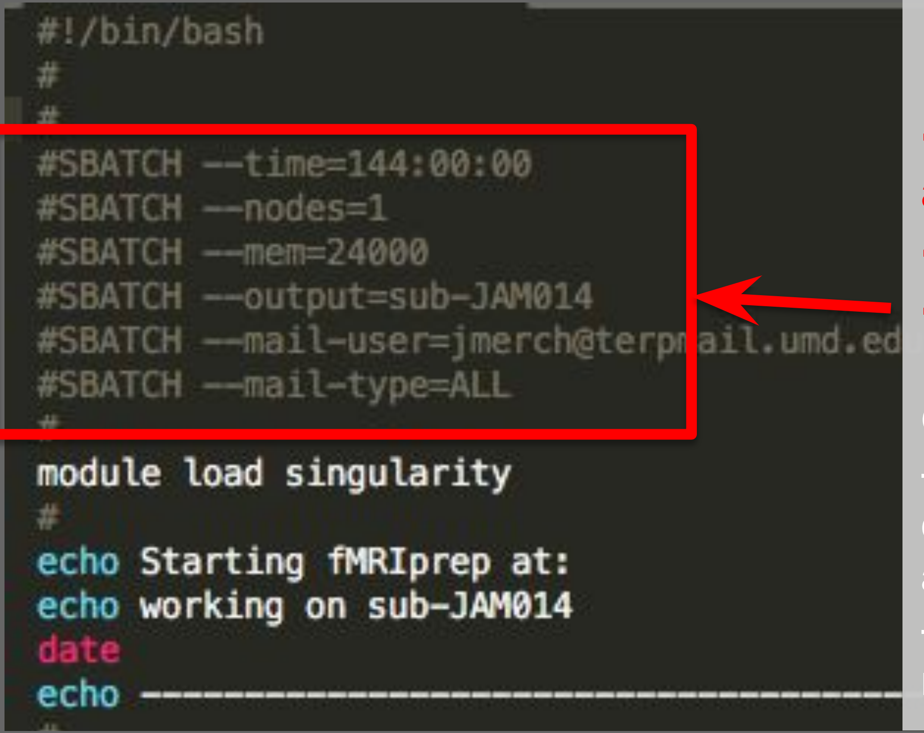
First line is called the 'shebang' and indicates what type of script it is.
In this case it is bash code, which is very general purpose

You can do python this way:
#!/bin/python

Or R:
#!/usr/bin/env Rscript
Matlab is a little different (more on this later)

SLURM Job Scripts

Before going too much further, we should look inside a job script



```
#!/bin/bash
#
#
#SBATCH --time=144:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
module load singularity
#
echo Starting fMRIprep at:
echo working on sub-JAM014
date
echo -------------------------------------------
```

The next few lines are sbatch options. These options can be specified within the job script, or outside of the script as I described before:

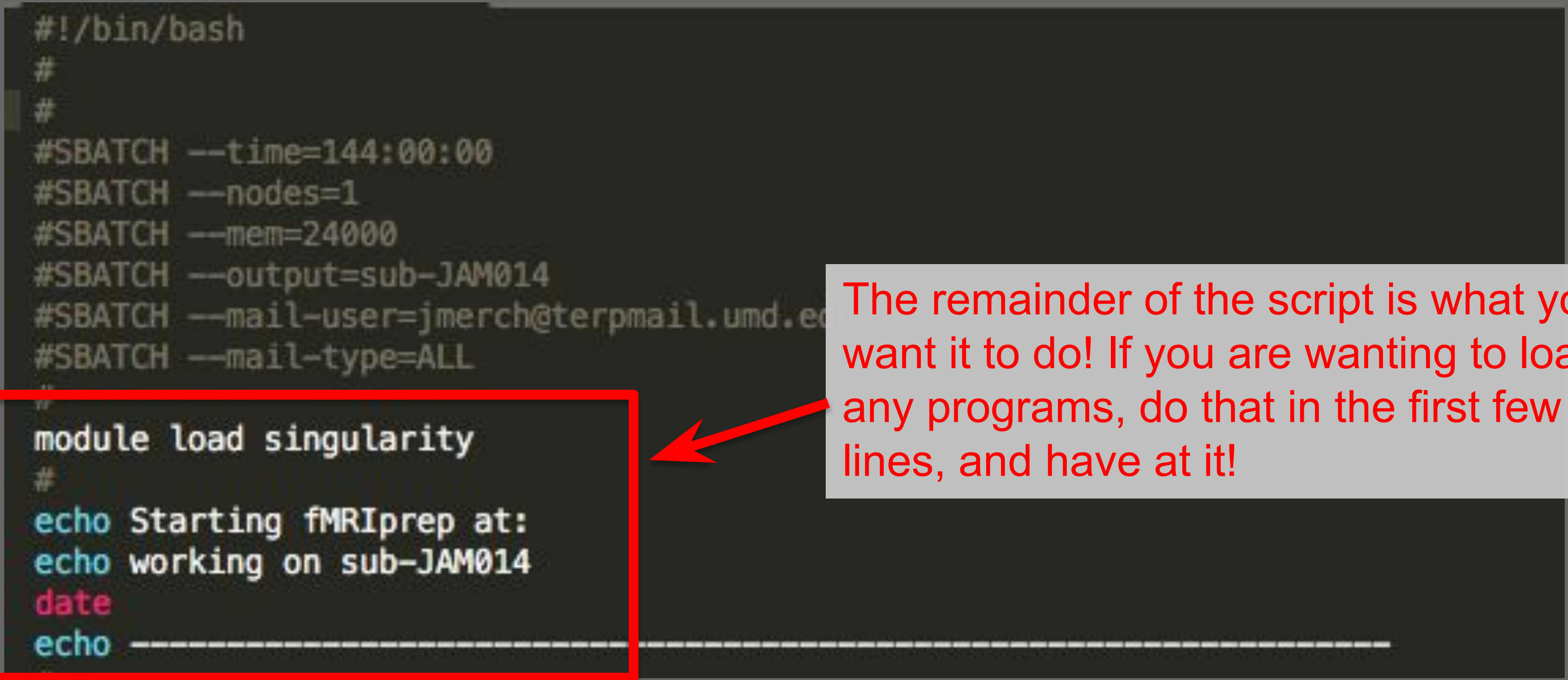
`sbatch [options] <job script>`

Required:
-time is the amount of time you want allocated in hours:minutes:seconds
-nodes is # of nodes
-mem is amount of RAM in megabytes

Optional:
-output - name of the output log file that contains what would be printed to terminal and any errors that occurred
-mail - give your umd email so it sends a message when the job starts and ends!

SLURM Job Scripts

Before going too much further, we should look inside a job script

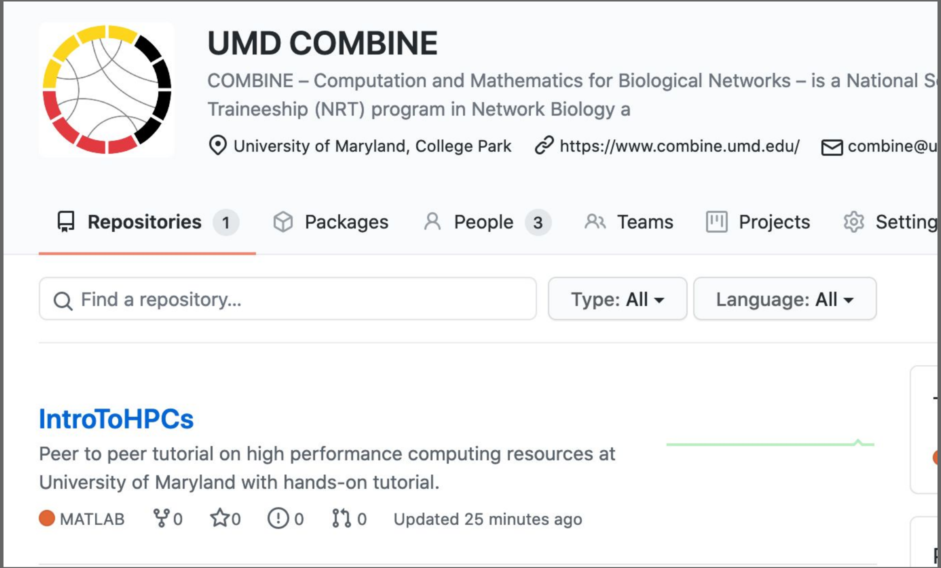


```
#!/bin/bash
#
#
#SBATCH --time=144:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=sub-JAM014
#SBATCH --mail-user=jmerch@terpmail.umd.ed
#SBATCH --mail-type=ALL
#
module load singularity
#
echo Starting fMRIprep at:
echo working on sub-JAM014
date
echo ------------------------------------------------------------
```

The remainder of the script is what you want it to do! If you are wanting to load any programs, do that in the first few lines, and have at it!

All the example code that I will show for the remainder of the time (and more!) can be found on the github repository we sent out:

https://github.com/UMD-COMBINE/IntroToHPCs



UMD COMBINE

COMBINE – Computation and Mathematics for Biological Networks – is a National S
Traineeship (NRT) program in Network Biology a

University of Maryland, College Park https://www.combine.umd.edu/ combine@u

IntroToHPCs

Peer to peer tutorial on high performance computing resources at University of Maryland with hands-on tutorial.

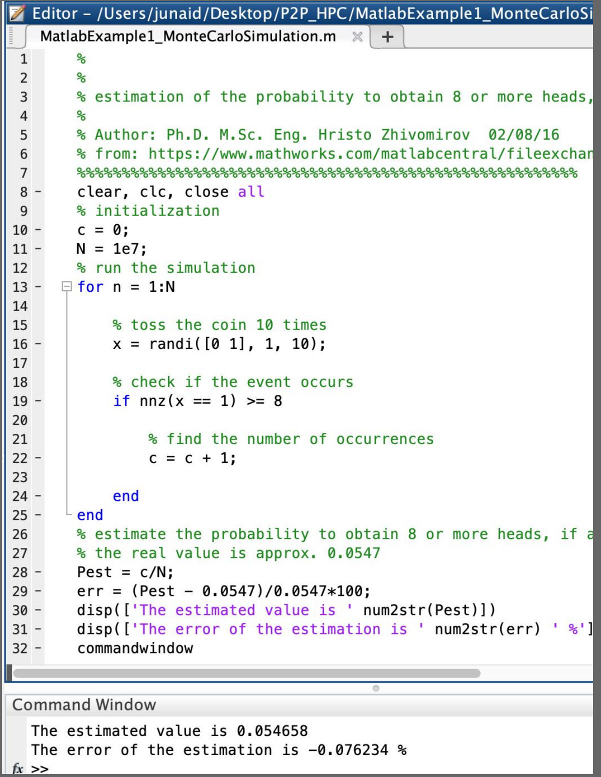
MATLAB 0 0 0 0 Updated 25 minutes ago

Matlab example: Monte Carlo simulation for estimation of the probability to obtain 8 or more heads, if a coin is tossed 10 times.

1) Write the standalone matlab script as you would run on your local workstation, and it outputs the solution in the command window.

2) Copy it up to the server

3) Write a wrapper script to submit it to a node using sbatch


Editor – /Users/junaid/Desktop/P2P_HPC/MatlabExample1_MonteCarloSi
MatlabExample1_MonteCarloSimulation.m
Command Window

```
%
%
% estimation of the probability to obtain 8 or more heads,
%
% Author: Ph.D. M.Sc. Eng. Hristo Zhivomirov  02/08/16
% from: https://www.mathworks.com/matlabcentral/fileexchan
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear, clc, close all
% initialization
c = 0;
N = 1e7;
% run the simulation
for n = 1:N

    % toss the coin 10 times
    x = randi([0 1], 1, 10);

    % check if the event occurs
    if nnz(x == 1) >= 8

        % find the number of occurrences
        c = c + 1;

    end
end
% estimate the probability to obtain 8 or more heads, if a
% the real value is approx. 0.0547
Pest = c/N;
err = (Pest - 0.0547)/0.0547*100;
disp(['The estimated value is ' num2str(Pest)])
disp(['The error of the estimation is ' num2str(err) ' %']
commandwindow
```

```
The estimated value is 0.054658
The error of the estimation is -0.076234 %
>>
```

This example can be found at:
https://github.com/UMD-COMBINE/IntroToHPCs/blob/main/MatlabExample1_MonteCarloSimulation.m

Code from:
https://www.mathworks.com/matlabcentral/fileexchange/55306-monte-carlo-estimation-examples-with-matlab

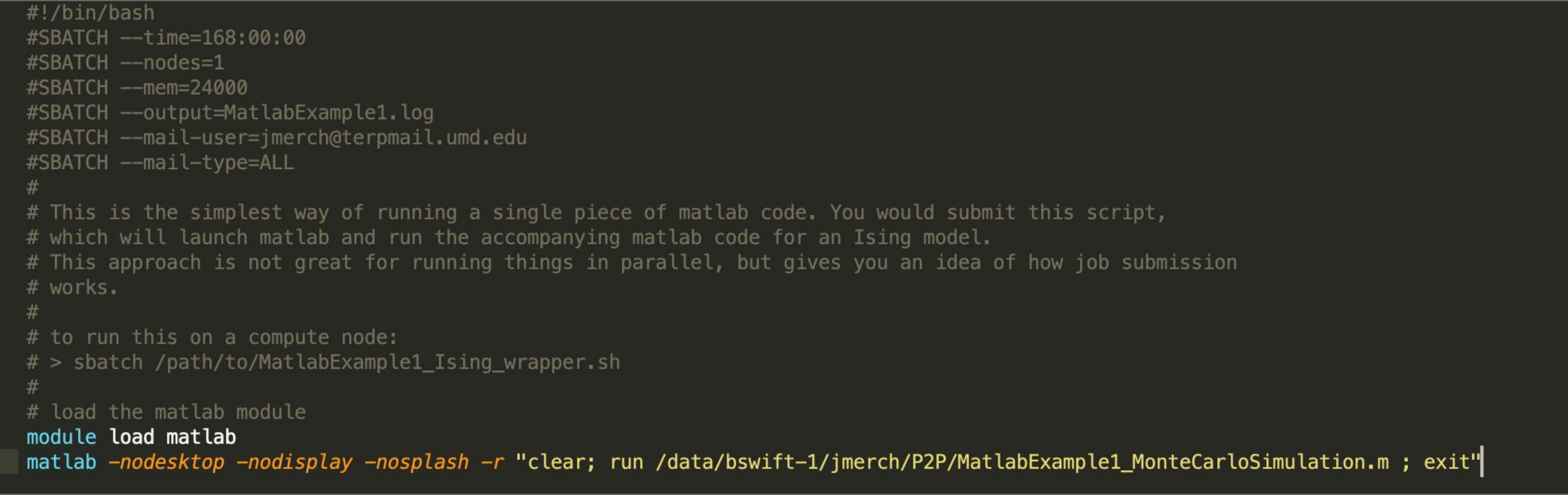
Matlab example: Monte Carlo simulation for estimation of the probability to obtain 8 or more heads, if a coin is tossed 10 times.

```
clear, clc, close all
% initialization
c = 0;
N = 1e7;
% run the simulation
for n = 1:N
% toss the coin 10 times
x = randi([0 1], 1, 10);
% check if the event occurs
if nnz(x == 1) >= 8
% find the number of occurrences
c = c + 1;
end
end
% estimate the probability to obtain 8 or more heads, if a coin is tossed 10 times
% the real value is approx. 0.0547
Pest = c/N;
err = (Pest - 0.0547)/0.0547*100;
disp(['The estimated value is ' num2str(Pest)])
disp(['The error of the estimation is ' num2str(err) ' %'])
commandwindow
```

SLURM Job Scripts: MATLAB Wrapper

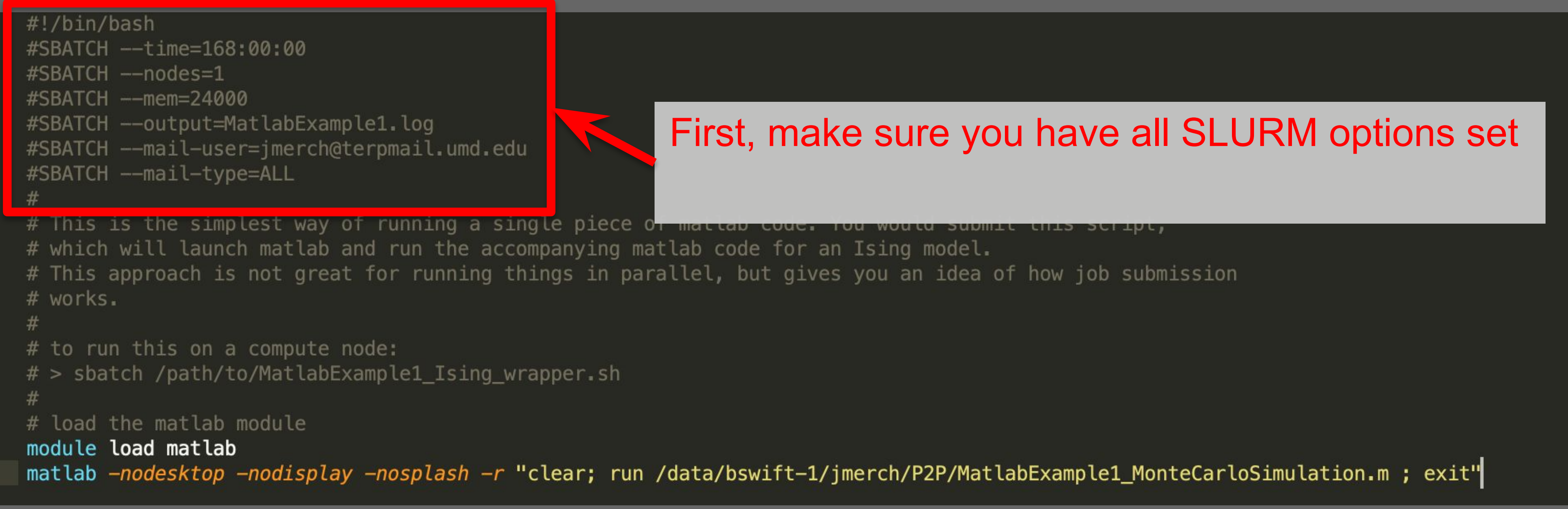
Now, let’s look at the special case of creating a job script with a MATLAB process.

For this, you want to create a bash script as before



```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=MatlabExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
# This is the simplest way of running a single piece of matlab code. You would submit this script,
# which will launch matlab and run the accompanying matlab code for an Ising model.
# This approach is not great for running things in parallel, but gives you an idea of how job submission
# works.
#
# to run this on a compute node:
# > sbatch /path/to/MatlabExample1_Ising_wrapper.sh
#
# load the matlab module
module load matlab
matlab -nodesktop -nodisplay -nosplash -r "clear; run /data/bswift-1/jmerch/P2P/MatlabExample1_MonteCarloSimulation.m ; exit"
```

SLURM Job Scripts: MATLAB Wrapper



```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=MatlabExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
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# which will launch matlab and run the accompanying matlab code for an Ising model.
# This approach is not great for running things in parallel, but gives you an idea of how job submission
# works.
#
# to run this on a compute node:
# > sbatch /path/to/MatlabExample1_Ising_wrapper.sh
#
# load the matlab module
module load matlab
matlab -nodesktop -nodisplay -nosplash -r "clear; run /data/bswift-1/jmerch/P2P/MatlabExample1_MonteCarloSimulation.m ; exit"
```
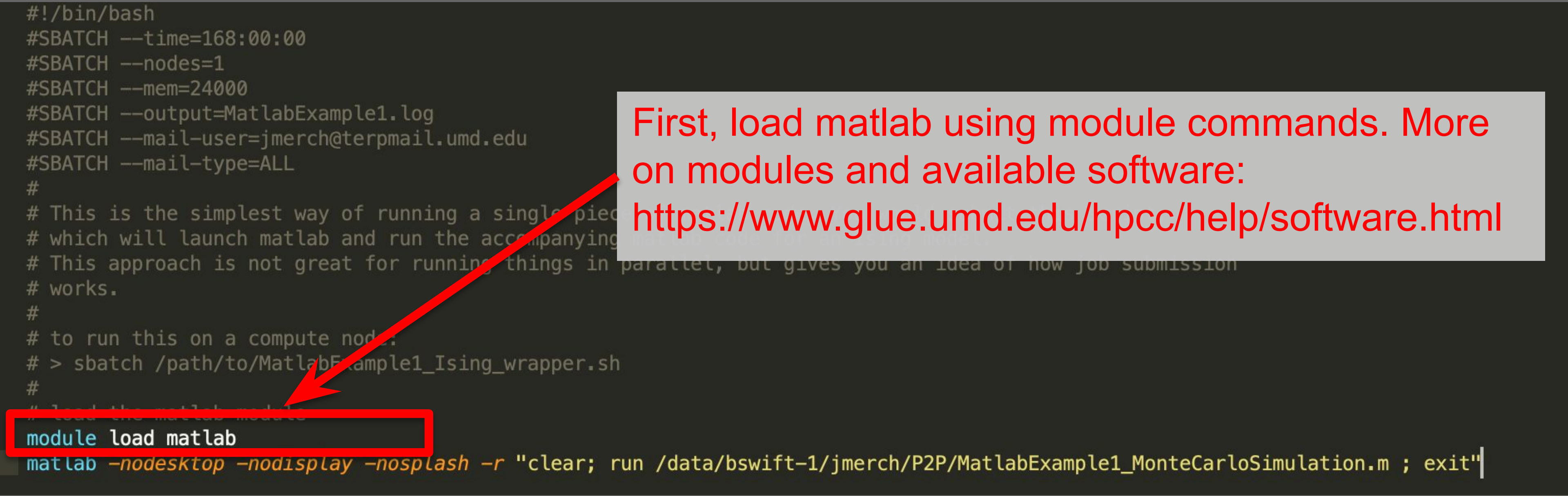

First, make sure you have all SLURM options set

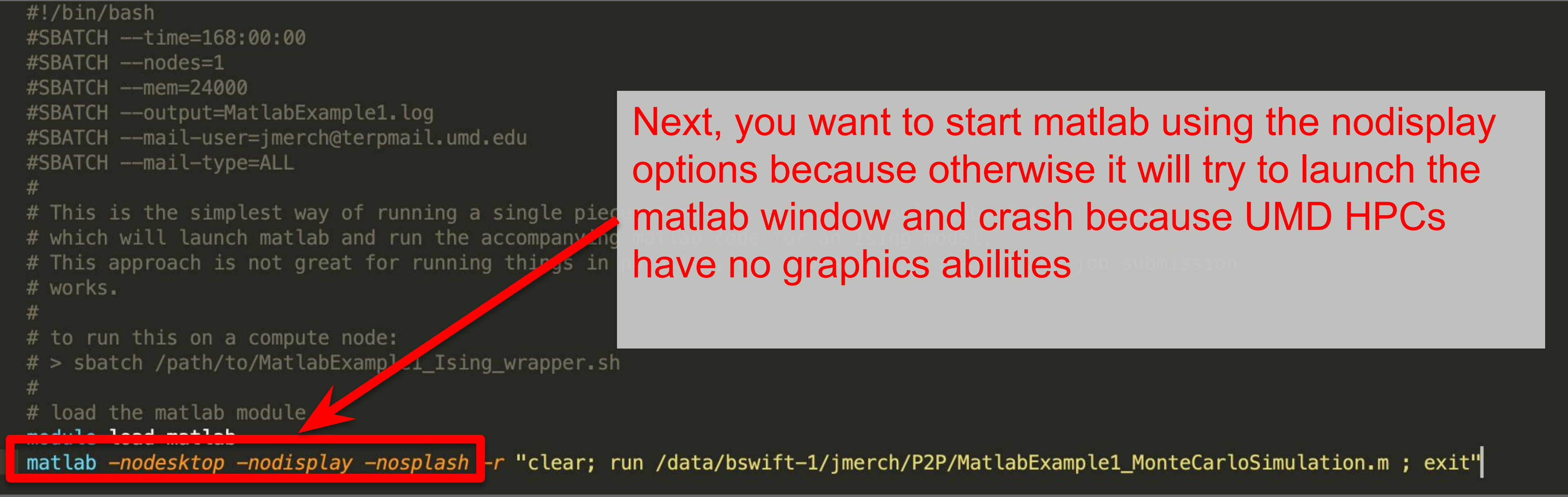
SLURM Job Scripts: MATLAB Wrapper



```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=MatlabExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
# This is the simplest way of running a single piec
# which will launch matlab and run the accompanying matlab code for the Ising model.
# This approach is not great for running things in parallel, but gives you an idea of how job submission
# works.
#
# to run this on a compute node:
# > sbatch /path/to/MatlabExample1_Ising_wrapper.sh
#
# load the matlab module
module load matlab
matlab -nodesktop -nodisplay -nosplash -r "clear; run /data/bswift-1/jmerch/P2P/MatlabExample1_MonteCarloSimulation.m ; exit"
```

First, load matlab using module commands. More on modules and available software: https://www.glue.umd.edu/hpcc/help/software.html

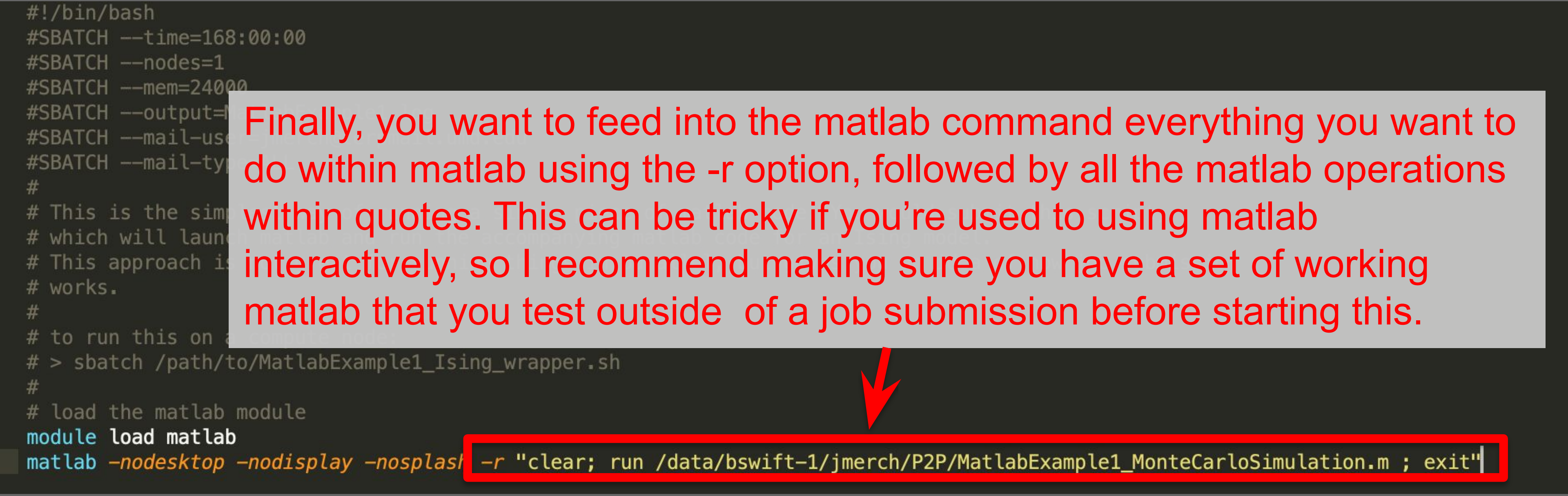
SLURM Job Scripts: MATLAB Wrapper



```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=MatlabExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
# This is the simplest way of running a single pie
# which will launch matlab and run the accompanying
# This approach is not great for running things in
# works.
#
# to run this on a compute node:
# > sbatch /path/to/MatlabExample1_Ising_wrapper.sh
#
# load the matlab module
module load matlab
matlab -nodesktop -nodisplay -nosplash -r "clear; run /data/bswift-1/jmerch/P2P/MatlabExample1_MonteCarloSimulation.m ; exit"
```

Next, you want to start matlab using the nodisplay options because otherwise it will try to launch the matlab window and crash because UMD HPCs have no graphics abilities

SLURM Job Scripts: MATLAB Wrapper



```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=
#SBATCH --mail-use
#SBATCH --mail-ty
#
# This is the sim
# which will launc
# This approach i
# works.
#
# to run this on a
# > sbatch /path/to/MatlabExample1_Ising_wrapper.sh
#
# load the matlab module
module load matlab
matlab -nodesktop -nodisplay -nosplash -r "clear; run /data/bswift-1/jmerch/P2P/MatlabExample1_MonteCarloSimulation.m ; exit"
```

Finally, you want to feed into the matlab command everything you want to do within matlab using the -r option, followed by all the matlab operations within quotes. This can be tricky if you're used to using matlab interactively, so I recommend making sure you have a set of working matlab that you test outside of a job submission before starting this.

SLURM Job Scripts: MATLAB Wrapper

```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=MatlabExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
# This is the simplest way of running a single piece of matlab code. You would submit this script,
# which will launch matlab and run the accompanying matlab code for an MC simulation.
# This approach is not great for running things in parallel, but gives you an idea of how job submission
# works.
#
# to run this on a compute node:
# > sbatch /path/to/MatlabExample1_MonteCarloSimulation.m
#
# load the matlab module
module load matlab
matlab -nodesktop -nodisplay -nosplash -r "clear; run /data/bswift-1/jmerch/P2P/MatlabExample1_MonteCarloSimulation.m ; exit"
```

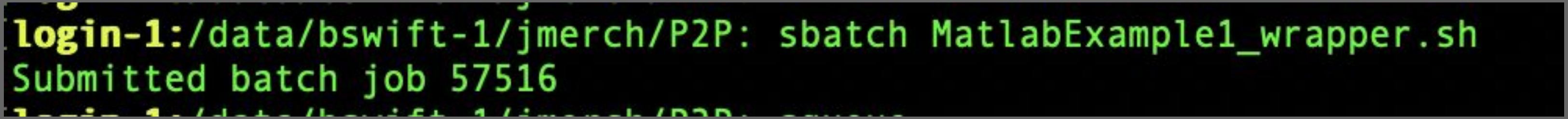
SLURM Job Scripts: MATLAB Wrapper

Now, to run this code, you can use the following command:

```
sbatch /path/to/MatlabExample1_wrapper.sh
```

specifically:

```
sbatch /data/bswift-1/jmerch/P2P/MatlabExample1_wrapper.sh
```

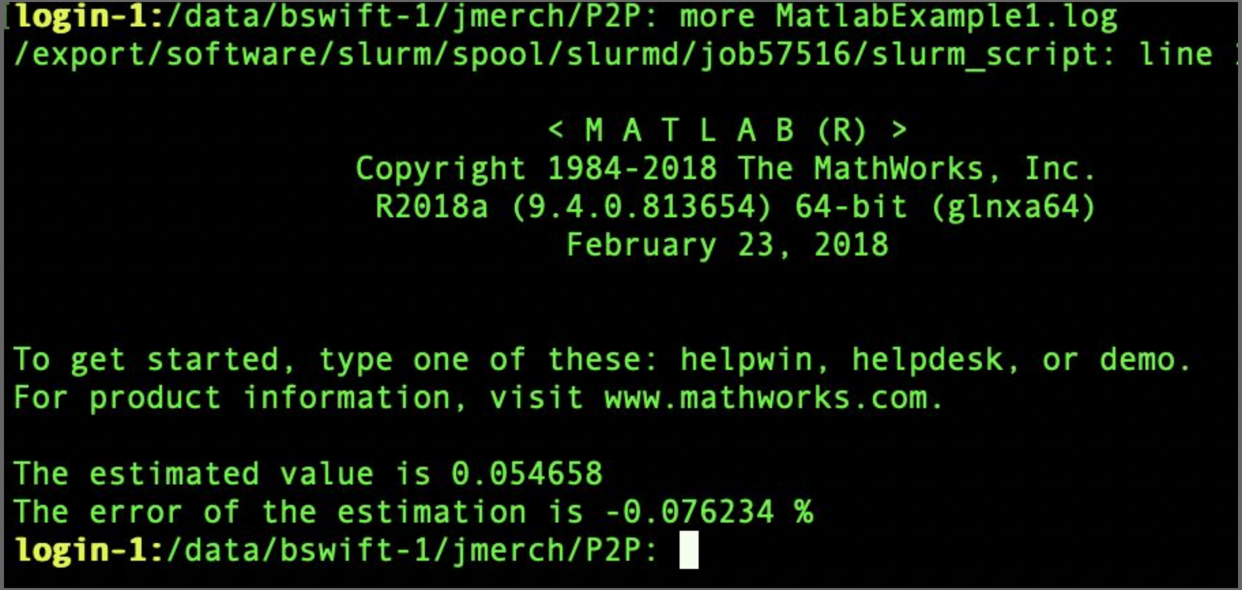


```
login-1:/data/bswift-1/jmerch/P2P: sbatch MatlabExample1_wrapper.sh
Submitted batch job 57516
```

SLURM Job Scripts: MATLAB Wrapper

Once it finishes, you can check the output file using the ‘more’ command, which captures everything that would have printed to screen:

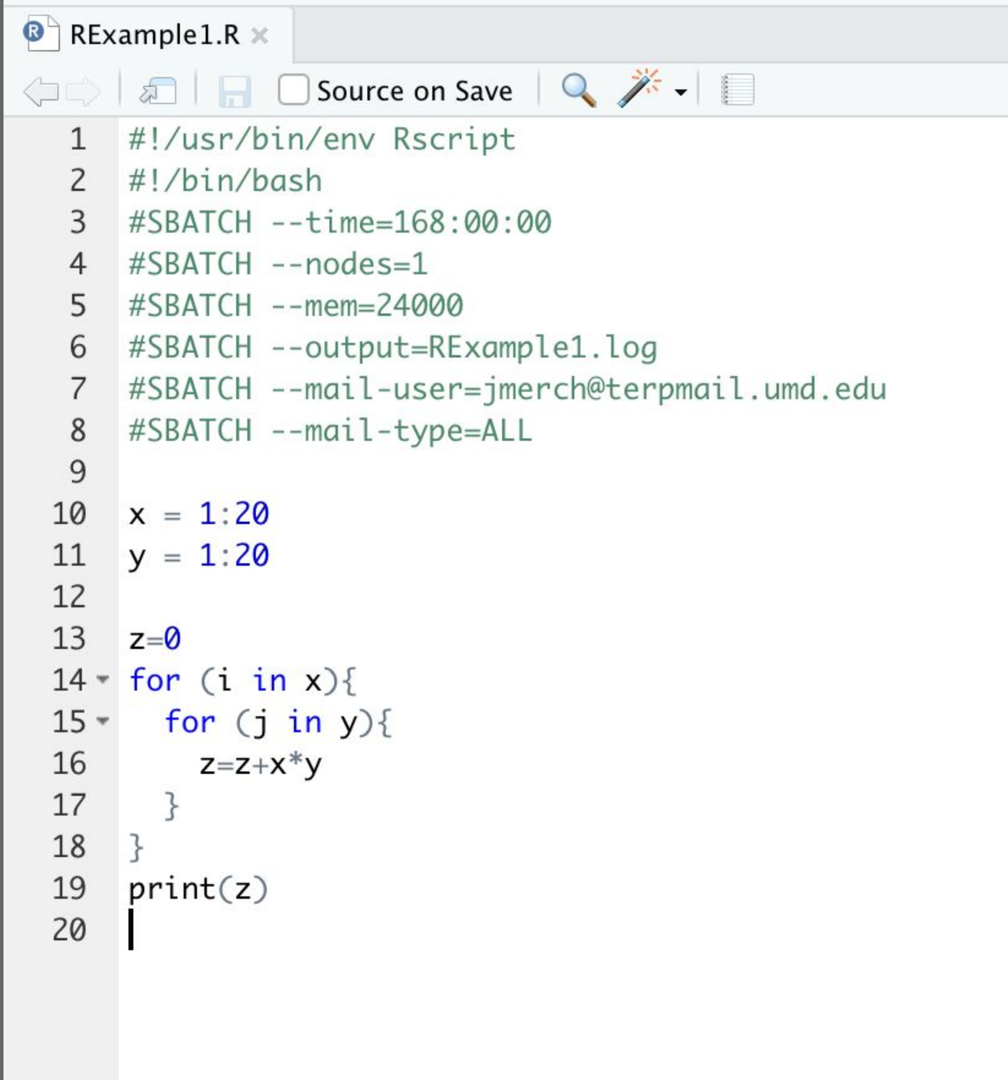
```
more /data/bswift-1/jmerch/P2P/MatlabExample1.log
```



```
login-1:/data/bswift-1/jmerch/P2P: more MatlabExample1.log
/export/software/slurm/spool/slurmd/job57516/slurm_script: line

                              < M A T L A B (R) >
                    Copyright 1984-2018 The MathWorks, Inc.
                     R2018a (9.4.0.813654) 64-bit (glnxa64)
                               February 23, 2018


To get started, type one of these: helpwin, helpdesk, or demo.
For product information, visit www.mathworks.com.

The estimated value is 0.054658
The error of the estimation is -0.076234 %
login-1:/data/bswift-1/jmerch/P2P:
```

R example

R and Python scripts are much easier because they don’t require a wrapper!

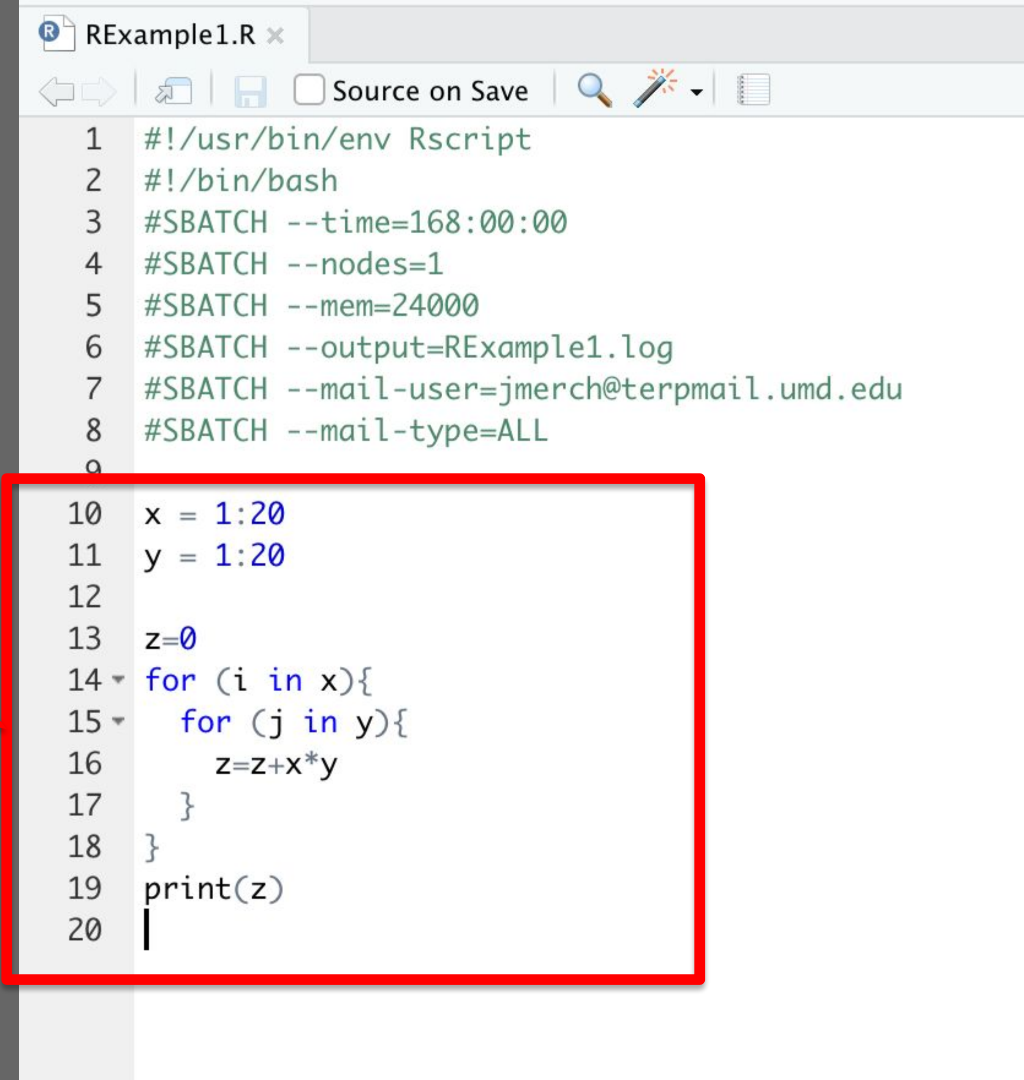


```
#!/usr/bin/env Rscript
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=RExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL

x = 1:20
y = 1:20

z=0
for (i in x){
  for (j in y){
    z=z+x*y
  }
}
print(z)

```

R example

R and Python scripts are much easier because they don't require a wrapper!

For example, this is a set of standalone R commands



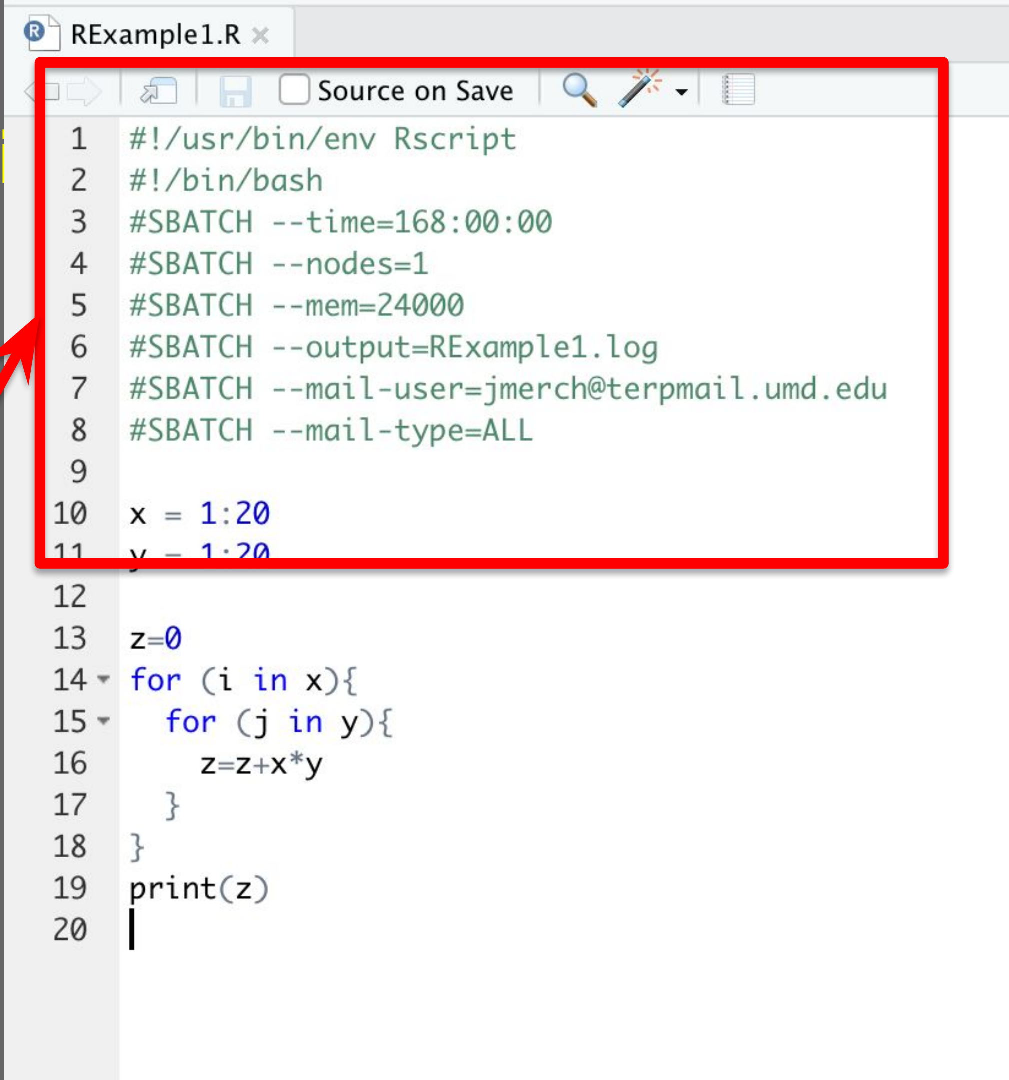
```
#!/usr/bin/env Rscript
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=RExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL

x = 1:20
y = 1:20

z=0
for (i in x){
  for (j in y){
    z=z+x*y
  }
}
print(z)
```

R example (will generali

R and Python scripts are much easier because they don't require a wrapper!

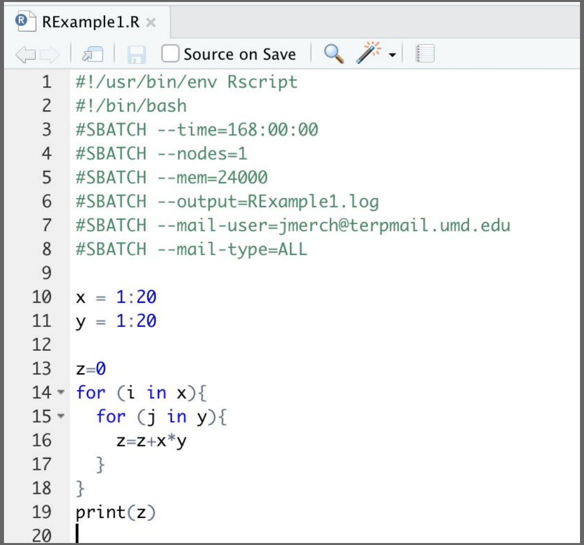
For example, this is a set of standalone R commands

As long as you add the shebang and SLURM options on top, this can run as-is!



```
#!/usr/bin/env Rscript
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=RExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL

x = 1:20
y = 1:20

z=0
for (i in x){
  for (j in y){
    z=z+x*y
  }
}
print(z)

```

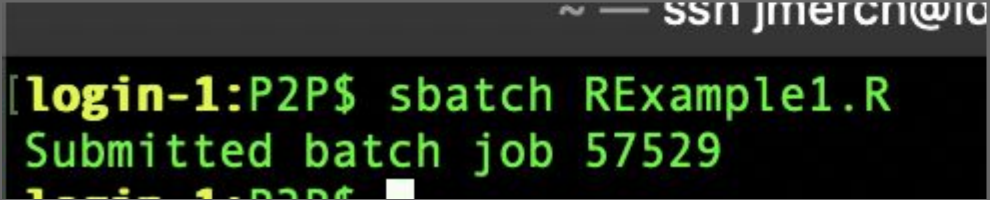
R example



```
#!/usr/bin/env Rscript
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=RExample1.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL

x = 1:20
y = 1:20

z=0
for (i in x){
  for (j in y){
    z=z+x*y
  }
}
print(z)

```

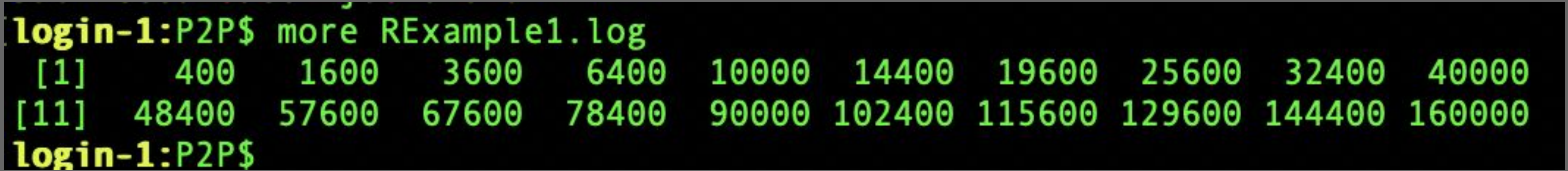
For instance:

```
sbatch /data/bswift-1/jmerch/P2P/RExample1.R
```



```
login-1:P2P$ sbatch RExample1.R
Submitted batch job 57529
```

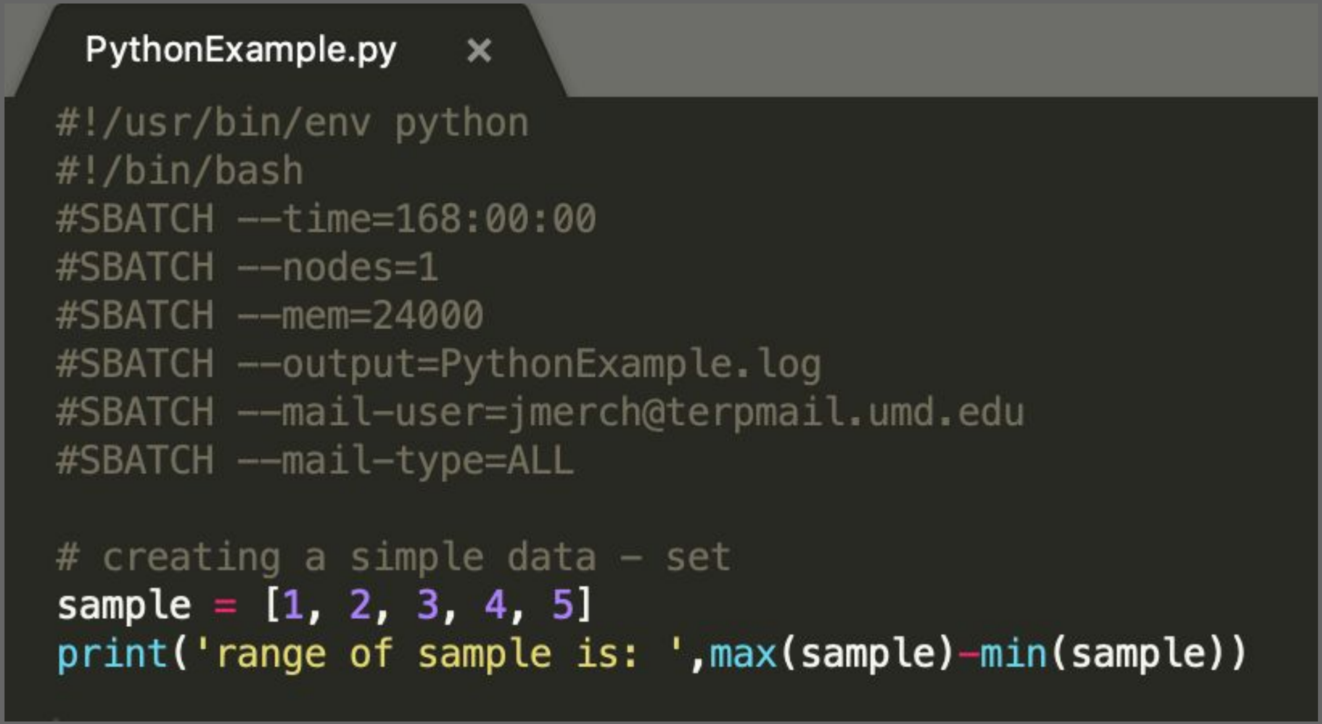
Then check output:



```
login-1:P2P$ more RExample1.log
 [1]     400    1600    3600    6400   10000   14400   19600   25600   32400   40000
[11]   48400   57600   67600   78400   90000  102400  115600  129600  144400  160000
login-1:P2P$
```

Python example

And the same holds true if you add the shebang and SLURM options to a Python script!



```
#!/usr/bin/env python
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --output=PythonExample.log
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL

# creating a simple data - set
sample = [1, 2, 3, 4, 5]
print('range of sample is: ',max(sample)-min(sample))
```

More Information and example code

https://github.com/UMD-COMBINE/IntroToHPCs

I have added additional example code that will let you really allow you to take advantage of a super computing. For example:

- A general MATLAB wrapper that will run any MATLAB script
- A wrapper for MATLAB functions that require input variables
- And an example of an Array job that will automatically run the code multiple times based on the specified input variables
    - This is how you parallelize efficiently
    - Can be used for things like parameter tuning etc

Questions?

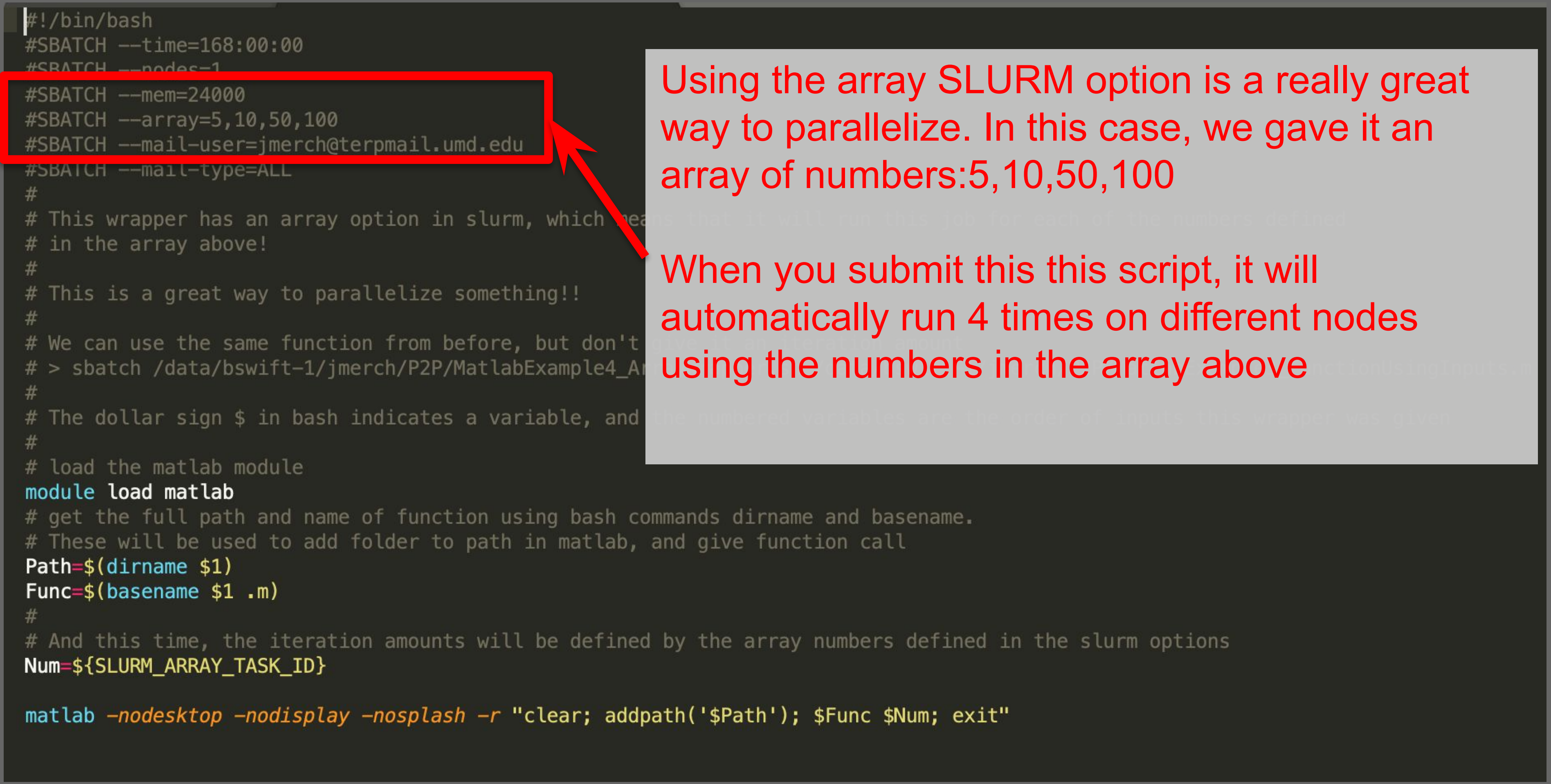
I’m available for consulting on how to get you set up on an HPC and running code, but I might ask for some compensation (i.e., cash, food, beer etc) since I’m really busy **&** underpaid!

#AlwaysLookingForASideHustle

Email: jmerch@umd.edu

@junaidsmerchant

SLURM Job Scripts: MATLAB Array example

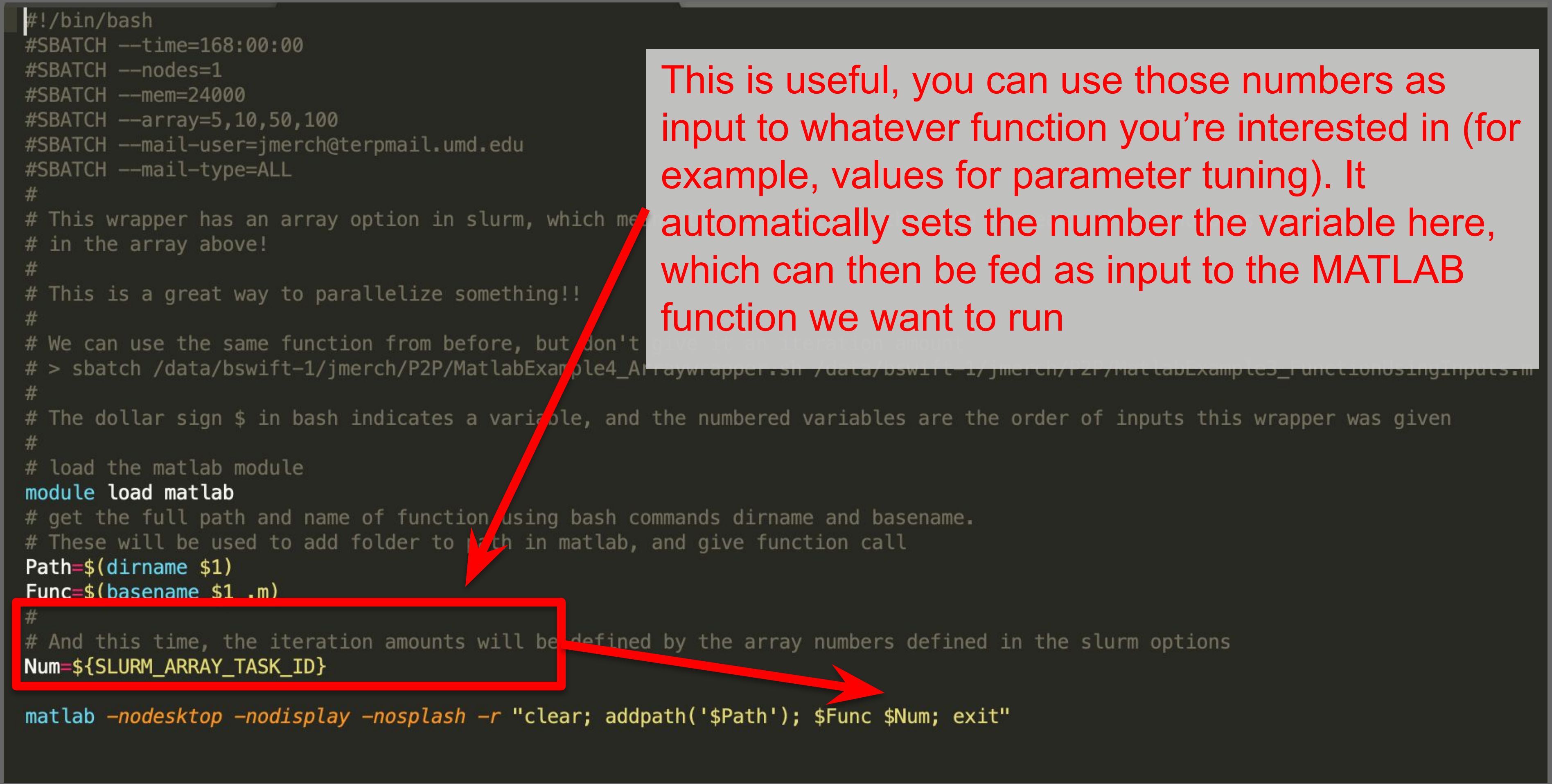


```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --array=5,10,50,100
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
# This wrapper has an array option in slurm, which means that it will run this job for each of the numbers defined
# in the array above!
#
# This is a great way to parallelize something!!
#
# We can use the same function from before, but don't give it an iteration amount
# > sbatch /data/bswift-1/jmerch/P2P/MatlabExample4_Ar[illegible]FunctionUsingInputs.m
#
# The dollar sign $ in bash indicates a variable, and the numbered variables are the order of inputs this wrapper was given
#
# load the matlab module
module load matlab
# get the full path and name of function using bash commands dirname and basename.
# These will be used to add folder to path in matlab, and give function call
Path=$(dirname $1)
Func=$(basename $1 .m)
#
# And this time, the iteration amounts will be defined by the array numbers defined in the slurm options
Num=${SLURM_ARRAY_TASK_ID}

matlab -nodesktop -nodisplay -nosplash -r "clear; addpath('$Path'); $Func $Num; exit"
```

Using the array SLURM option is a really great way to parallelize. In this case, we gave it an array of numbers:5,10,50,100

When you submit this this script, it will automatically run 4 times on different nodes using the numbers in the array above

SLURM Job Scripts: MATLAB Array example



```
#!/bin/bash
#SBATCH --time=168:00:00
#SBATCH --nodes=1
#SBATCH --mem=24000
#SBATCH --array=5,10,50,100
#SBATCH --mail-user=jmerch@terpmail.umd.edu
#SBATCH --mail-type=ALL
#
# This wrapper has an array option in slurm, which me
# in the array above!
#
# This is a great way to parallelize something!!
#
# We can use the same function from before, but don't give it an iteration amount
# > sbatch /data/bswift-1/jmerch/P2P/MatlabExample4_Arraywrapper.sh /data/bswift-1/jmerch/P2P/MatlabExample3_FunctionUsingInputs.m
#
# The dollar sign $ in bash indicates a variable, and the numbered variables are the order of inputs this wrapper was given
#
# load the matlab module
module load matlab
# get the full path and name of function using bash commands dirname and basename.
# These will be used to add folder to path in matlab, and give function call
Path=$(dirname $1)
Func=$(basename $1 .m)
#
# And this time, the iteration amounts will be defined by the array numbers defined in the slurm options
Num=${SLURM_ARRAY_TASK_ID}

matlab -nodesktop -nodisplay -nosplash -r "clear; addpath('$Path'); $Func $Num; exit"
```

This is useful, you can use those numbers as input to whatever function you're interested in (for example, values for parameter tuning). It automatically sets the number the variable here, which can then be fed as input to the MATLAB function we want to run