

HIGH-PERFORMANCE COMPUTING + EFFICIENCY



OPERATIONS
RESEARCH
CENTER

IAP 15.S60 Session 8

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(Adapted from Alex Schmid)

Today's Learning Objectives

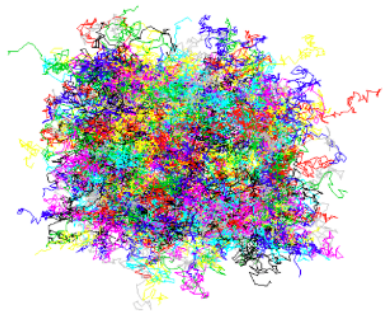
- Submit interactive jobs, batch jobs, and job arrays on a computing cluster
- Recognize parallelizable code and implement a simple parallel job with shared memory
- Design a reproducible and efficient pipeline for scientific computing

Clusters

Why do we use computing clusters?

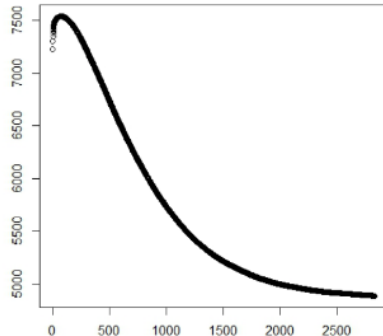
In optimization and stats, we often need a lot of computational power:

Deep learning on a
large dataset



GPU

Simulations (e.g. Monte-Carlo)



CPU

Hard optimization problems

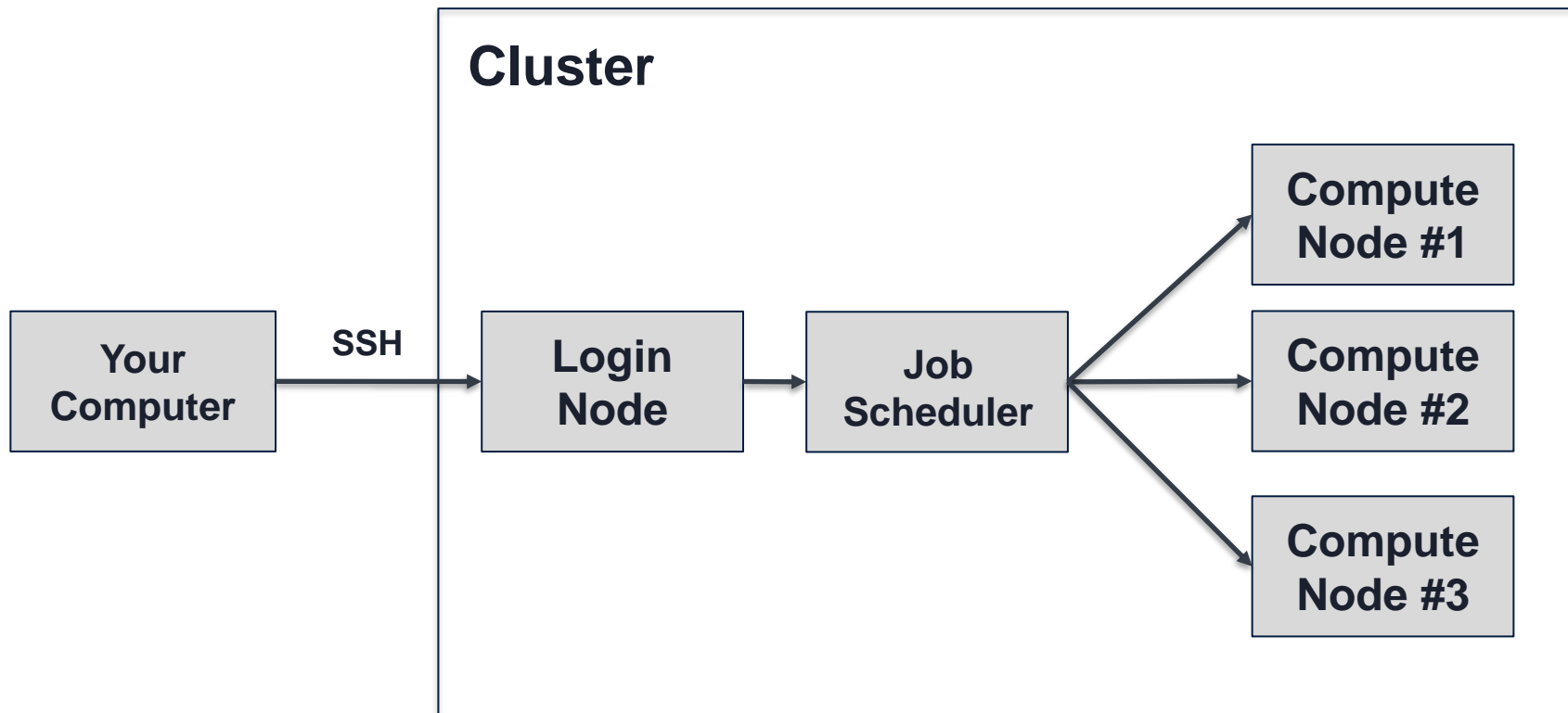


GUROBI
OPTIMIZATION

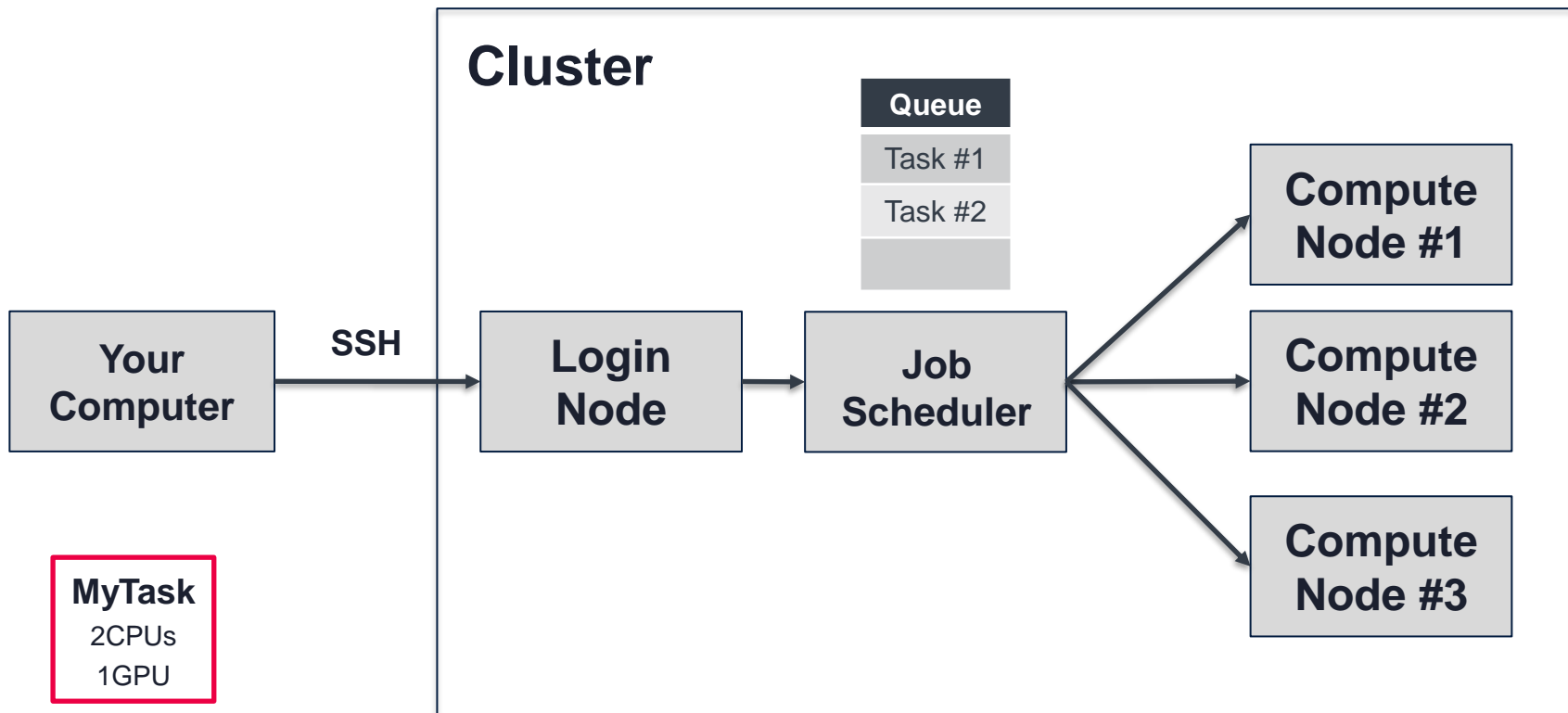
MEMORY

Usually need a
lot of:

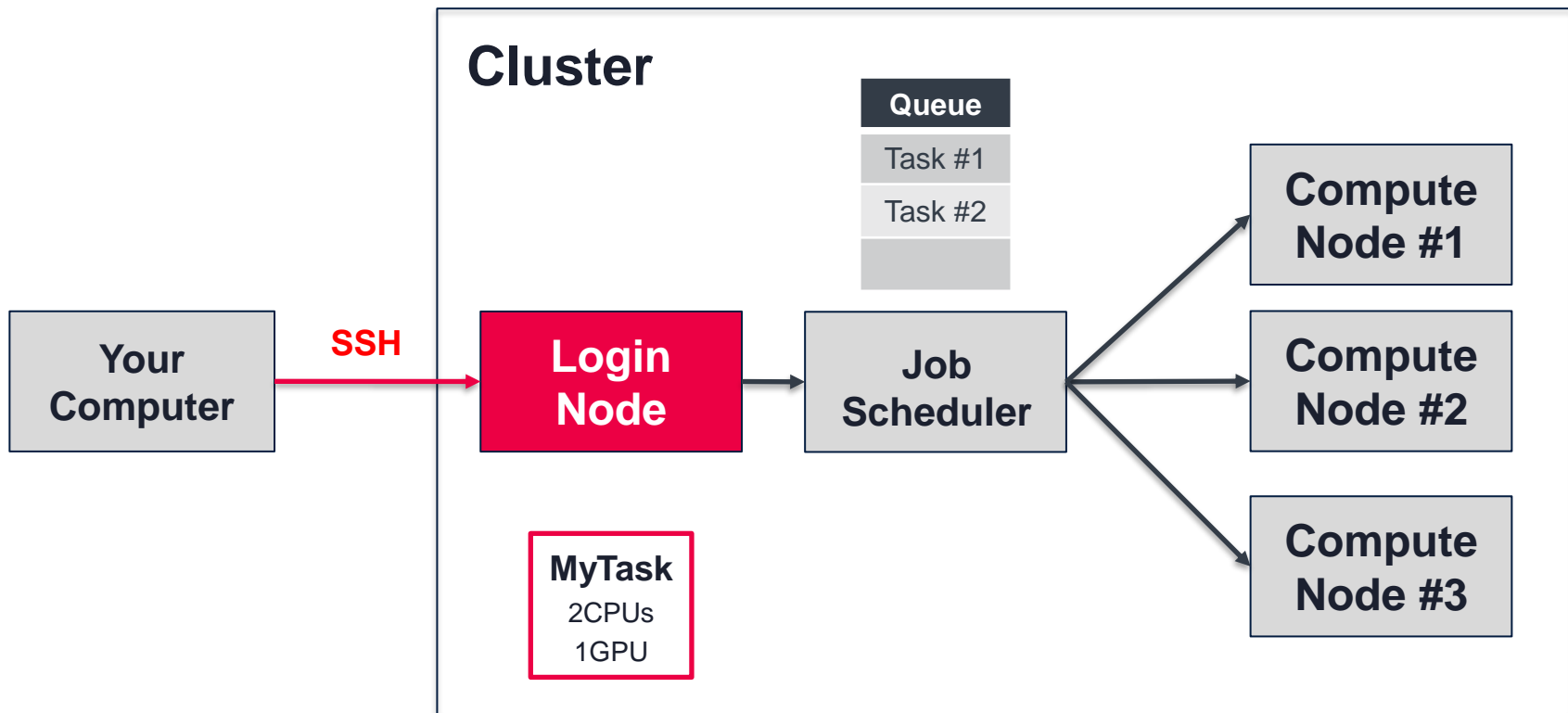
Using a cluster



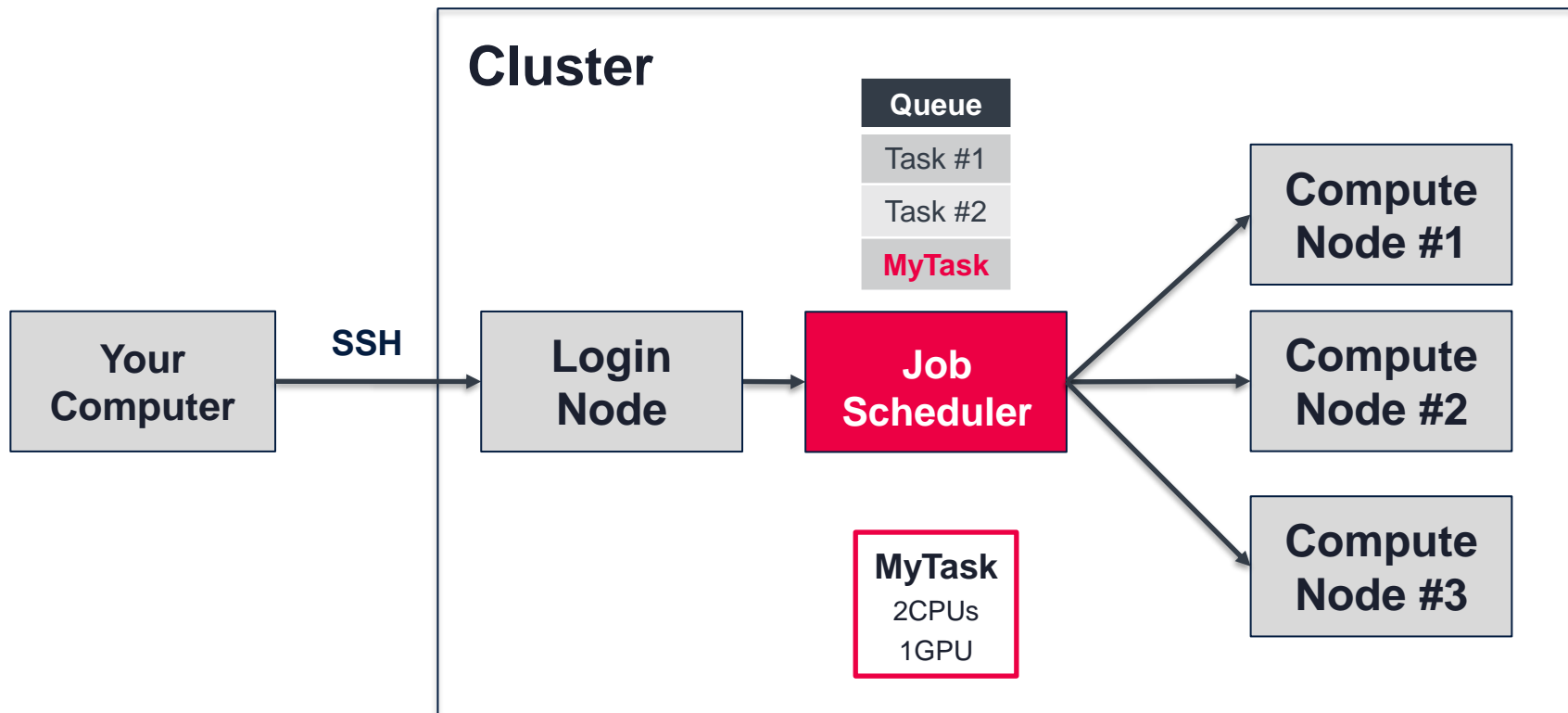
Using a cluster



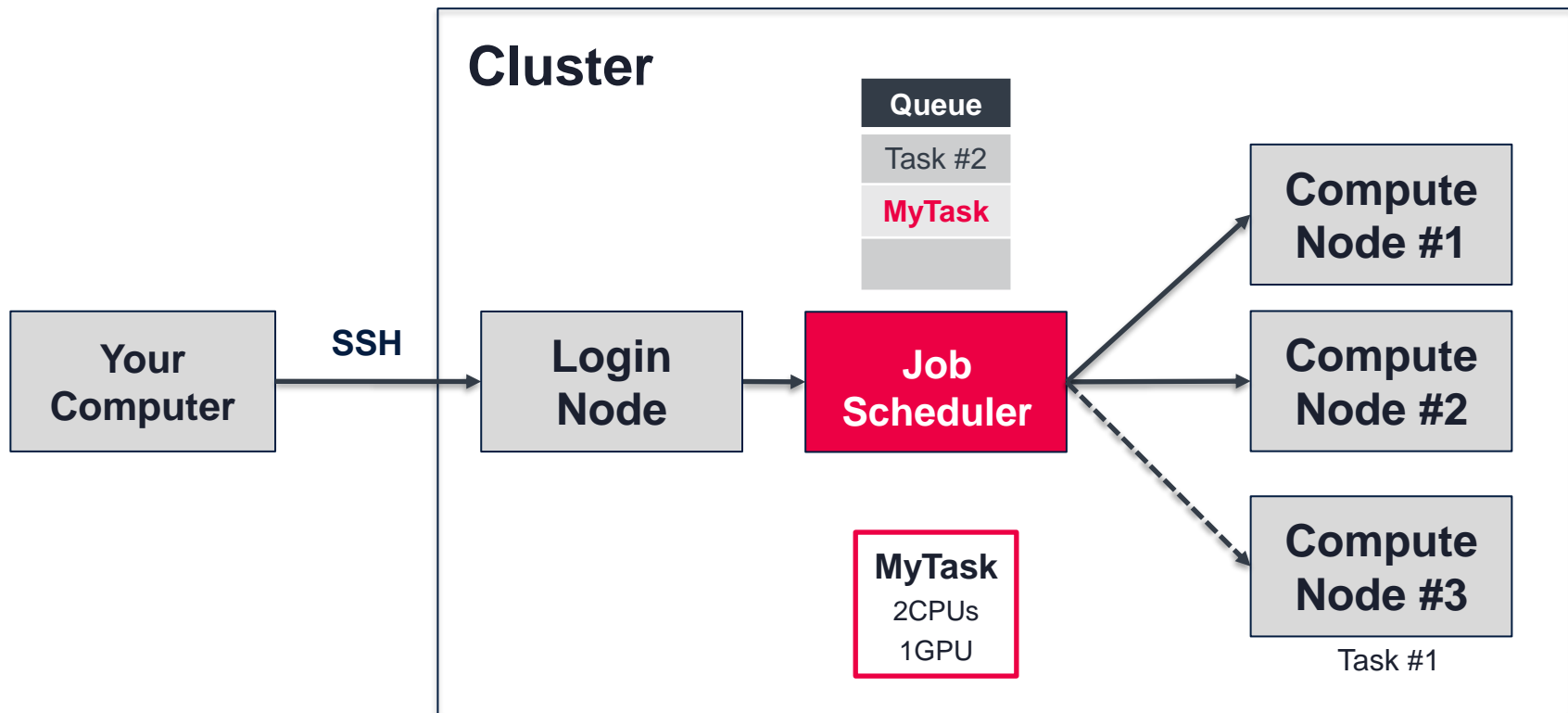
Using a cluster



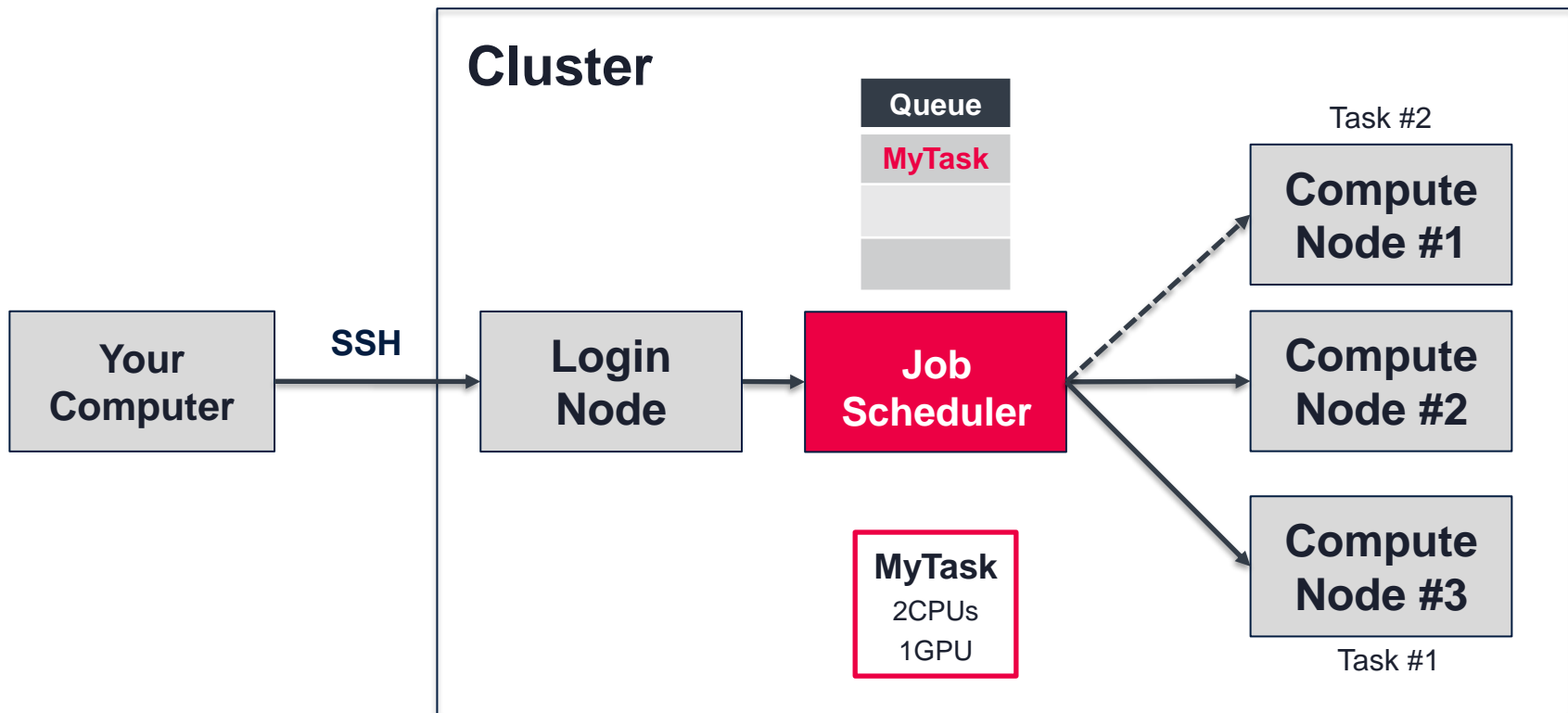
Using a cluster



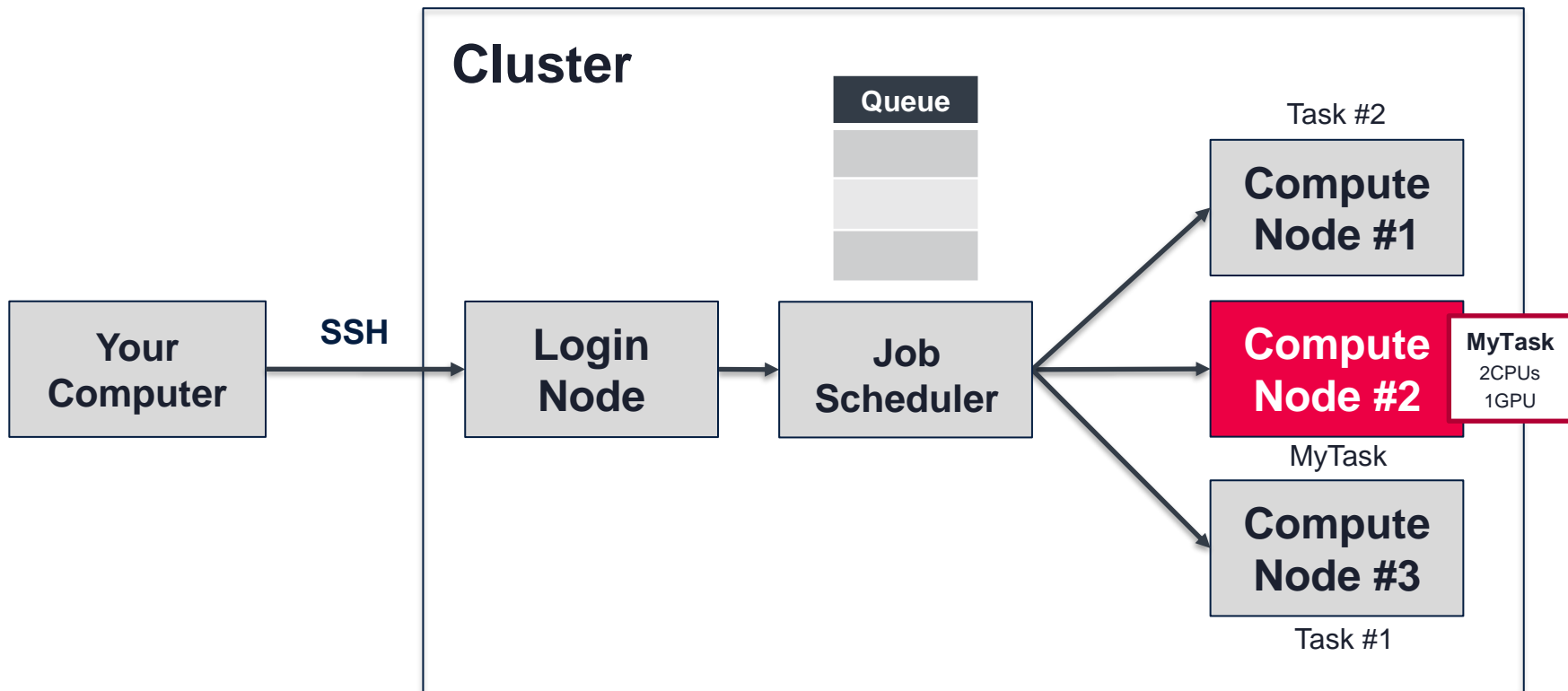
Using a cluster



Using a cluster



Using a cluster



Poll Question

pollev.com/georgemargaritis537

What cluster are you using today?

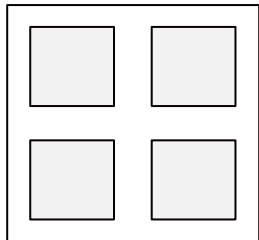
- A.) Engaging OnDemand
- B.) Engaging with Sloan resources
- C.) SuperCloud

Partitions

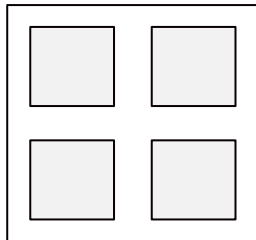
Clusters have many **nodes**, grouped into **partitions**

Engaging

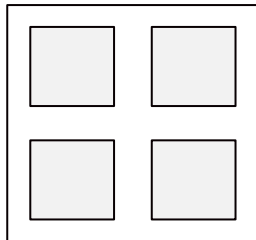
sched_any_quicktest



sched_any

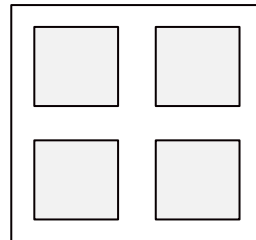


newnodes

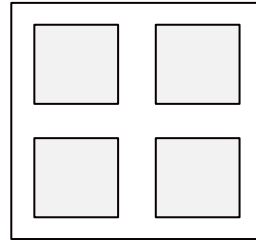


Sloan

sched_mit_sloan_
interactive

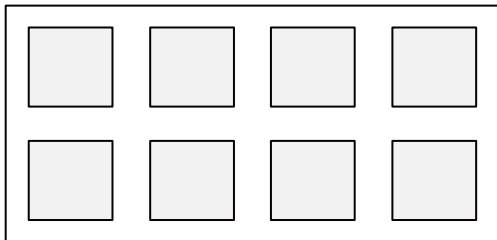


sched_mit_sloan_
batch

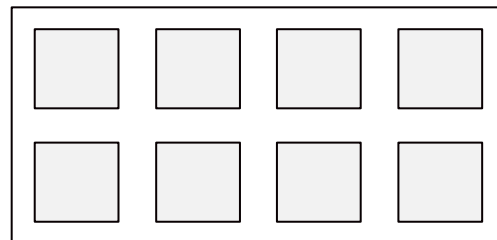


SuperCloud

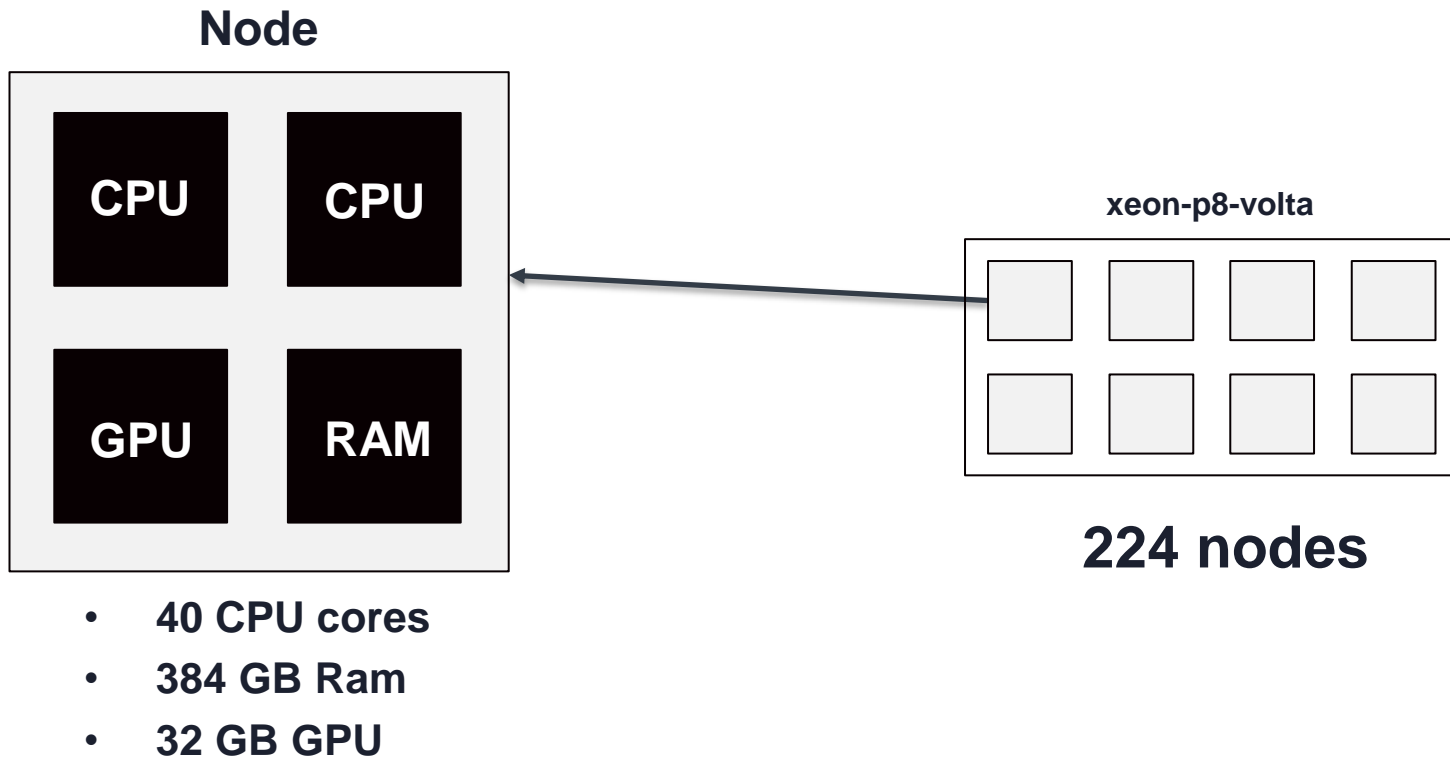
xeon-p8



xeon-p8-volta



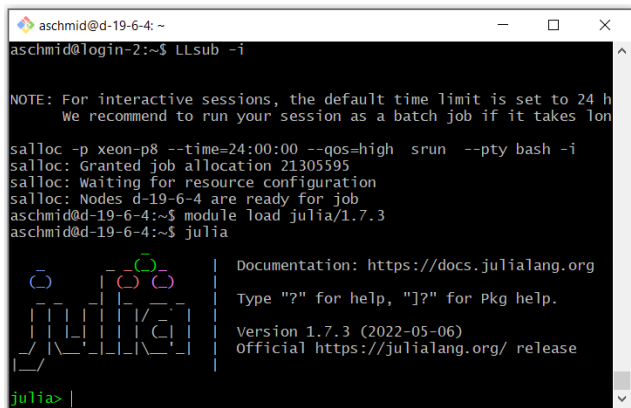
Node example: Supercloud



Types of Jobs

Interactive jobs

- Use cluster resources to interact with your code as you would locally
- Prototyping, testing, long jobs



```
aschmid@d-19-6-4: ~  
aschmid@login-2:~$ LLsub -i  
  
NOTE: For interactive sessions, the default time limit is set to 24 h  
We recommend to run your session as a batch job if it takes lon  
  
salloc -p xeon-p8 --time=24:00:00 --qos=high srun --pty bash -i  
salloc: Granted job allocation 21305595  
salloc: Waiting for resource configuration  
salloc: Nodes d-19-6-4 are ready for job  
aschmid@d-19-6-4:~$ module load julia/1.7.3  
aschmid@d-19-6-4:~$ julia  
  
Documentation: https://docs.julialang.org  
Type "?" for help, "]"? for pkg help.  
Version 1.7.3 (2022-05-06)  
Official https://julialang.org/ release  
  
julia> |
```

Batch jobs

- Set it and forget it! Request cluster resources to run scripts, then check back later for your results
- “Official” runs, running multiple scripts

```
1#!/bin/bash  
2#SBATCH -a 151-300  
3#SBATCH --cpus-per-task=2  
4#SBATCH --mem=32G  
5#SBATCH --partition=sched_mit_sloan_batch  
6#SBATCH --time=1-00:00  
7#SBATCH -o /home/aschmid/warehouse-task-assignment/outerr/train_both_\%a.out  
8#SBATCH -e /home/aschmid/warehouse-task-assignment/outerr/train_both_\%a.err  
9#SBATCH --mail-type=BEGIN,END,FAIL  
10#SBATCH --mail-user=aschmid@mit.edu  
11  
12module load julia/1.5.2  
13module load gurobi/8.1.1  
14  
15julia run_gettrainingdata_both.jl $SLURM_ARRAY_TASK_ID
```

Log in to the cluster with SSH

Open a terminal or Git Bash window

Engaging OnDemand:

```
ssh username@eofe7.mit.edu
```

```
ssh username@eofe8.mit.edu
```

Engaging via Sloan:

```
ssh username@eosloan.mit.edu
```

SuperCloud:

```
ssh username@txe1-login.mit.edu
```


Productivity Hack #1

ssh config: (`~/.ssh/config` file)

```
Host engaging-login-simple
  HostName eosloan.mit.edu
  User USERNAME
  IdentityFile ~/.ssh/id_rsa
```

Productivity Hack #1

ssh config: (`~/.ssh/config` file)

```
Host engaging-login-simple
  HostName eosloan.mit.edu
  User USERNAME
  IdentityFile ~/.ssh/id_rsa
```



Login Node

This will land you on the cluster login node

```
aschmid@login-2:~$
```

Don't run code on the login node! It doesn't have many compute resources and you may cause issues for others trying to log in.

- **Exception:** on SuperCloud, only the login node has internet access, so you must use it to install new software, add packages, clone repos, etc.

File system on the cluster

- Analogous to the file system on your local machine
 - We must move files and data to the cluster to run them
- **Engaging:** `/home/username`
- **SuperCloud:** `/home/gridsan/username`

Interacting with file system

Usual terminal commands

```
pwd, ls, cd
```

Move files from local to cluster

```
scp filename username@hostname:destination_file_path
```

e.g. `scp filename username@eofe7.mit.edu:/home/username/<destfolder>`

```
scp filename username@eosloan.mit.edu:/home/username/<destfolder>
```

```
scp filename username@txel-login.mit.edu:/home/gridsan/username/<destfolder>
```

Move **folder** from local to cluster

```
scp -r foldername/ username@hostname:destination_file_path
```

File Transfer – Try it out

Open a **second** terminal window to manipulate local files and run the following:

1. **Local window:** Create a new file on your local machine

```
touch newfile.txt
```

2. **Local window:** Move the file to your home directory on the cluster

```
scp newfile.txt user@eofe7.mit.edu:/home/user  
scp newfile.txt user@txel-login.mit.edu:/home/gridsan/user
```

3. **Cluster window:** Create a new folder on the cluster

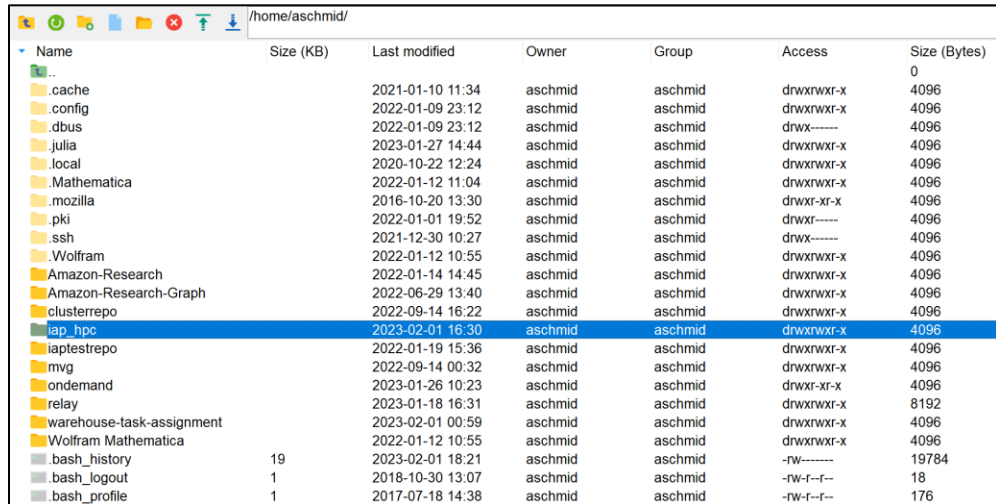
```
mkdir newfolder
```

4. **Local:** Move the new folder to your machine

```
scp -r user@eofe7.mit.edu:/home/user/newfolder/ ./  
scp -r user@txel-login.mit.edu:/home/gridsan/user/newfolder/ ./
```

Aside: Graphical Interface for Files

- Engaging OnDemand has a [GUI](#) interface for viewing and manipulating your files
- Windows users can also download and use [MobaXterm](#), which has a nice GUI file system in addition to a shell for running slurm commands
- You can view the SuperCloud file system through the [web portal](#)



Name	Size (KB)	Last modified	Owner	Group	Access	Size (Bytes)
..						0
.cache		2021-01-10 11:34	aschmid	aschmid	drwxrwxr-x	4096
.config		2022-01-09 23:12	aschmid	aschmid	drwxrwxr-x	4096
.dbus		2022-01-09 23:12	aschmid	aschmid	drwx-----	4096
.julia		2023-01-27 14:44	aschmid	aschmid	drwxrwxr-x	4096
.local		2020-10-22 12:24	aschmid	aschmid	drwxrwxr-x	4096
.Mathematica		2022-01-12 11:04	aschmid	aschmid	drwxrwxr-x	4096
.mozilla		2016-10-20 13:30	aschmid	aschmid	drwxr-xr-x	4096
.pki		2022-01-01 19:52	aschmid	aschmid	drwxr-----	4096
.ssh		2021-12-30 10:27	aschmid	aschmid	drwx-----	4096
.Wolfram		2022-01-12 10:55	aschmid	aschmid	drwxrwxr-x	4096
Amazon-Research		2022-01-14 14:45	aschmid	aschmid	drwxrwxr-x	4096
Amazon-Research-Graph		2022-06-29 13:40	aschmid	aschmid	drwxrwxr-x	4096
clusterrepo		2022-09-14 16:22	aschmid	aschmid	drwxrwxr-x	4096
lap_hpc		2023-02-01 16:30	aschmid	aschmid	drwxrwxr-x	4096
laptestrepo		2022-01-19 15:36	aschmid	aschmid	drwxrwxr-x	4096
mvq		2022-09-14 00:32	aschmid	aschmid	drwxrwxr-x	4096
ondemand		2023-01-26 10:23	aschmid	aschmid	drwxr-xr-x	4096
relay		2023-01-18 16:31	aschmid	aschmid	drwxrwxr-x	8192
warehouse-task-assignment		2023-02-01 00:59	aschmid	aschmid	drwxrwxr-x	4096
Wolfram Mathematica		2022-01-12 10:55	aschmid	aschmid	drwxrwxr-x	4096
.bash_history	19	2023-02-01 18:21	aschmid	aschmid	-rw-----	19784
.bash_logout	1	2018-10-30 13:07	aschmid	aschmid	-rw-r--r--	18
.bash_profile	1	2017-07-18 14:38	aschmid	aschmid	-rw-r--r--	176

Productivity Hack #2

MacOS: **Forklift** (personally I bought it – full worth)

Windows: **WinSCP**

Linux:

Productivity Hack #2

MacOS: **Forklift** (personally I bought it – full worth)

Windows: **WinSCP**

Linux: 🦴



We can also use Git and Github!

In the terminal logged in to your cluster, clone today's repo into your home directory:

```
git clone https://github.com/lisaxeverest/15.S60_2025.git
```

If you get an error about certificate verification, you may need to run:

```
git config --global http.sslVerify false
```

Go to the folder `8_hpc_and_efficiency` . Four folders for today's four examples:

- `1_interactive` (`_sc` for SuperCloud or `_eng` for Engaging)
- `2_batch`
- ...

Interactive Jobs

Starting an interactive job

Launch an interactive job with default resources

Engaging

```
srun --pty --partition=sched_any_quicktest bash
```

SuperCloud

```
LLsub -i
```

You can also specify your resources

Engaging

```
srun --pty --partition=sched_any_quicktest  
--cpus-per-task=1 --mem=2G bash
```

SuperCloud

```
LLsub -i -s 20 -g volta:1
```

Cpus

1 GPU

Loading Software

A variety of software is installed on the cluster, including many versions of Python, Julia, R, etc. To use them, we must load the appropriate module.

Load a known module

```
module load julia/1.8.5
```

See all modules

```
module avail
```

See specific modules, e.g. Julia

```
module avail julia
```

Start an Interactive Job

1. Start your interactive job

```
srun --pty --partition=sched_any_quicktest bash
```

```
LLsub -i
```

2. Load Julia

```
module load julia/1.8.5
```

3. Navigate to the first directory for today

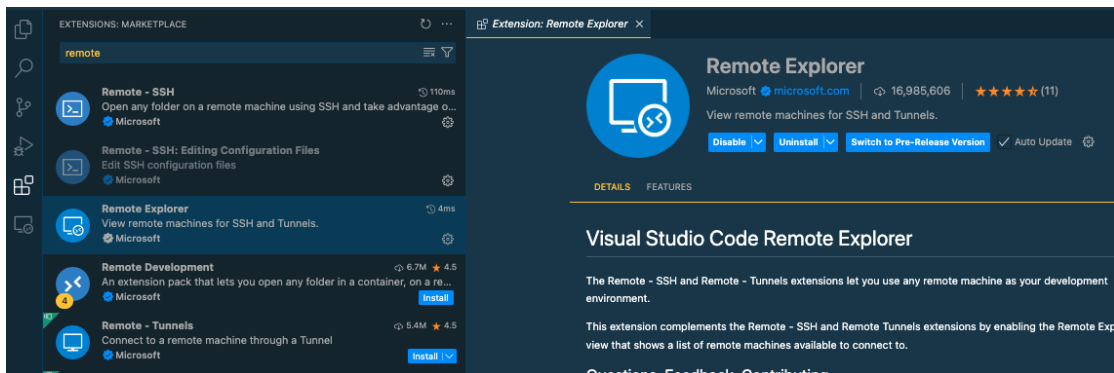
```
cd 1_interactive_sc or cd 1_interactive_eng
```

4. Run our test script

```
julia testscript.jl
```

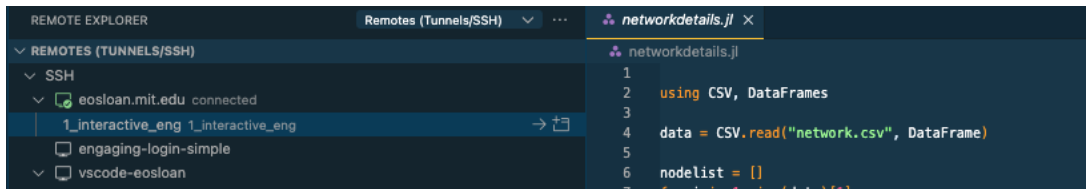
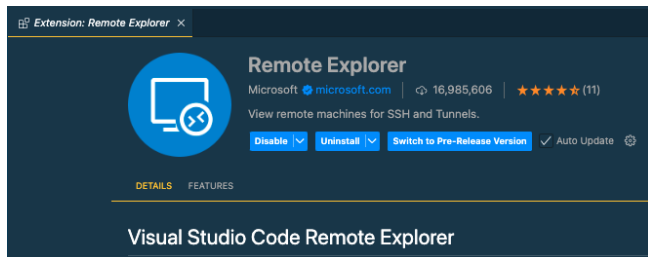
Productivity Hack #3

VSCode + Remote Development (Remote Explorer Extension)



Productivity Hack #3

VSCode + Remote Development (Remote Explorer Extension)



Passing Arguments

Let's run some of the scripts in `1_interactive` which find the shortest path between two nodes in the network given in the CSV file

1. First, let's check out the network details

```
julia networkdetails.jl
```

2. Let's find the shortest path between node 1 and node 20

```
julia shortestpath_noargs.jl
```

3. Now, let's pass two arguments to find the shortest path between nodes 6 and 7

```
julia shortestpath_args.jl 6 7
```

The .bashrc file

The problem:

- In order to load Julia, I need to run `module load julia/1.8.5`
- I need to do that **every time** before running my code
- Can I avoid that? Can I tell the cluster to automatically load Julia?

What is .bashrc ?

- File that is executed **every time** you log into the cluster or a node
- Can be edited using `nano ~/.bashrc`
- Append any code you want to automatically run every time **at the end of the file**

Batch Jobs

Batch Jobs

Instead of interacting directly, we'll tell the cluster to run a set of commands on its own time!

- Run scripts with long computational time or that require lots of resources
- Running many scripts at once (e.g. testing an algorithm on 100 different datasets or instances)

Shell scripts

We tell the cluster what commands to execute with a shell script:

```
#!/bin/bash
```

“shebang”

```
#Set up computing environment
```

```
#SBATCH --cpus-per-task=2
```

```
#SBATCH --mem=16G
```

```
#SBATCH --partition=sched_mit_sloan_batch
```

```
#SBATCH --time=1-00:00
```

```
#SBATCH -o outputlog.out
```

**request resources
(optional)**

```
#Load software
```

```
module load julia/1.7.3
```

```
module load gurobi/9.0.3
```

load software

```
#Run the script as usual
```

```
julia myscript.jl
```

**run script, pass
arguments**

Kicking off a batch job

Write your batch shell script!

```
touch mybatchfile.sh  
nano mybatchfile.sh
```

Kickoff job

```
sbatch mybatchfile.sh
```

Monitor your jobs

Engaging:

```
eo-show-myjobs
```

SuperCloud:

```
LLstat
```

Batch Job – Try it out

1. Navigate to the folder `2_batch_sc` or `2_batch_eng`

2. Take a look at the batch file

```
cat batchjob.sh
```

3. Kick it off, check it out, then look at the results!

```
sbatch batchjob.sh
```

```
eo-show-myjobs or LLstat
```

```
cat outputlog.out
```

Resources

Task	Syntax
CPUs	<code>--cpus-per-task=1</code>
Memory	<code>--mem=4G</code>
Time	<code>--time=1-00:00</code>

Engaging

Check partition resources with:

```
eo-show-partition
```

SuperCloud

Check available resources with:

```
LLfree
```

When the cluster is busy, your job will be queued until the resources are available.
The job will fail if you use more than the requested memory.

Takeaways

- **Interactive** jobs let you code as if the cluster were your computer, while **batch jobs** run without your intervention
- Use **interactive** jobs when **prototyping** and **testing**, use **batch** jobs to kick off your **final runs**
- **Never run your scripts on the login node!** Use `sbatch` to start a batch job, or `srun / LLsub -i` to start an interactive job
- **DOCUMENTATION (IMPORTANT):**

<https://engaging-web.mit.edu/eofe-wiki/> (OLDER, SLIGHTLY DEPRECATED)

<https://orcd-docs.mit.edu/> (MORE RECENT, MORE OFFICIAL)

Break

Job Arrays

Submitting many batch jobs at once

We have a script and we want to run it for several different parameters.

e.g. testing a new optimization model or algorithm on many instances

Let's check out an example in this folder:

`3_array_eng/`

or

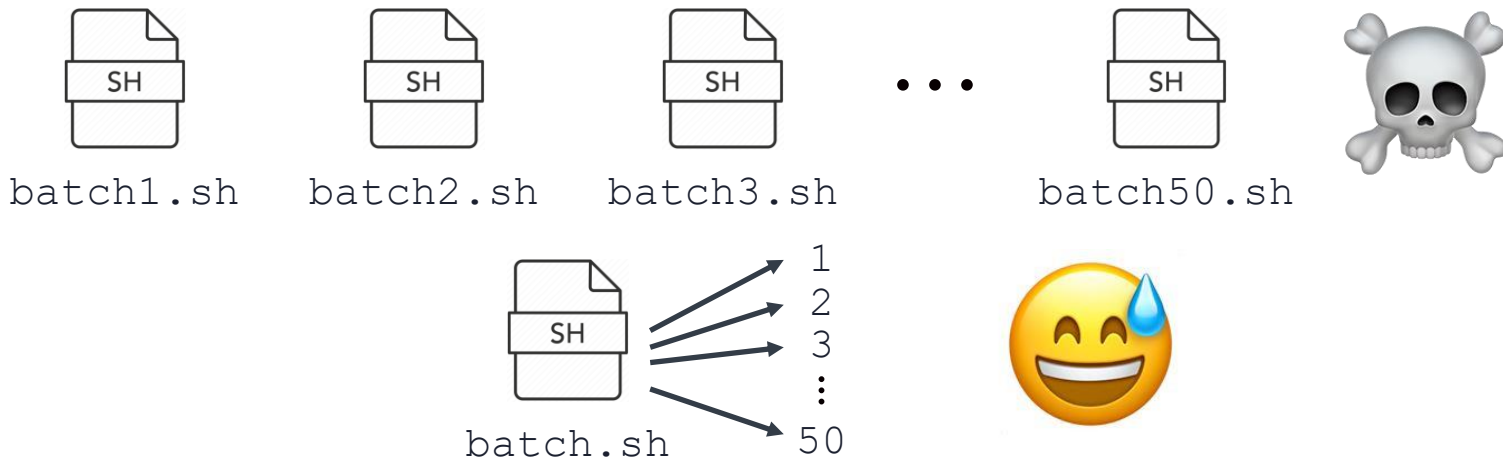
`3_array_sc/`

How would you approach this?

Script: `shortestpath_one.jl`

Instance list: `data/`

How can we use the cluster to accomplish this?



Job Array Batch Script - Engaging

```
#!/bin/bash
```

```
#SBATCH -a 1-50
```

```
#SBATCH --cpus-per-task=1
```

```
#SBATCH --mem=2G
```

```
#SBATCH --partition=sched_mit_sloan_batch
```

```
#SBATCH --time=0-00:10
```

```
#SBATCH -o /home/aschmid/iap_hpc/run_\%a.out
```

```
#SBATCH -e /home/aschmid/iap_hpc/run_\%a.err
```

```
#Load software
```

```
module load julia/1.7.3
```

```
#Run the script as usual
```

```
julia shortestpath_one.jl $SLURM_ARRAY_TASK_ID
```

Job Array Batch Script - [SuperCloud](#)

```
#!/bin/bash
```

```
#SBATCH -o array.sh.log-%a
```

```
#SBATCH -a 1-3
```

```
#Load software
```

```
module load julia/1.7.3
```

```
julia shortestpath_many.jl $SLURM_ARRAY_TASK_ID
```

```
$SLURM_ARRAY_TASK_COUNT
```

Modifying our Julia script

We need to tell Julia that we'll be passing arguments and specify how she should handle them. For example,

```
runid = parse{Int, ARGS[1]}

networkfile = string("data/network", runid, ".csv")
outputfile = string("outputs/network", runid, ".csv")
```


Kickoff Job Array – Try it out

1. Kick off the batch job

```
sbatch array.sh
```

2. Once it completes, check out the `outputs` folder

```
ls outputs/
```

3. Run the script `combineoutputfiles.jl` to gather the outputs from the experiments into one file (use an interactive job to avoid login node!)

```
srun... or LLsub -i  
module load julia/1.7.3  
julia combineoutputfiles.jl
```

4. Check out the combined file

```
cat outputs/combined.csv
```

Poll Question

pollev.com/georgemargaritis537

What if instead of having each of the 50 runs write to its own output file, we had them all write to one file?

- A.) All 50 would write to the output file, but the rows may be in a random order
- B.) Some of the 50 may overwrite each other, leaving an incomplete output file
- C.) An error, as all jobs are trying to access the same file at the same time

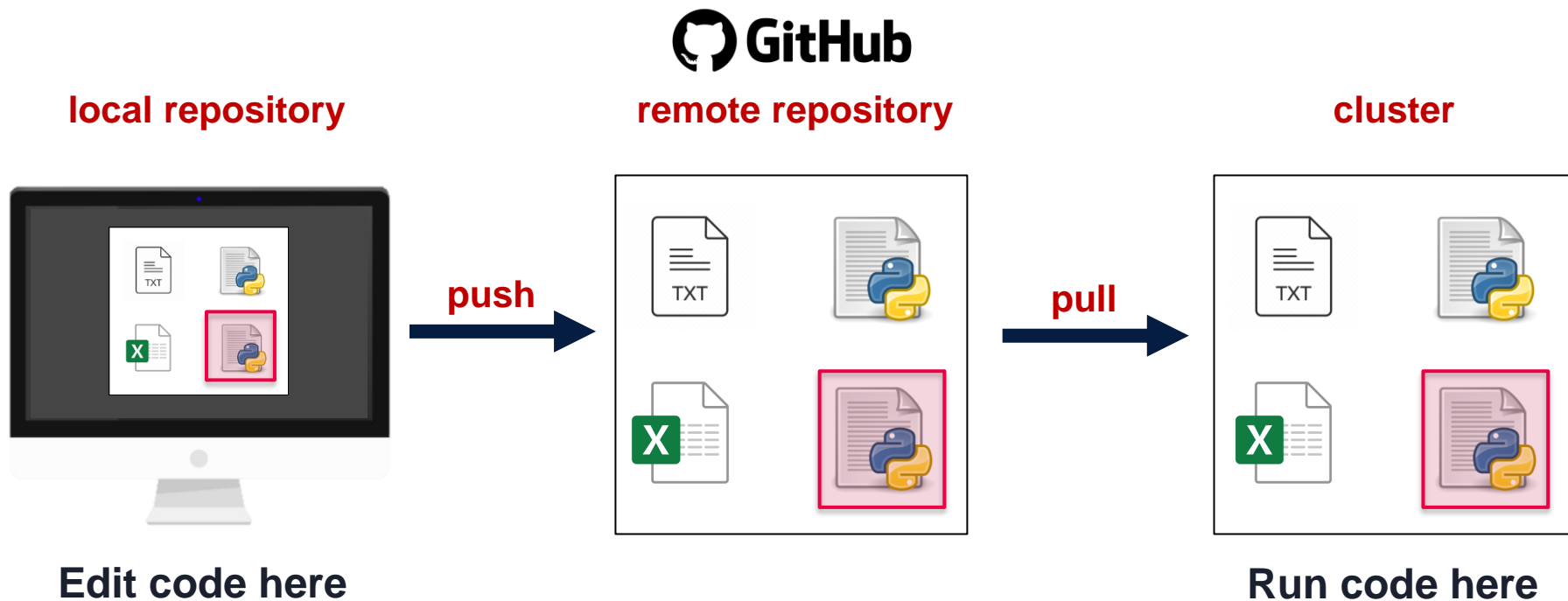
Best Practices

- Before kicking off n jobs (where n is large), test code locally, then perhaps interactively, then kick-off 1-3 batch runs to avoid having all n fail
- Be mindful about the resources you request! The scheduler may give you lower priority if you run jobs requesting a lot of resources, so make sure you request what you need
- To automate the last step (gathering files), check out [LLMapReduce](#) if you're using SuperCloud

Collaboration Tips

Collaborating with the Cluster

We know we can use Git/Github on the cluster. We can then:



Connecting Engaging to Github

Follow the link below for instructions on how to generate an SSH key for your Github account, add your key to the SSH agent, then add the key to your Github account <https://docs.github.com/en/get-started/quickstart/set-up-git>

Aside: Data Storage on the Cluster

- If your data is small, you can just store it on Github
- Otherwise, SuperCloud has a nice collaboration features that lets you create a shared group directory, which will be stored in `/home/gridsan/groups`
 - To request a group directory, send email to `supercloud@mit.edu` ([details](#))

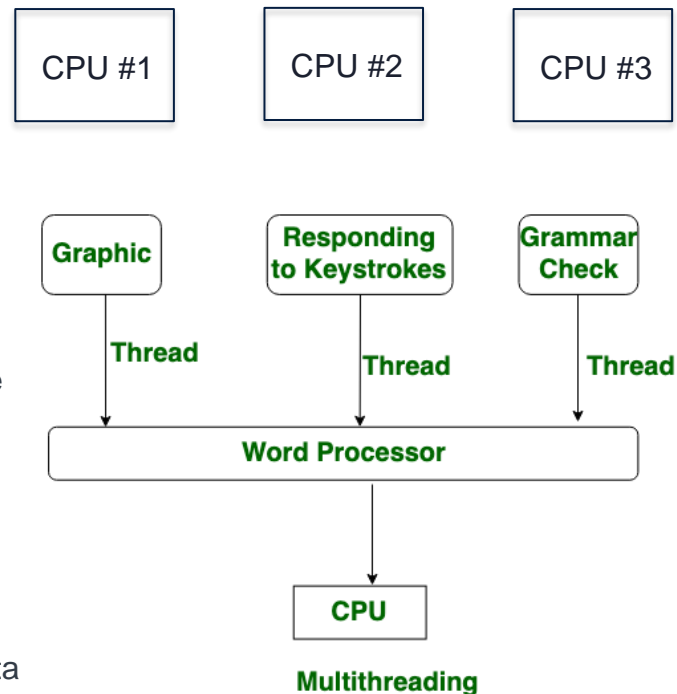
Storage space:

- **Engaging:** `/home/username` (100GB per user)
`/pool001/username` (1TB per user)
- **SuperCloud:** `/home/gridsan/username` (no limit)

Parallel Computing: Multithreading

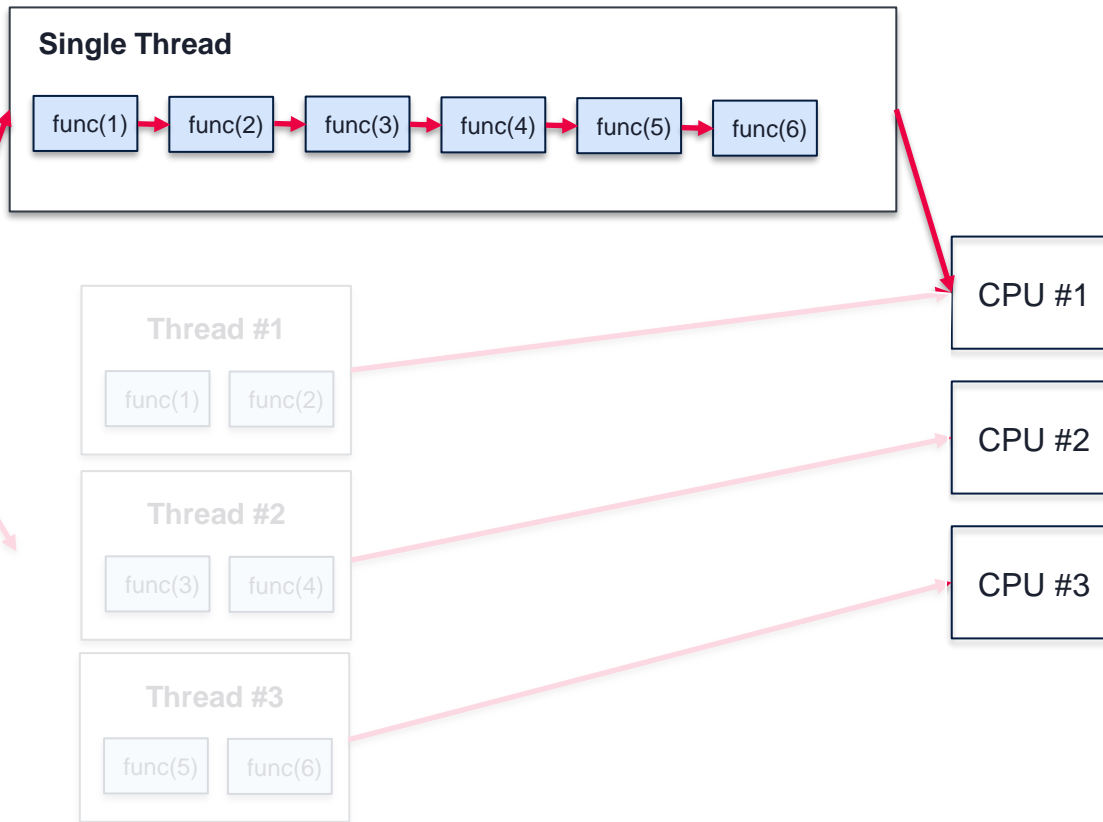
Multithreading

- Multithreading allows a computer program to perform multiple tasks concurrently.
- **Thread:** A lightweight unit of a process that can execute independently. Think of it as a small unit of work within a program.
- If we have multiple CPUs, multiple threads can be processed at the same time by our CPUs:
 - **Program can run much faster!**
- Biggest challenge:
 - **Race conditions:** Occur when multiple threads access shared data at the same time. May lead to unpredictable outcomes



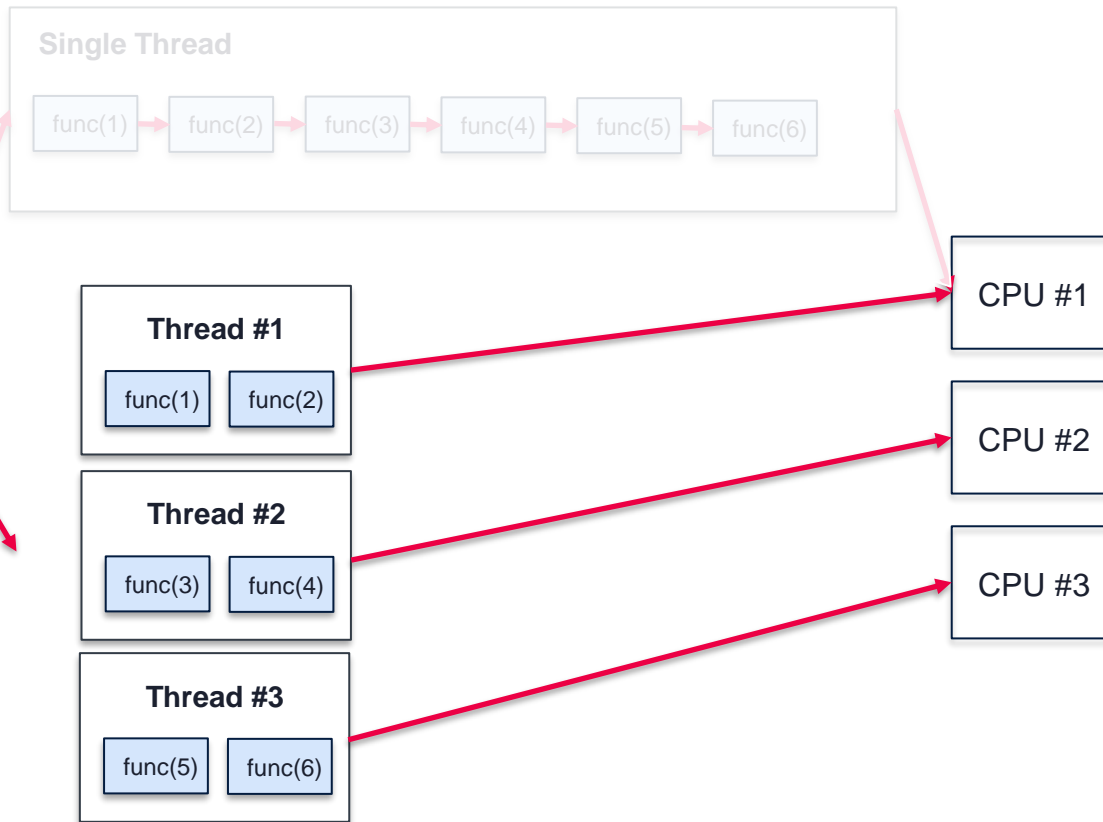
Single-threading vs Multithreading

```
r = 0
for i=1...6
  r += func(i)
end
```



Single-threading vs Multithreading

```
r = 0
for i=1...6
  r += func(i)
end
```



Parallelizing Julia for loops

File: loop_1.jl

```
1 using Base.Threads
2
3 function my_long_running_function(i)
4     sleep(1) # Waits for 1 second
5     return i
6 end
7
8 result = 0
9 a = 5
10
11 @time begin # This counts the execution time of the block
12     for i in -a:a # Loop from -a to a with step 1
13         global result = result + my_long_running_function(i)
14     end
15 end;
16
17 println("Result: $(result)")
18
```

- Assume we only have 1 CPU:
 - **Supercloud:** LLsub -i -s 1
 - **Engage:** srun --pty --cpus-per-task=1 bash
- Answer the following:
 - Loop execution time?
 - Result?

Parallelizing Julia for loops

File: loop_1.jl

```
1 using Base.Threads
2
3 function my_long_running_function(i)
4     sleep(1) # Waits for 1 second
5     return i
6 end
7
8 result = 0
9 a = 5
10
11 @time begin # This counts the execution time of the block
12     for i in -a:a # Loop from -a to a with step 1
13         global result = result + my_long_running_function(i)
14     end
15 end;
16
17 println("Result: $(result)")
18
```

- Assume we only have 1 CPU:
 - **Supercloud:** LLsub -i -s 1
 - **Engage:** srun --pty --cpus-per-task=1 bash
- Answer the following:
 - Loop execution time? **11 seconds**
 - Result? **0**

Parallelizing Julia for loops

File: loop_1.jl

```
1 using Base.Threads
2
3 function my_long_running_function(i)
4     sleep(1) # Waits for 1 second
5     return i
6 end
7
8 result = 0
9 a = 5
10
11 @time begin # This counts the execution time of the block
12     for i in -a:a # Loop from -a to a with step 1
13         global result = result + my_long_running_function(i)
14     end
15 end;
16
17 println("Result: $(result)")
18
```

- Assume we have 11 CPUs:
 - **Supercloud:** LLsub -i -s 11
 - **Engage:** srun --pty --cpus-per-task=11 bash
- Answer the following:
 - Loop execution time?
 - Result?

Parallelizing Julia for loops

File: loop_1.jl

```
1 using Base.Threads
2
3 function my_long_running_function(i)
4     sleep(1) # Waits for 1 second
5     return i
6 end
7
8 result = 0
9 a = 5
10
11 @time begin # This counts the execution time of the block
12     for i in -a:a # Loop from -a to a with step 1
13         global result = result + my_long_running_function(i)
14     end
15 end;
16
17 println("Result: $(result)")
18
```

- Assume we have 11 CPUs:
 - **Supercloud:** LLsub -i -s 11
 - **Engage:** srun --pty --cpus-per-task=11 bash
- Answer the following:
 - Loop execution time? **11 seconds**
 - Result? **0**

Parallelizing Julia for loops

File: loop_2.jl

```
1 using Base.Threads
2
3 function my_long_running_function(i)
4     sleep(1) # Waits for 1 second
5     return i
6 end
7
8 result = 0
9 a = 5
10
11 @time begin # This counts the execution time of the block
12     @threads for i in -a:a # Loop from -a to a with step 1
13         global result = result + my_long_running_function(i)
14     end
15 end;
16
17 println("Result: $(result)")
18
```

- Assume we have 11 CPUs:
 - **Supercloud:** `LLsub -i -s 11`
 - **Engage:** `srun --pty --cpus-per-task=11 bash`
- Answer the following:
 - Loop execution time?
 - Result?

This macro **parallelizes** the loop and runs it across multiple threads. Make sure to run `julia -t <num_threads> loop_2.jl` to run Julia with multiple threads, where `<num_threads>=<num_cpus>`

Parallelizing Julia for loops

File: loop_2.jl

```
1 using Base.Threads
2
3 function my_long_running_function(i)
4     sleep(1) # Waits for 1 second
5     return i
6 end
7
8 result = 0
9 a = 5
10
11 @time begin # This counts the execution time of the block
12     @threads for i in -a:a # Loop from -a to a with step 1
13         global result = result + my_long_running_function(i)
14     end
15 end;
16
17 println("Result: $(result)")
18
```

This macro **parallelizes** the loop and runs it across multiple threads. Make sure to run `julia -t <num_threads> loop_2.jl` to run Julia with multiple threads, where `<num_threads>=<num_cpus>`

- Assume we have 11 CPUs:
 - **Supercloud:** `LLsub -i -s 11`
 - **Engage:** `srun --pty --cpus-per-task=11 bash`
- Answer the following:
 - Loop execution time? **1 seconds**
 - Result? **Unknown!!!!**

↓
Threads read/write to the same variable `result` at the same time: **"Race condition"**

Race Condition

Shopping List on Google Sheets



Read 1

Item	Quantity
Apples	1
...	...

Read 1

I need 2 more Apples
for a smoothie:

Total apples = 1+2=3



John

I need 3 more Apples
for Apple pie:

Total apples = 1+3=4



Julia

Race Condition

Shopping List on Google Sheets



Item	Quantity
Apples	1
...	...

I need **2** more Apples
for a smoothie:

Total apples = 1+2=3



John

Write **3**

I need **3** more Apples
for Apple pie:

Total apples = 1+3=4



Julia

Race Condition

Shopping List on Google Sheets



Item	Quantity
Apples	1
...	...

I need **2** more Apples
for a smoothie:

Total apples = 1+2=3



John

Write **3**

I need **3** more Apples
for Apple pie:

Total apples = 1+3=4



Julia

Write **4**

Race Condition

Shopping List on Google Sheets



Item	Quantity
Apples	?
...	..

I need 2 more Apples
for a smoothie:

Total apples = 1+2=3



John

Write 3

**Wrong/Unknown
value!**

I need 3 more Apples
for Apple pie:

Total apples = 1+3=4



Julia

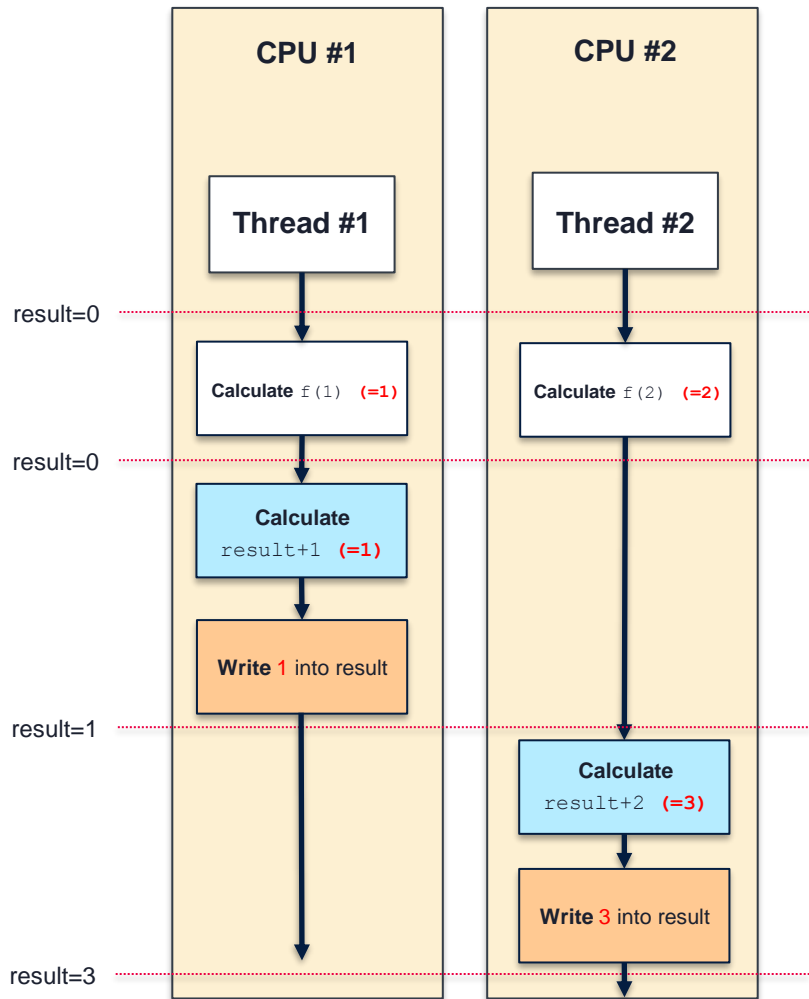
Write 4

Correct value = 6

Race Condition

```
1  using Base.Threads
2
3  function f(i)
4      sleep(1)
5      return i
6  end
7
8  result = 0
9
10 @threads for i in 1:2 # Loop from 1 to 2
11     global result = result + f(i)
12 end
13
14 println("Result: $(result)")
15
```

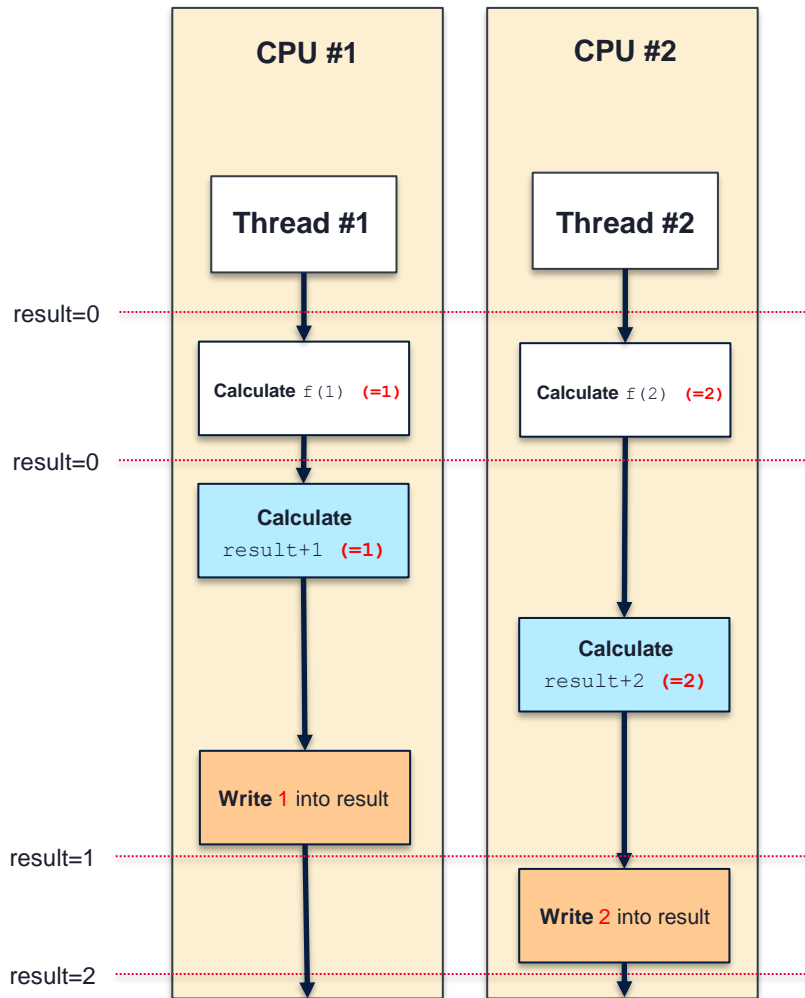
Correct value!



Race Condition

```
1  using Base.Threads
2
3  function f(i)
4      sleep(1)
5      return i
6  end
7
8  result = 0
9
10 @threads for i in 1:2 # Loop from 1 to 2
11     global result = result + f(i)
12 end
13
14 println("Result: $(result)")
15
```

Incorrect value!



Parallelizing Julia for loops

File: loop_3.jl

```
1 using Base.Threads
2 using SharedArrays
3
4 function my_long_running_function(i)
5     sleep(1) # Waits for 1 second
6     return i
7 end
8
9 a = 5
10
11 # Array of size 11 used to hold the individual results.
12 # This array is "Shared" by the threads
13 results = SharedArray{Int}(2*a+1)
14
15
16 @time begin # This counts the execution time of the block
17     @threads for i in -a:a # Loop from -a to a with step 1
18         results[i+a+1] = my_long_running_function(i)
19     end
20 end;
21
22 result = sum(results)
23
24 println("Result: $(result)")
```

- 1 We first write the individual results in a thread-safe array
- 2 We accumulate in the end

- Assume we have 11 CPUs:
 - **Supercloud:** `LLsub -i -s 11`
 - **Engage:** `srun --pty --cpus-per-task=11 bash`
- Answer the following:
 - Loop execution time?
 - Result?

Parallelizing Julia for loops

File: loop_3.jl

```
1 using Base.Threads
2 using SharedArrays
3
4 function my_long_running_function(i)
5     sleep(1) # Waits for 1 second
6     return i
7 end
8
9 a = 5
10
11 # Array of size 11 used to hold the individual results.
12 # This array is "Shared" by the threads
13 results = SharedArray{Int}(2*a+1)
14
15
16 @time begin # This counts the execution time of the block
17     @threads for i in -a:a # Loop from -a to a with step 1
18         results[i+a+1] = my_long_running_function(i)
19     end
20 end;
21
22 result = sum(results)
23
24 println("Result: $(result)")
```

- 1 We first write the individual results in a thread-safe array
- 2 We accumulate in the end

- Assume we have 11 CPUs:
 - **Supercloud:** `LLsub -i -s 11`
 - **Engage:** `srun --pty --cpus-per-task=11 bash`
- Answer the following:
 - Loop execution time? **1 seconds**
 - Result? **0!**

Multithreading is language-specific: Python

```
import ray
import time

# Define a remote function that performs the computation on a single element
@ray.remote
def long_running_function(i):
    time.sleep(1)
    return i

if __name__ == "__main__":

    # Start Ray
    ray.init(num_cpus=4)

    tasks = [long_running_function.remote(i) for i in range(-5, 6)]

    # Retrieve the results from the remote tasks
    results = ray.get(tasks)

    r = sum(results)

    # Print the results
    print("Result: ", r)
```

- Python code that performs exactly the same Julia task we saw before
- Personal opinion: Best parallelization library in python is **ray**

Takeaways

- Increasing CPU count **does not** necessarily make your program faster:
 - **First**, examine if your program can use multiple CPUs
 - **Then**, request more than 1 CPUs: Be mindful about the resources you request
- Some libraries (e.g. Gurobi, numpy) already exploit multiple cores
- ≠ If you write your own code, you need to parallelize it **yourself**:
 - Each language has its own syntax for multiprocessing/multithreading
 - Be careful about **Race Conditions**:
 - **Multiple threads accessing the same variable at the same time**
 - Consider using “**thread-safe**” variables or **mutexes/locks**. [More Info](#)

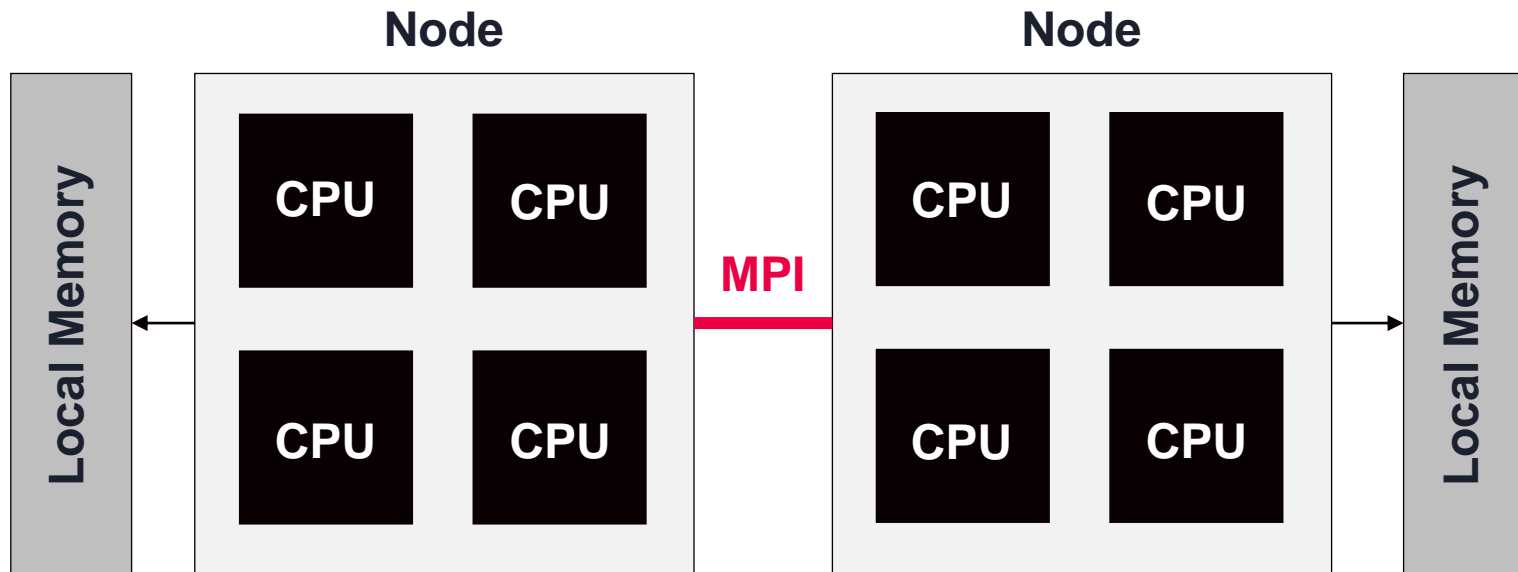
Parallel Computing on SuperCloud: MPI

Adapted from Alex Schmid & Lauren Milechin

Distributed computing

- Multithreading can only happen in the **same node**
- Multithreading is limited by the **number of CPUs** in the node:
 - Using more threads than CPUs doesn't increase performance
- How can we parallelize across nodes & CPUs?
- **MPI!**

Distributed computing



Parallelization

We can use **MPI (Message Passing Interface)** to parallelize our code!

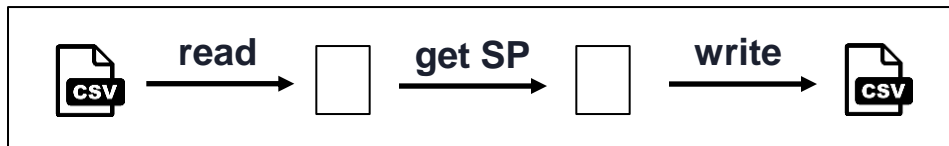
Unlike the commands we've run so far today, integrating MPI requires language-specific code

→ We will use **MPI.jl** to integrate parallelization into our Julia code

```
1 using MPI
2
3 # Initialize MPI environment
4 MPI.Init()
5
6 # Get MPI process rank id
7 rank = MPI.Comm_rank(MPI.COMM_WORLD)
8
9 # Get number of MPI processes in this communicator
10 nproc = MPI.Comm_size(MPI.COMM_WORLD)
11
12 # Print hello world message
13 print("Hello world, I am rank $(rank) of $(nproc)
14 processors\n")
15
16
```

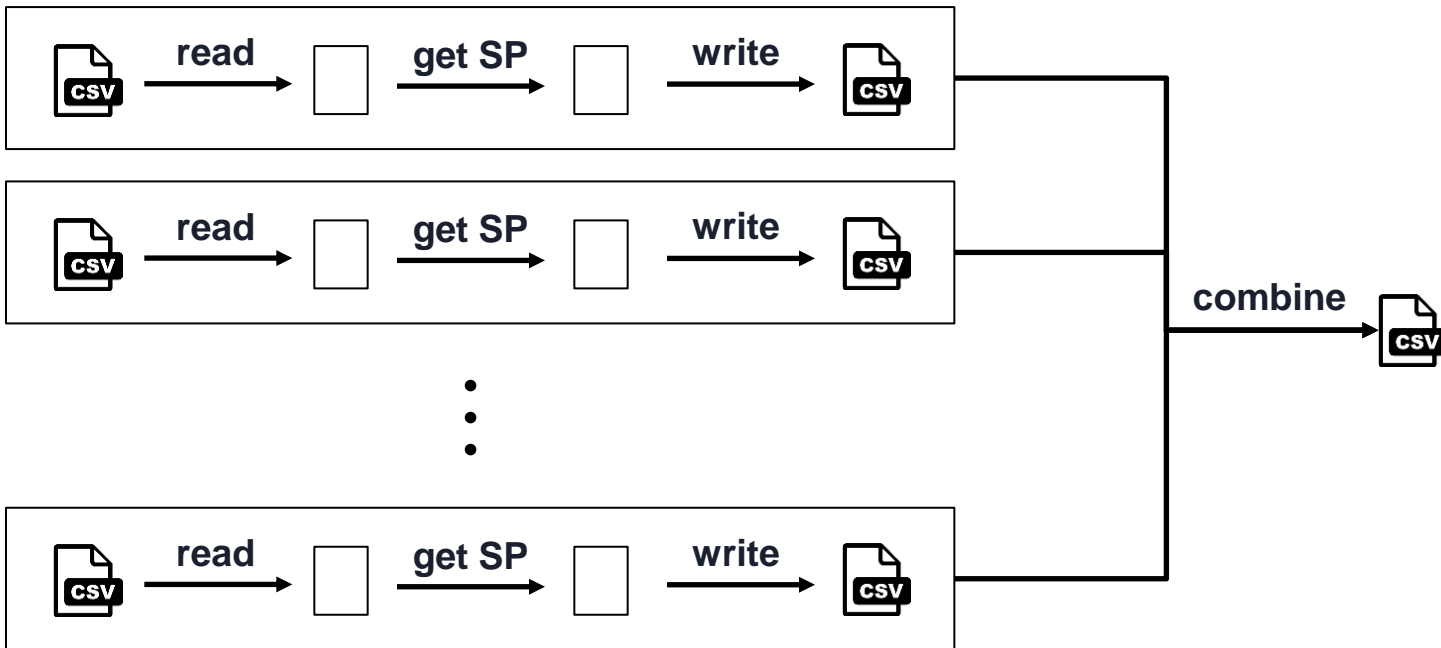
Option 1: One big for loop

```
for runid in 1:50
```

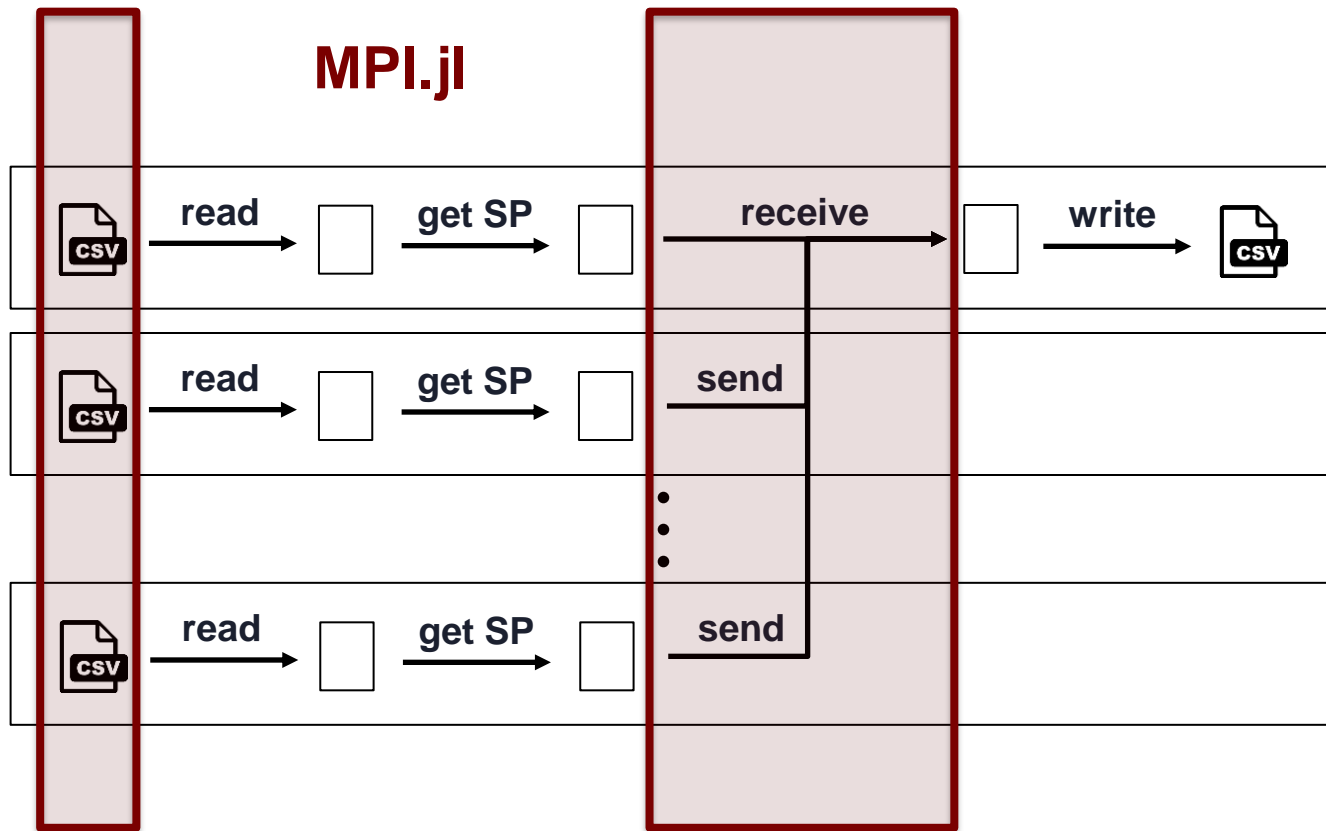


```
end
```


Option 2: Job array / MapReduce



Option 3: Parallelize across nodes & cores



MPI Commands

Initialize MPI environment

```
MPI.Init()
```

MPI communicator

```
MPI.COMM_WORLD
```

The number of MPI processes

```
MPI.Comm_size
```

The rank / ID of a given process

```
MPI.Comm_rank
```

Send message

```
MPI.send(message, recvr_rank, my_id, comm)
```

Receive message

```
MPI.recv(sender_rank, my_id, comm)
```

Running parallelized code with MPI

1. Navigate to `5_parallel_mpi`

2. Load `mpi`, add `MPI.jl`, and build `MPI.jl`

```
module load Julia/1.8.5
module load mpi/openmpi-4.1.5
julia
using Pkg
Pkg.add("MPI")
Pkg.build("MPI")
```

If you get a wrong MPI version warning during `mpirun`:

```
Pkg.add("MPIPreferences")
julia --project -e 'using MPIPreferences; MPIPreferences.use_system_binary()'
```

3. Kickoff `hello_mpi.jl` with `mpi` and four cores

```
mpirun -n 4 julia hello_mpi.jl
```

Running parallelized code with MPI

1. Navigate to `5_parallel_mpi`
2. Run `sbatch sp_mpi.sh` which runs the following script:

This runs the shortest path algorithm we saw in previous parts, but it uses MPI to split the scenarios across the different CPUs

3. Observe the output file:

```
1  #!/bin/bash
2
3  #Slurm sbatch options
4  #SBATCH -n 4
5
6  #Load software
7  module load julia/1.7.3
8  module load mpi
9
10 #Run the script as usual
11 mpirun julia shortestpath_mpi.jl
```

```
gmargaritis@login-4:~/15_S60_2024/8_hpc_and_efficiency/4_parallel_sc$ cat slurm-24903907.out
Hello, World! I am rank 1 of 4 processors, running 2:4:50.
Hello, World! I am rank 2 of 4 processors, running 3:4:47.
Hello, World! I am rank 3 of 4 processors, running 4:4:48.
Hello, World! I am rank 0 of 4 processors, running 1:4:49.

2: Sending data 2 -> 0
3: Sending data 3 -> 0
1: Sending data 1 -> 0
```

Questions?

Final assignment in `assignment`

Due: Saturday, Feb 1 at 11:59pm (hard deadline)

Best of luck in the upcoming semester 😊

Thank you!