HIGH-PERFORMANCE COMPUTING + EFFICIENCY

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

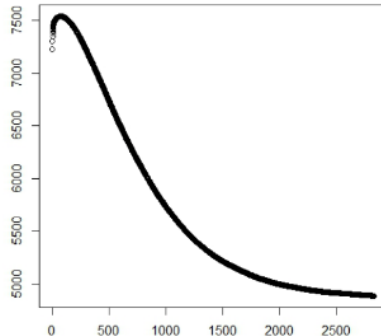# Clusters

Why do we use computing clusters?

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

Deep learning on a
large dataset
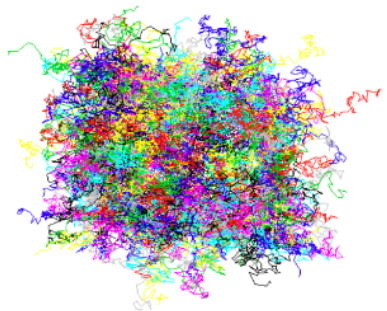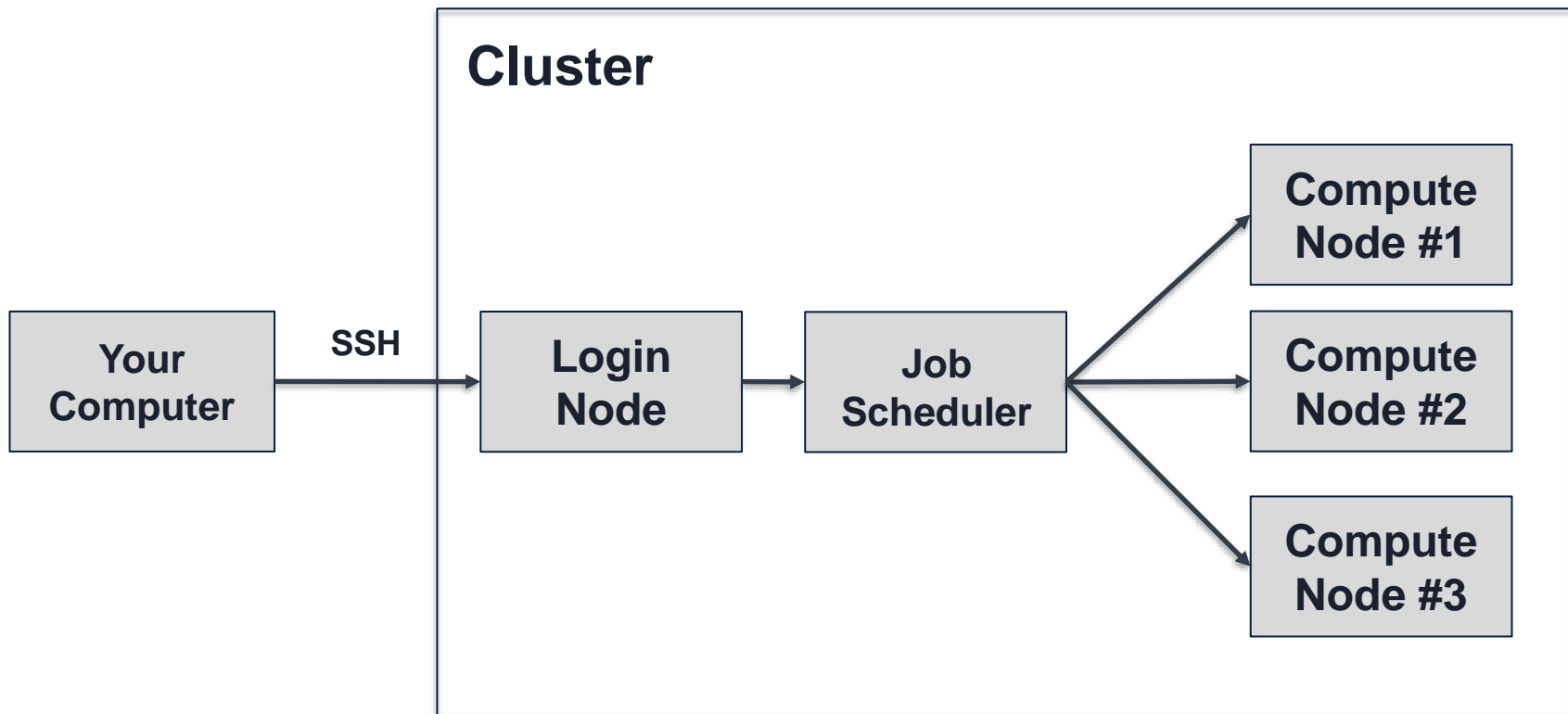
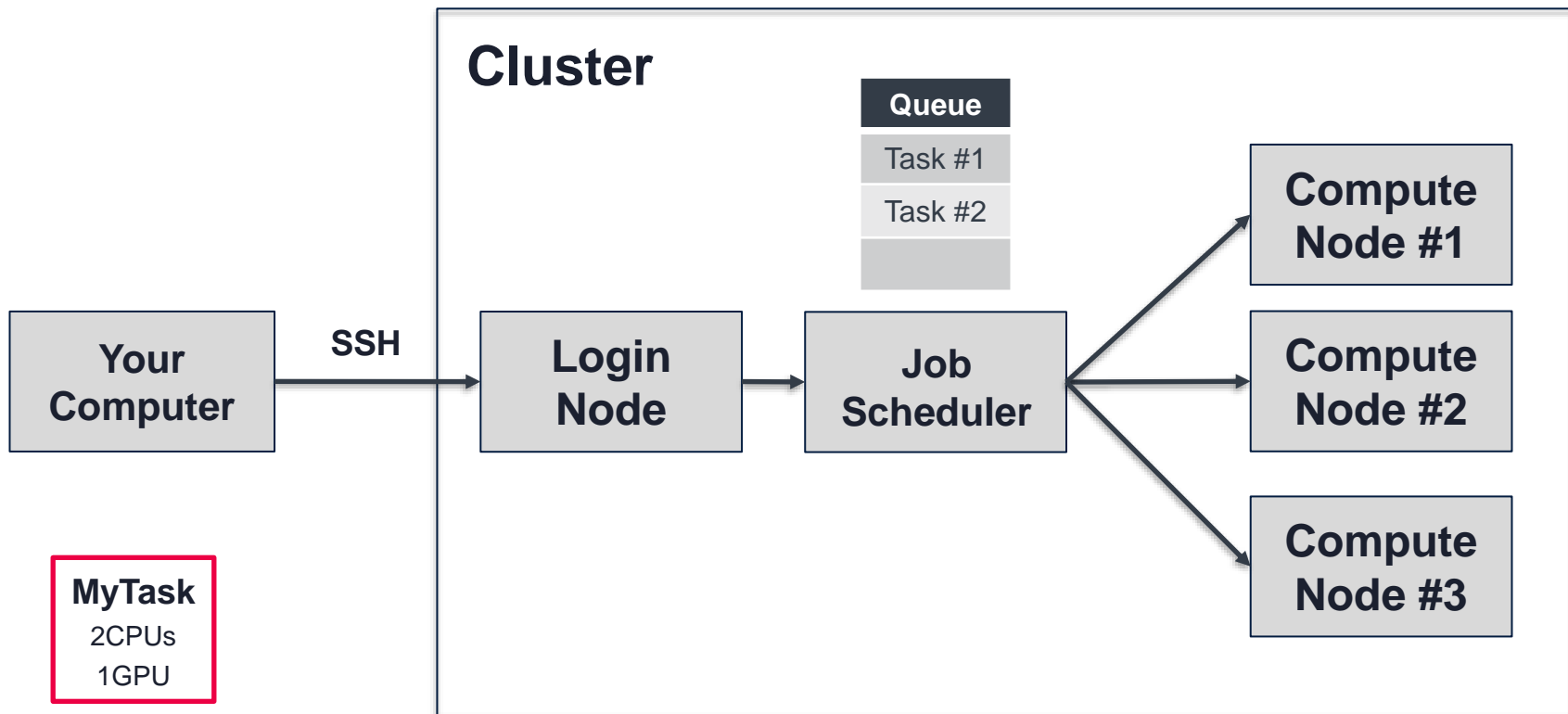Simulations (e.g. Monte-Carlo)

Hard optimization problems

Usually need a
lot of:

GPU

CPU

MEMORY

Using a cluster

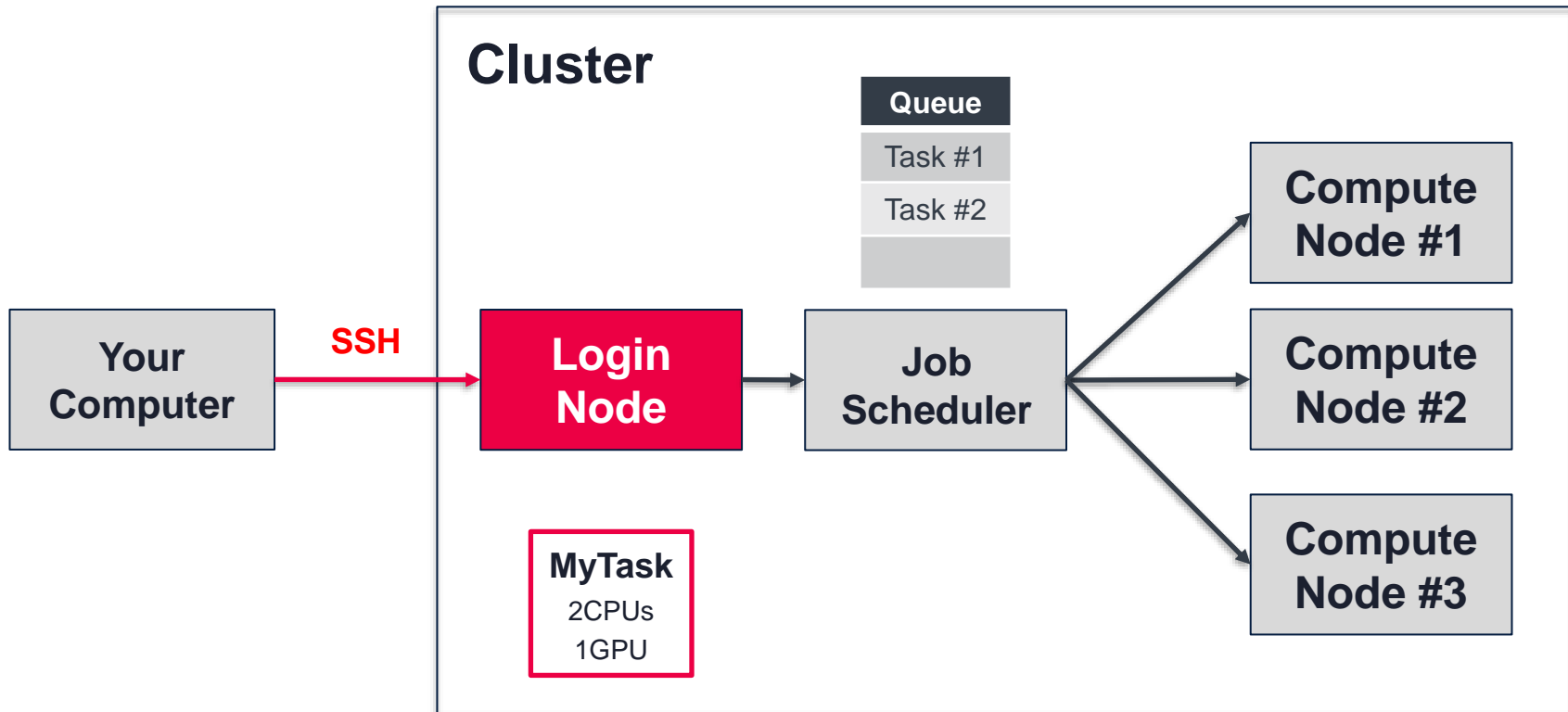# Using a cluster

Using a cluster
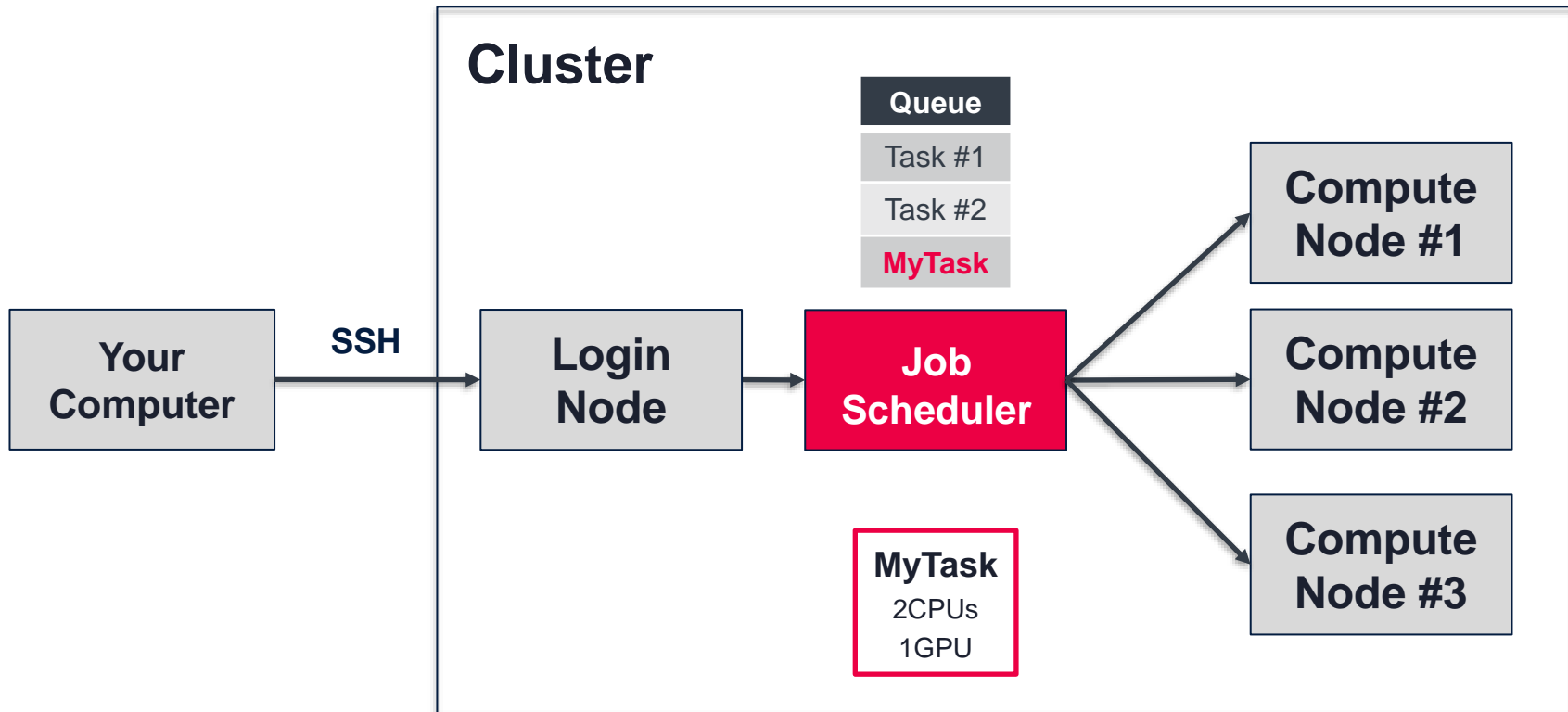
Using a cluster
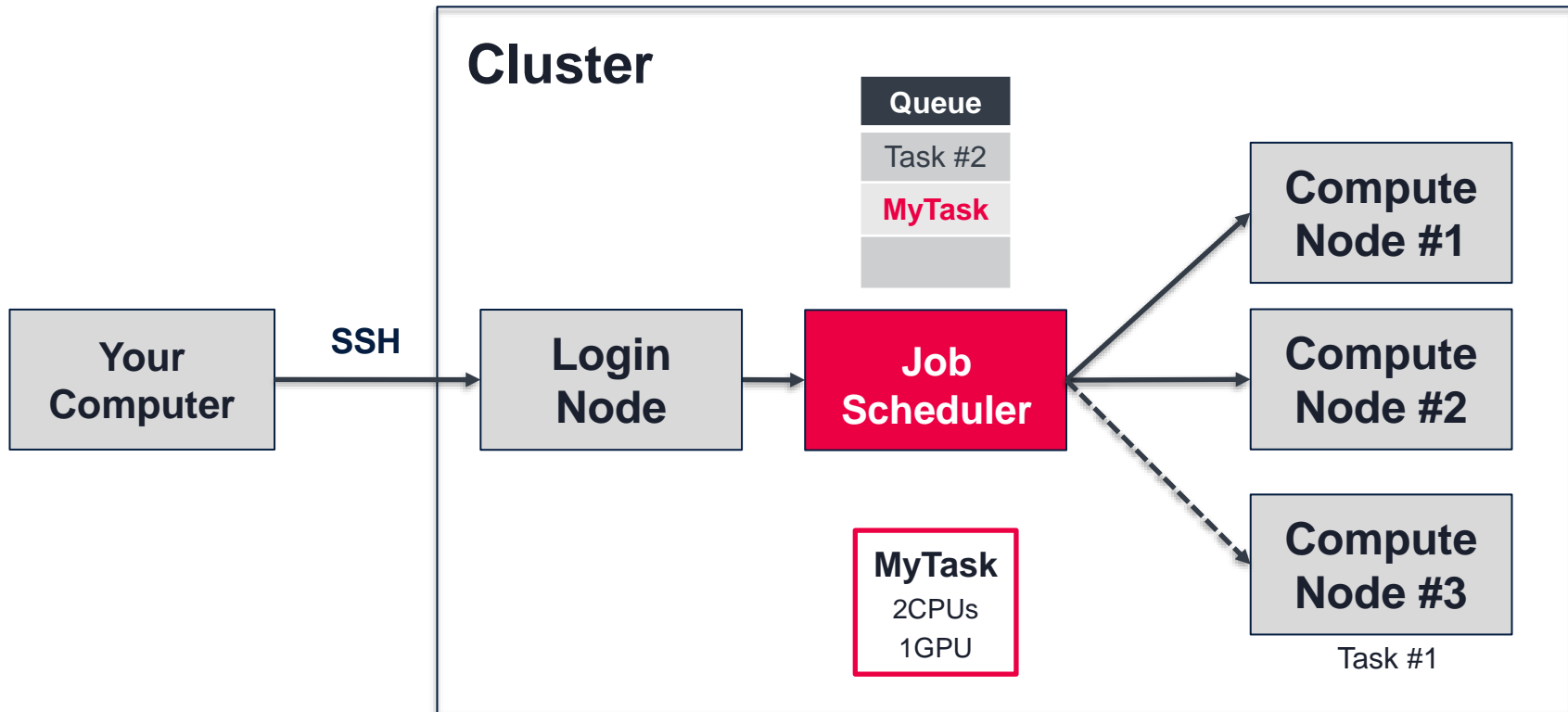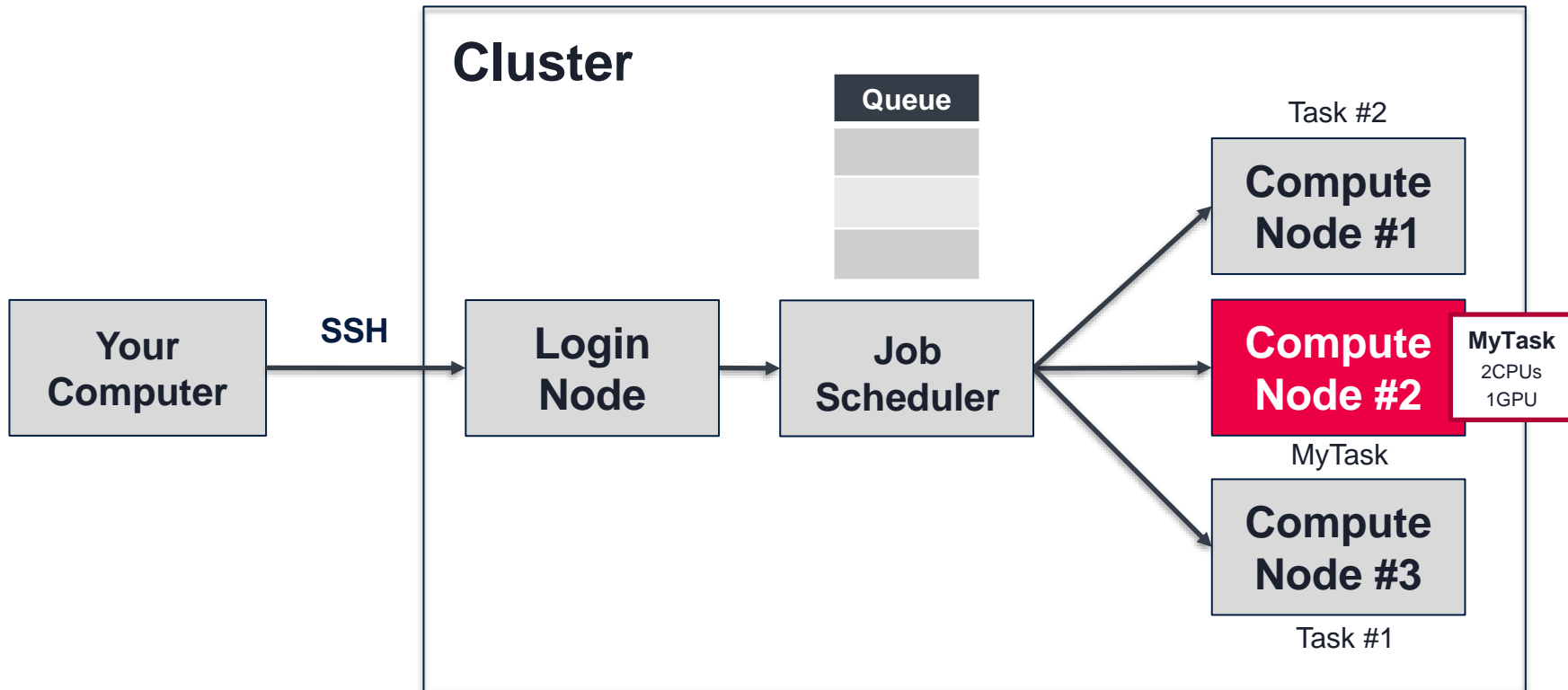
Using a cluster

Using a cluster

Using a cluster

Poll Question

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
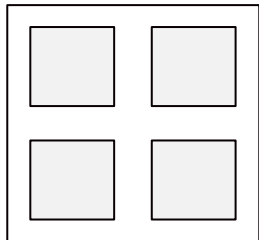
sched_any
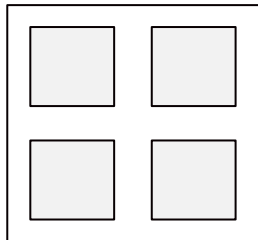
newnodes
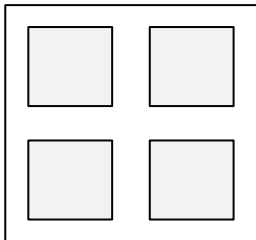
Sloan

sched_mit_sloan_interactive
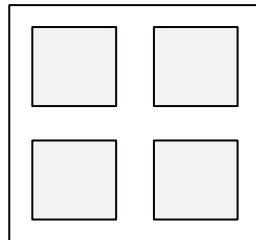
sched_mit_sloan_batch
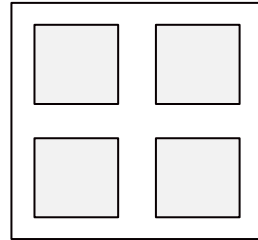
SuperCloud

xeon-p8
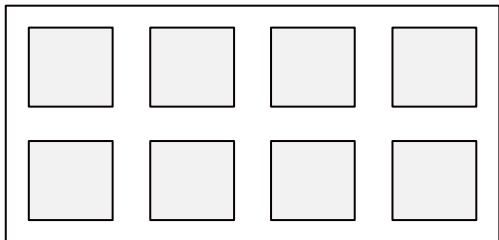
xeon-p8-volta
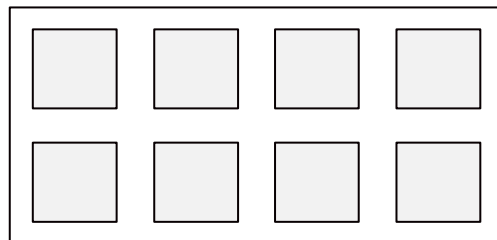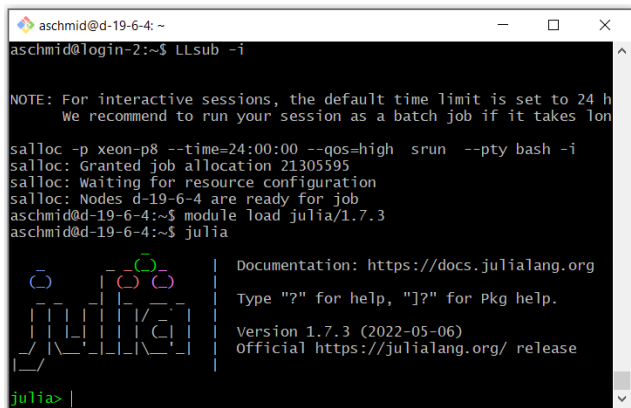
Node example: Supercloud

Node

CPU   CPU

GPU   RAM

- **40 CPU cores**
- **384 GB Ram**
- **32 GB GPU**

xeon-p8-volta

224 nodes
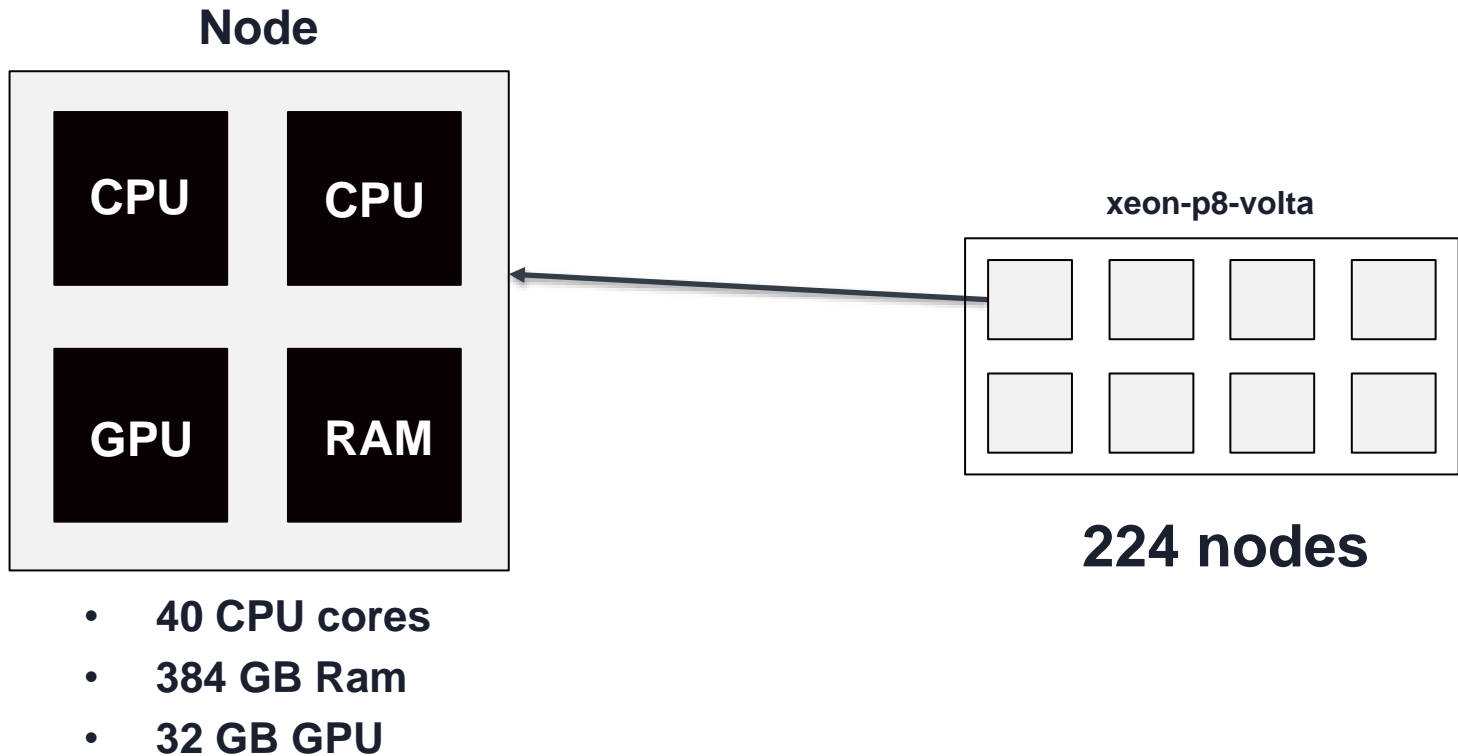
Types of Jobs

Interactive jobs

- Use cluster resources to interact with your code as you would locally

- Prototyping, testing, long jobs

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

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
```

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@txe1-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@txe1-login.mit.edu:/home/gridsan/user
```

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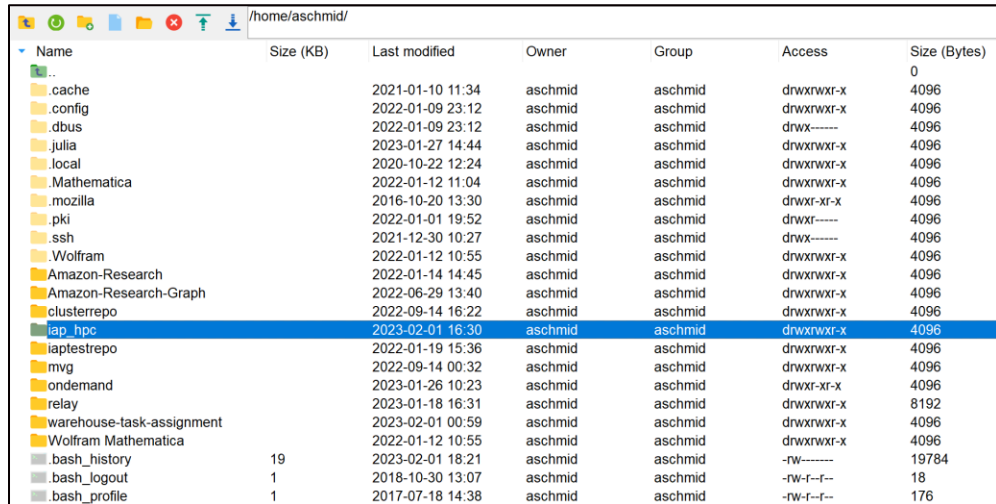
```
mkdir newfolder
```

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

```
     scp –r user@eofe7.mit.edu:/home/user/newfolder/  ./
scp -r user@txe1-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

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/angkoulouras/15.S60_2024.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/1.7.3`
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/1.7.3
   ```

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
   ```

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/1.7.3`

- 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:

```bash
#!/bin/bash

#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

#Load software
module load julia/1.7.3
module load gurobi/9.0.3

#Run the script as usual
julia myscript.jl
```

"shebang"

request resources *(optional)*

load software

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	`--cpus-per-task=1`
Memory	`--mem=4G`
Time	`--time=1-00:00`

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 before running your scripts

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:

<div align="center">

`3_array_eng/`

or

`3_array_sc/`

</div>

How would you approach this?

Script: `shortestpath_one.jl`

Instance list: `data/`

How can we use the cluster to accomplish this?
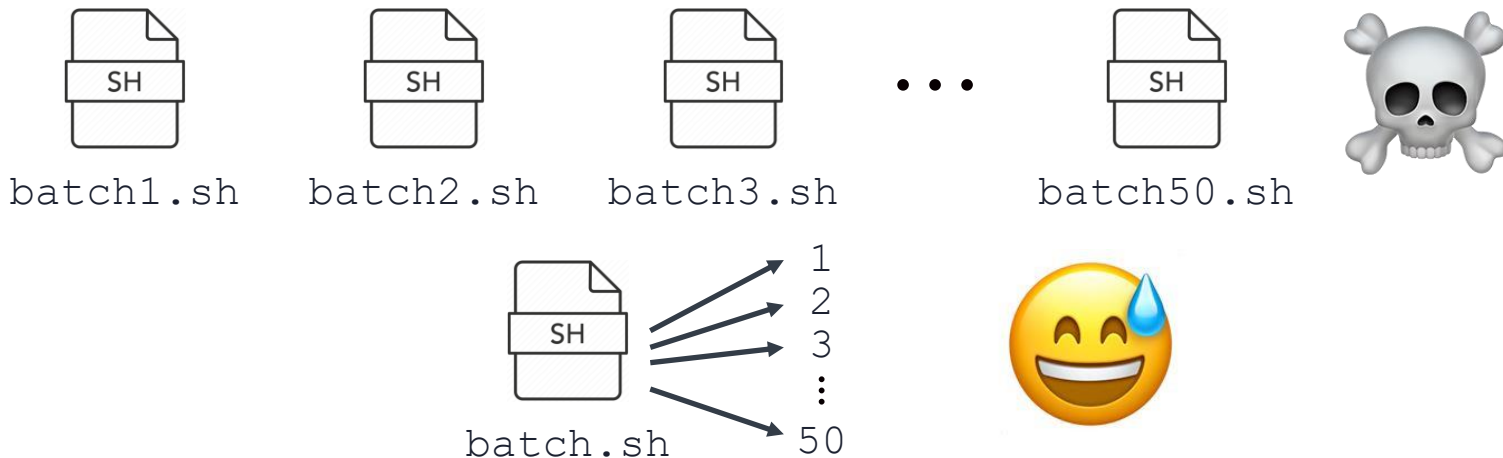
Job Array Batch Script - Engaging

```bash
#!/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](#)

```bash
#!/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

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:

local repository   remote repository   cluster

push

pull

Edit code here   **Run code here**
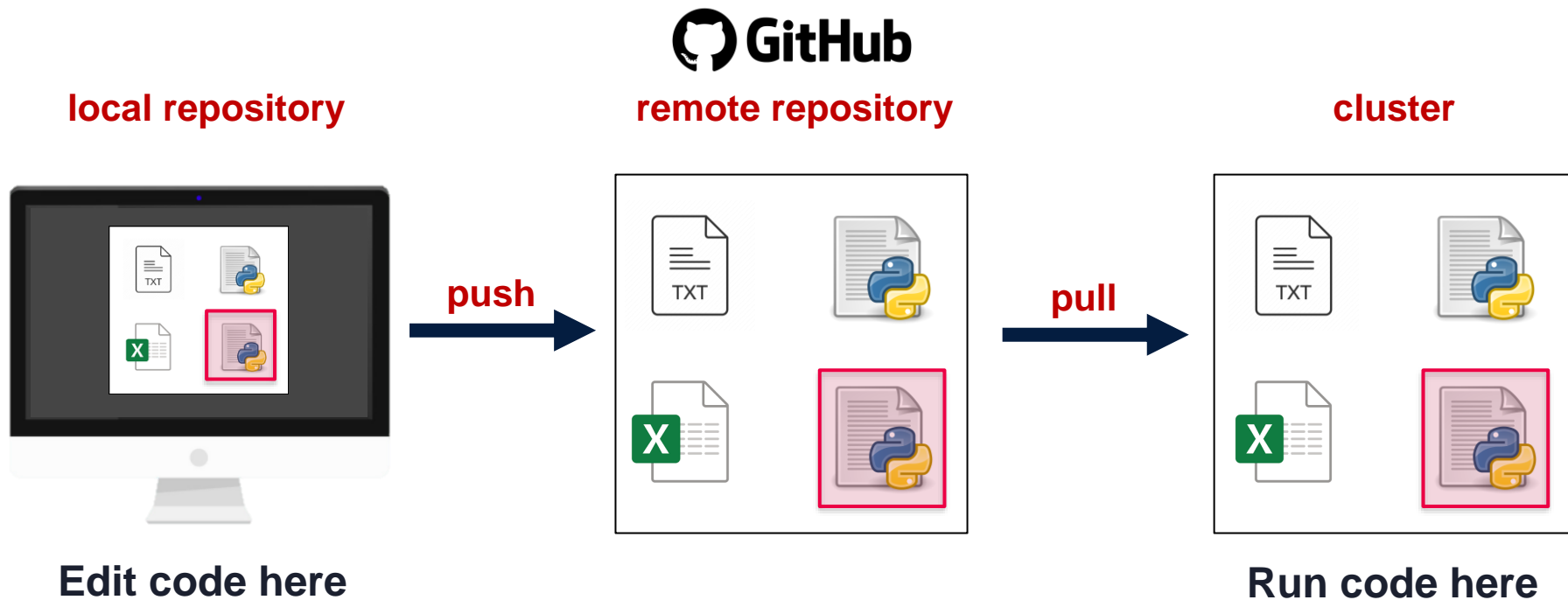
Connecting Engaging to Github

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
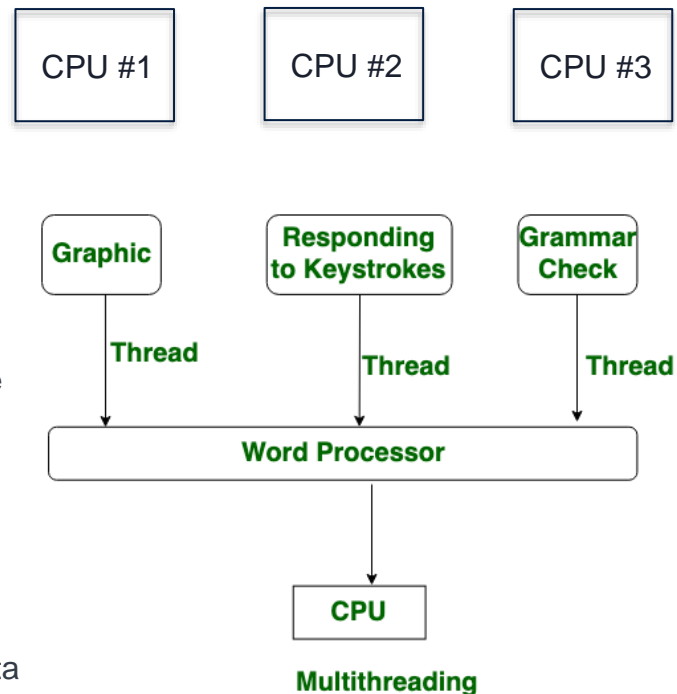
Single-threading vs Multithreading
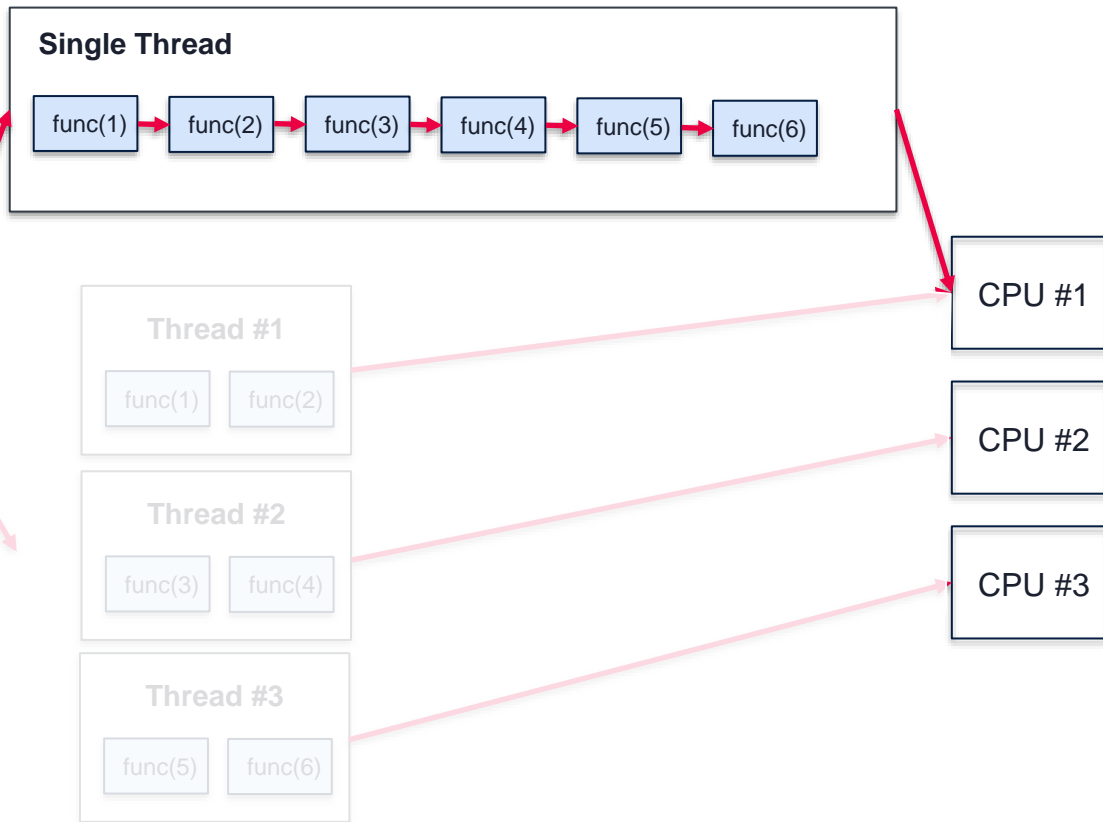
Single Thread

func(1) → func(2) → func(3) → func(4) → func(5) → func(6)

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

Thread #1

func(1) func(2)

Thread #2

func(3) func(4)

Thread #3

func(5) func(6)

CPU #1

CPU #2

CPU #3

Single-threading vs Multithreading

Single Thread

func(1) → func(2) → func(3) → func(4) → func(5) → func(6)

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

Thread #1

func(1) func(2)

Thread #2

func(3) func(4)

Thread #3

func(5) func(6)

CPU #1

CPU #2

CPU #3
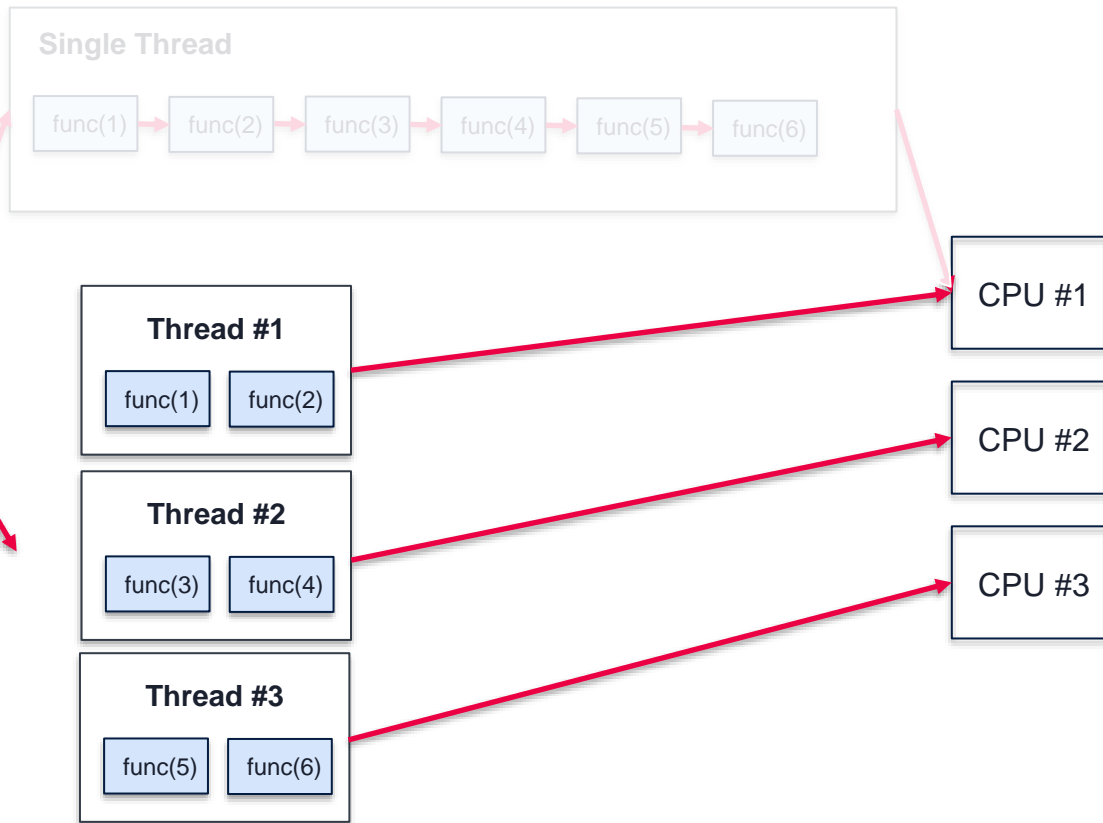
Parallelizing Julia for loops

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`

```julia
using Base.Threads

function my_long_running_function(i)
    sleep(1) # Waits for 1 second
    return i
end

result = 0
a = 5

@time begin # This counts the execution time of the block
    for i in -a:a # Loop from -a to a with step 1
        global result = result + my_long_running_function(i)
    end
end;

println("Result: $(result)")
```

- 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`

```julia
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`

```julia
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`

```julia
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?
  - Result?

Parallelizing Julia for loops

File: `loop_2.jl`

```julia
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)")
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```

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

```julia
using Base.Threads

function f(i)
    sleep(1)
    return i
end

result = 0

@threads for i in 1:2 # Loop from 1 to 2
    global result = result + f(i)
end

println("Result: $(result)")
```


Correct value!

Race Condition

```julia
using Base.Threads

function f(i)
    sleep(1)
    return i
end

result = 0

@threads for i in 1:2 # Loop from 1 to 2
    global result = result + f(i)
end

println("Result: $(result)")
```


Incorrect value!

Parallelizing Julia for loops

File: `loop_3.jl`

```julia
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
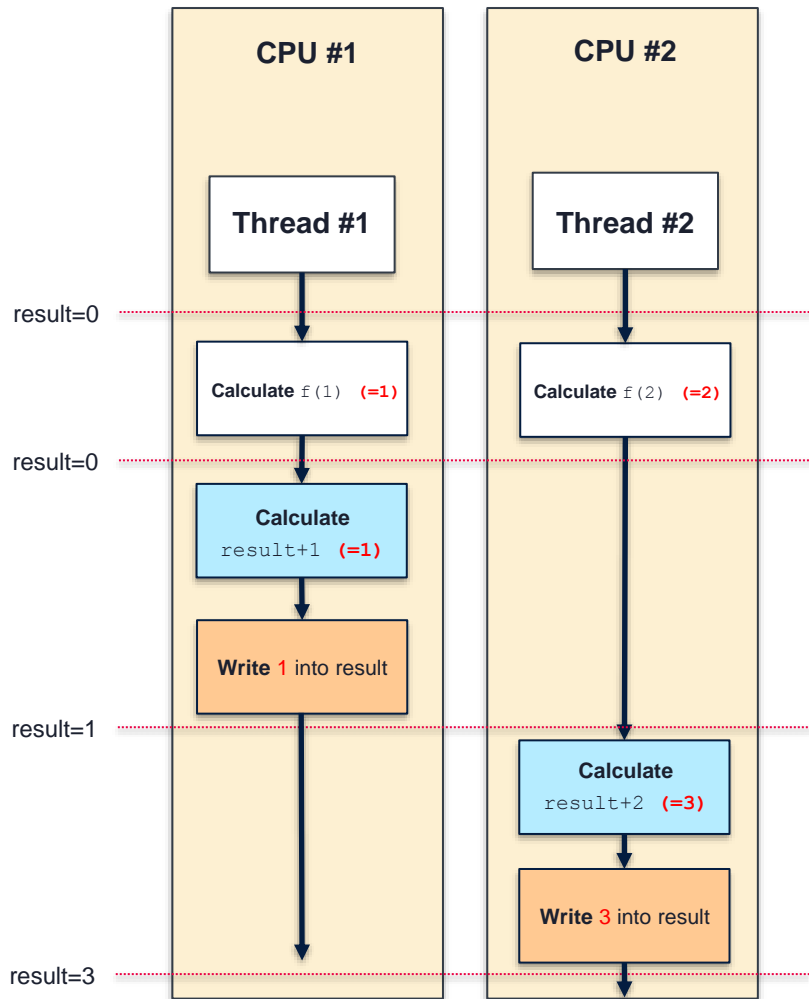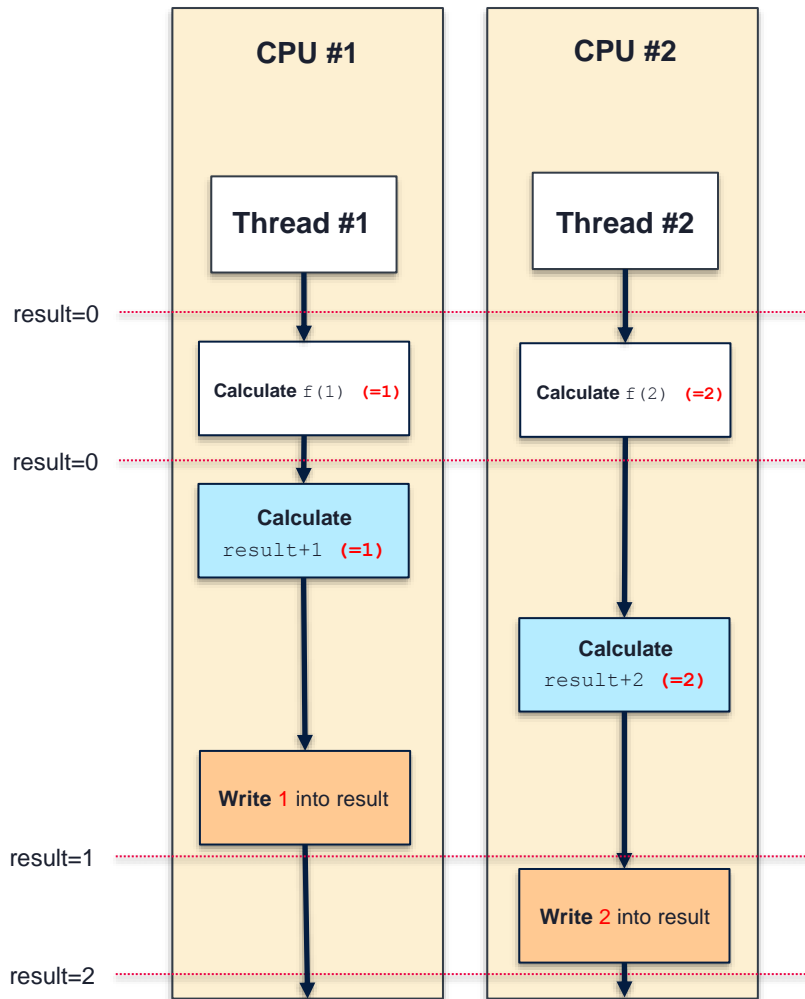2. We accumulate in the end

- 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`

```julia
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

```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
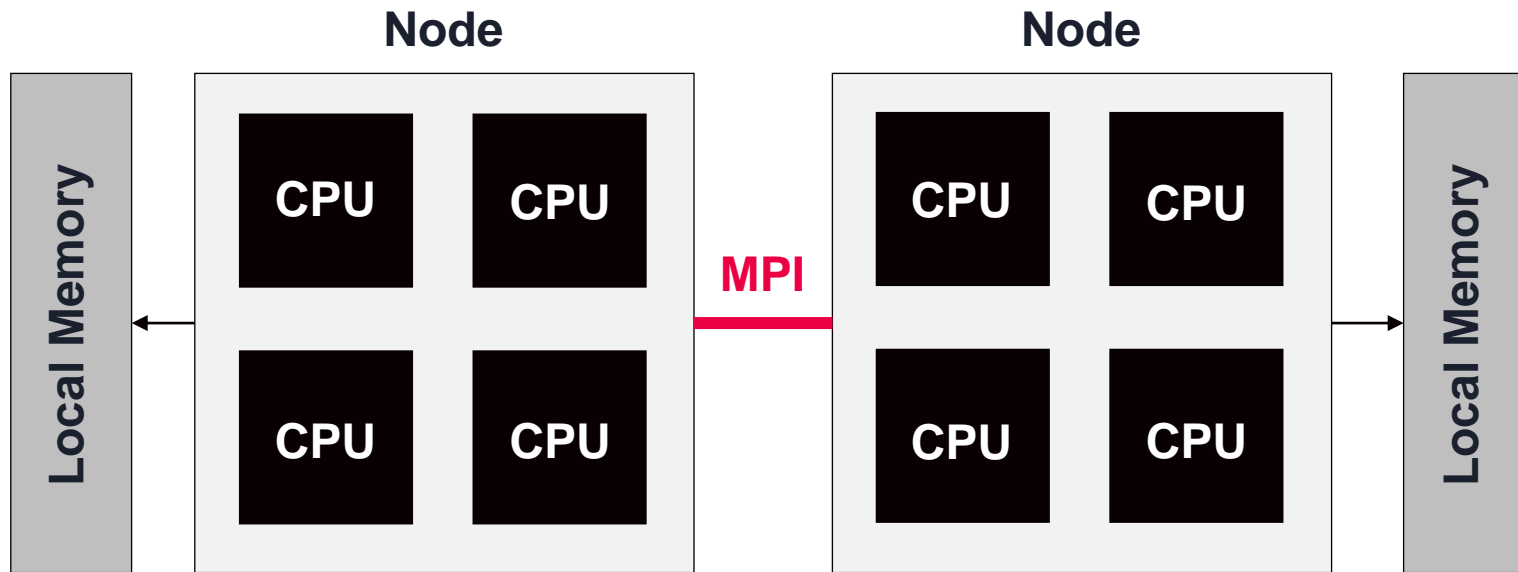
Parallelization

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

```julia
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
```
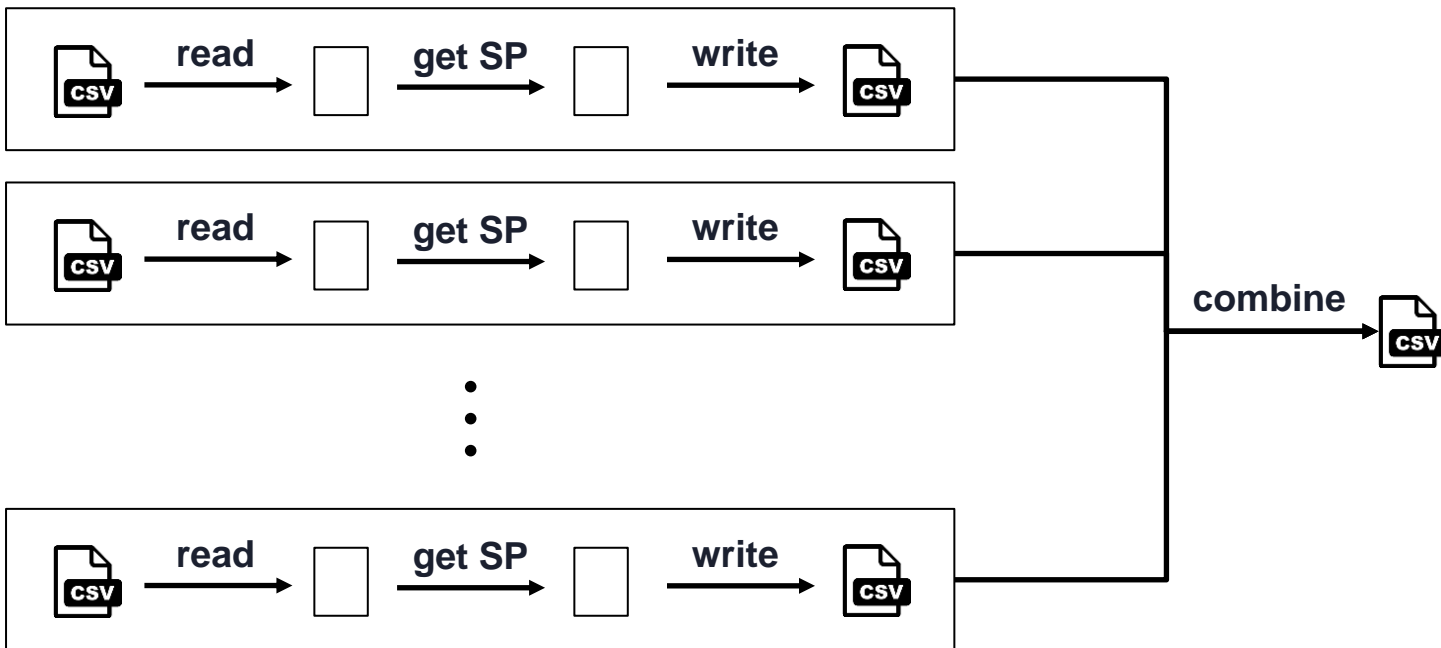
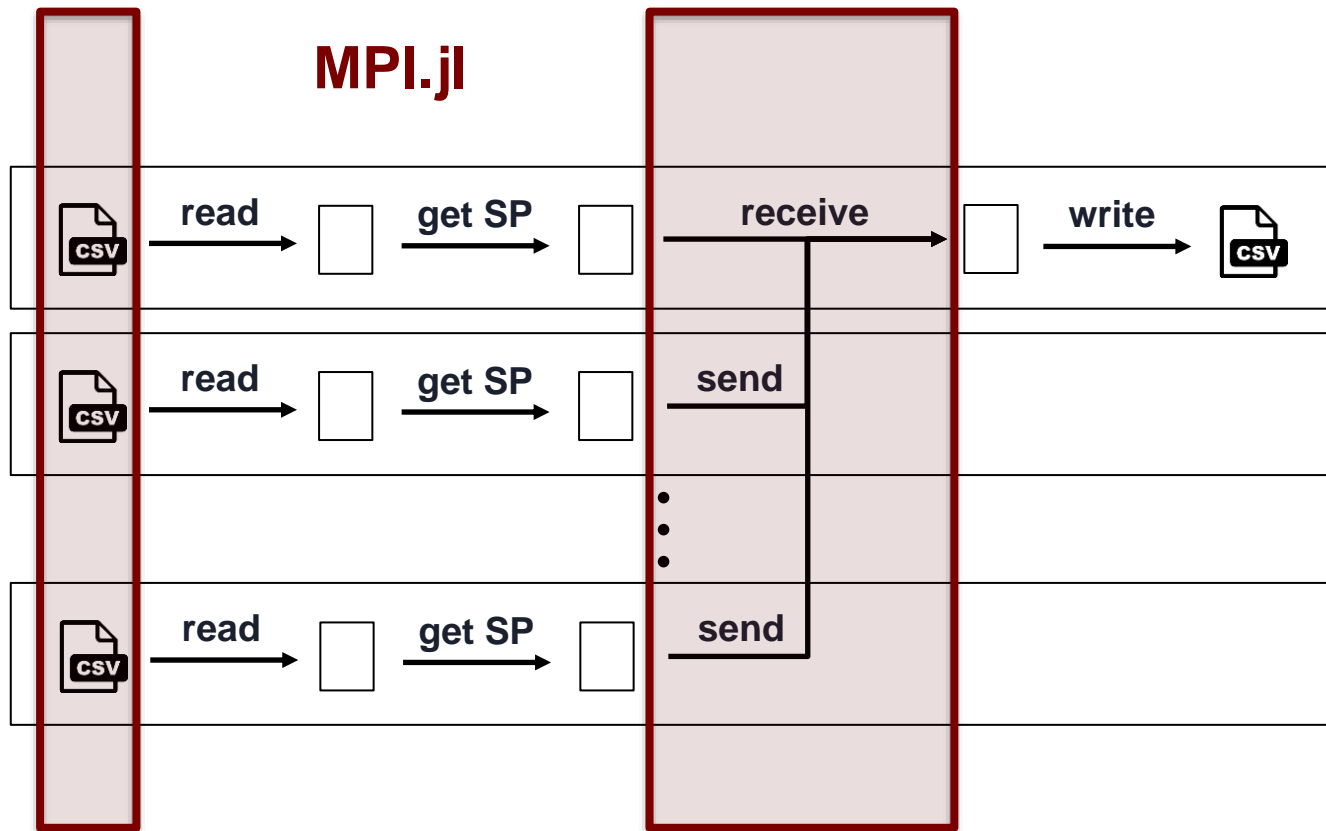# Option 1: One big for loop

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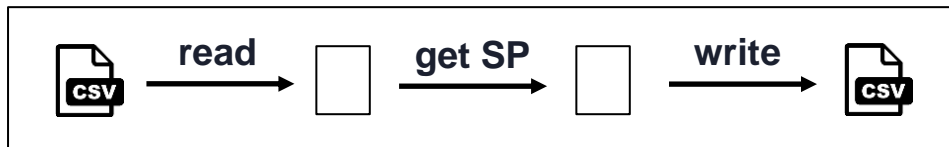


```
end
```

Option 2: Job array / MapReduce

Option 3: Parallelize across nodes & cores

MPI.jl

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
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

```bash
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
```

3. Observe the output file:

```
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: Monday, Saturday. Feb 3 at 11:59pm **(hard deadline)**

Best of luck in the upcoming semester ☺

Thank you!