Georgia Advanced Computing Resource Center
UNIVERSITY OF GEORGIA

Job Parallelization with GNU Parallel and Slurm Arrays

Georgia Advanced Computing Resource Center
University of Georgia
Isaiah Davis
isaiah.davis@uga.edu

Job Parallelism

Job parallelism refers to the practice of dividing a computational task into smaller tasks that can be run concurrently, typically across multiple processors or computers.

Benefits:

- Speed – Complete tasks faster by working on multiple parts at once.
- Scalability – Handle larger datasets or more complex simulations.
- Efficiency – Make better use of available hardware resources.

Types of parallelism:

- Embarrassingly Parallel
- Complex Parallelization (*e.g. Interdependent Tasks*)

Embarrassingly Parallel vs. Complex Parallelization

Type	Description	Examples	Challenges
Embarrassingly Parallel	Tasks can run completely independently with no need to communicate or share data.	Image rendering, Monte Carlo simulations, batch data processing.	Minimal—easy to implement and scale.
Complex Parallelization	Tasks are interdependent and may need to exchange data during execution.	Simulations with shared state, machine learning training, weather modeling.	Requires coordination, synchronization, and efficient data sharing.

Job Parallelism

Covered Today:

Embarrassingly parallel problems, using GNU Parallel and Slurm Array jobs.

Not Covered Today:

Programming libraries for parallelism.

e.g. doParallel (R), multiprocessing (Python), OpenMP, Pthreads, OpenMPI

Job Parallelism

Today's Focus:

Running multiple instances of the same command at the same time.

```
command input1
command input2
command input3
command input4
command input5
```

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem=1G

process_data input1.csv
process_data input2.csv
process_data input3.csv
process_data input4.csv
process_data input5.csv
```

Manually write out the command for each input.

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

1) Create a file containing the name of each input.

2) Iterate through the file using a for loop.

inputs.txt

```
input1.csv
input2.csv
input3.csv
input4.csv
input5.csv
```

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem=1G

for FILE in $(cat inputs.txt)
do
  process_data ${FILE}
done
```

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

Sequential Execution

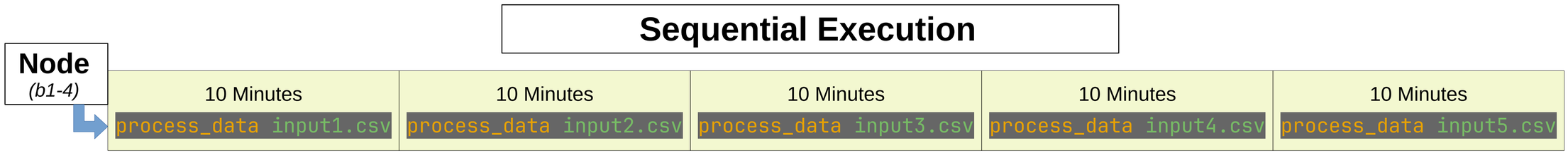
```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem=1G

process_data input1.csv
process_data input2.csv
process_data input3.csv
process_data input4.csv
process_data input5.csv
```

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=01:00:00
#SBATCH --mem=1G

for FILE in $(cat inputs.txt)
do
  process_data ${FILE}
done
```

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`



Total Time: 50 Minutes

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

Parallel Execution

10 Minutes `process_data input1.csv`
10 Minutes `process_data input2.csv`
10 Minutes `process_data input3.csv`
10 Minutes `process_data input4.csv`
10 Minutes `process_data input5.csv`

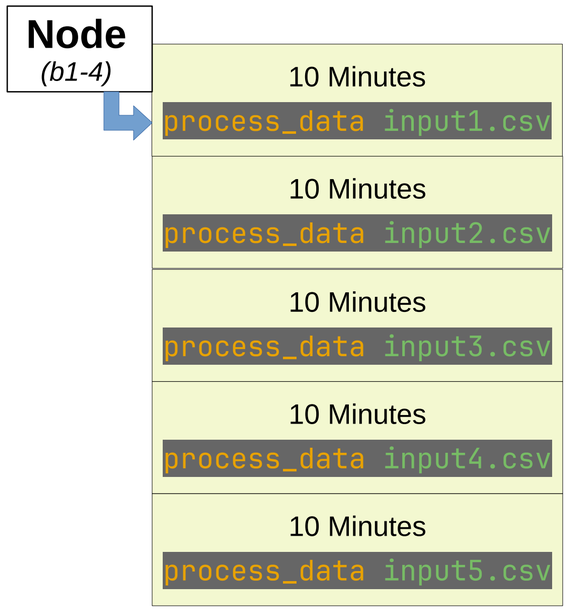
Total Time: ~10 Minutes

(*parallelization incurs some overhead)*

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`



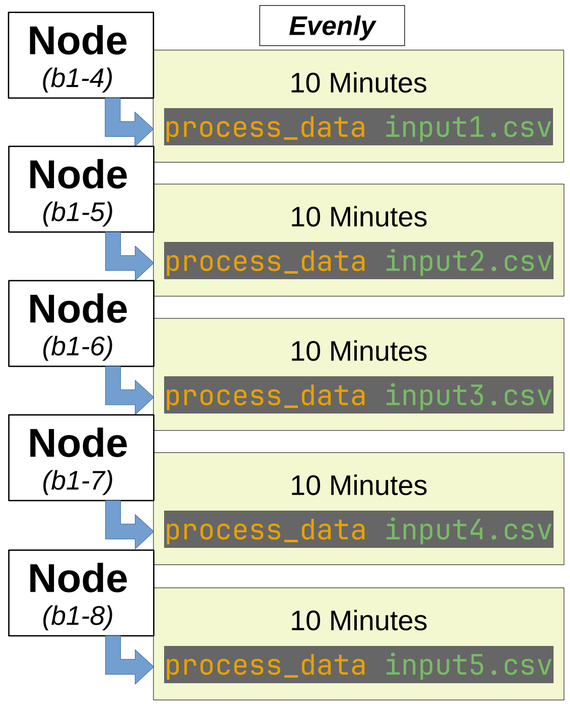
Utilize multiple cores on a single Sapelo2 node.

Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

Spread commands equally across multiple nodes on Sapelo2.

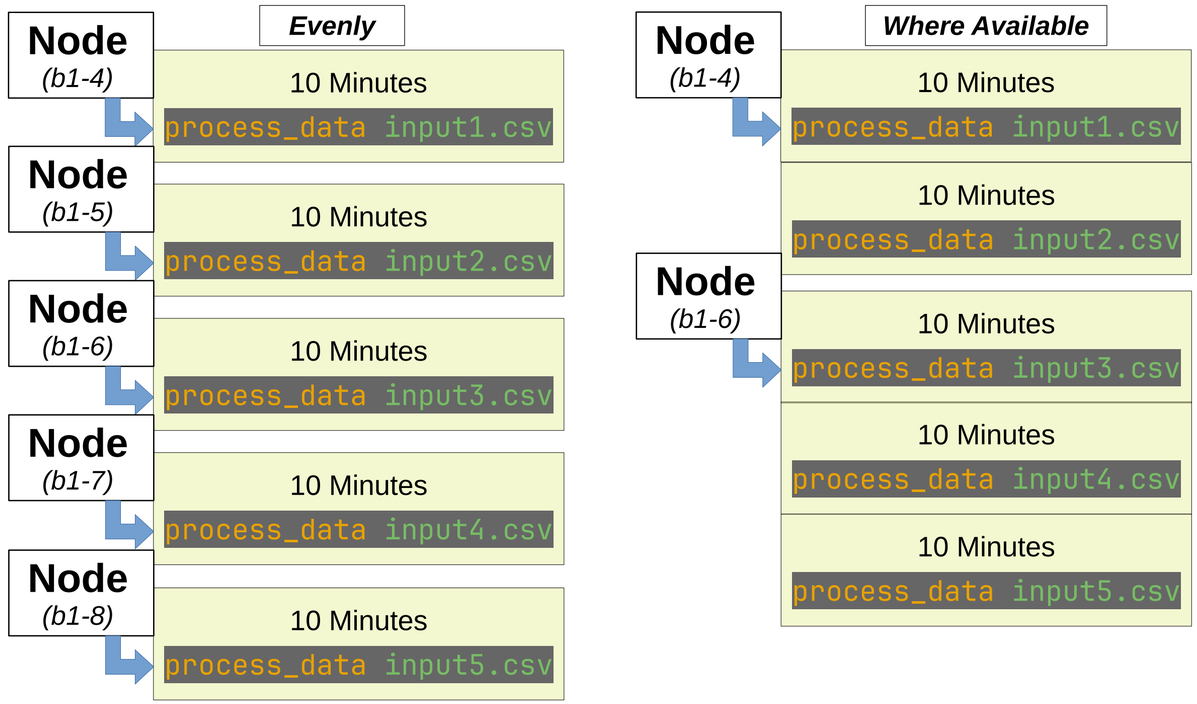


Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`

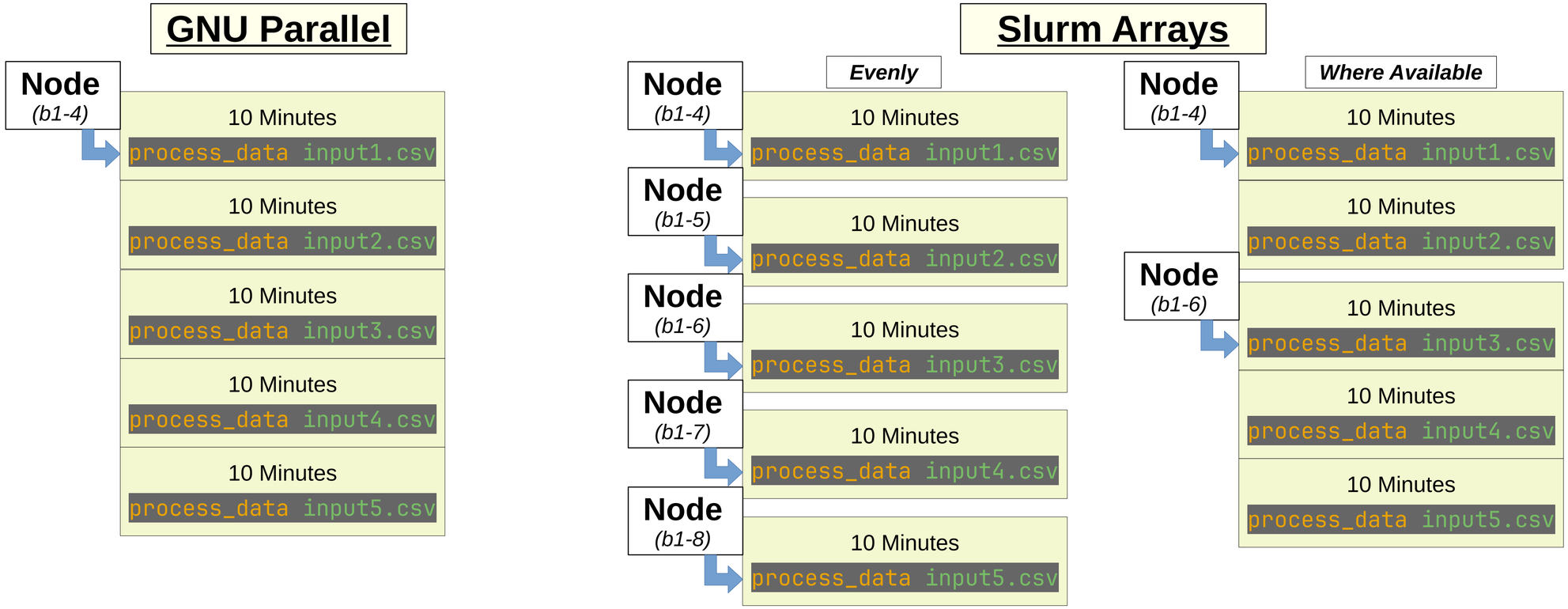
Spread commands across multiple nodes on Sapelo2 wherever available.



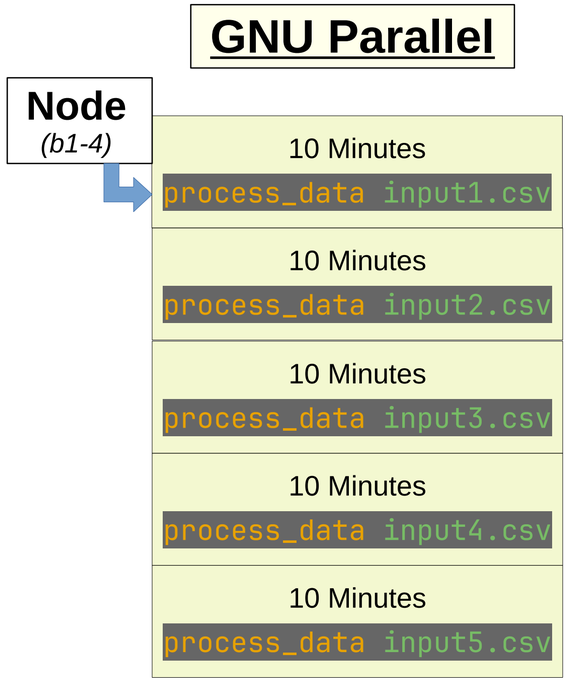
Example

Use the `process_data` command with the files:

`input1.csv` `input2.csv` `input3.csv` `input4.csv` `input5.csv`



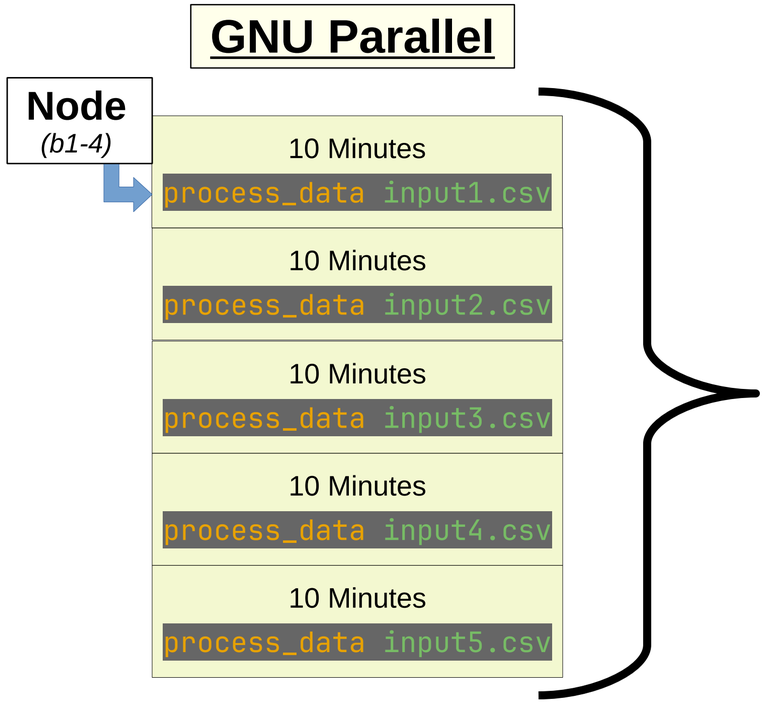
GNU Parallel



GNU Parallel

GNU Parallel is a general parallelizer to run multiple serial command line programs in parallel without changing them.

GNU Parallel

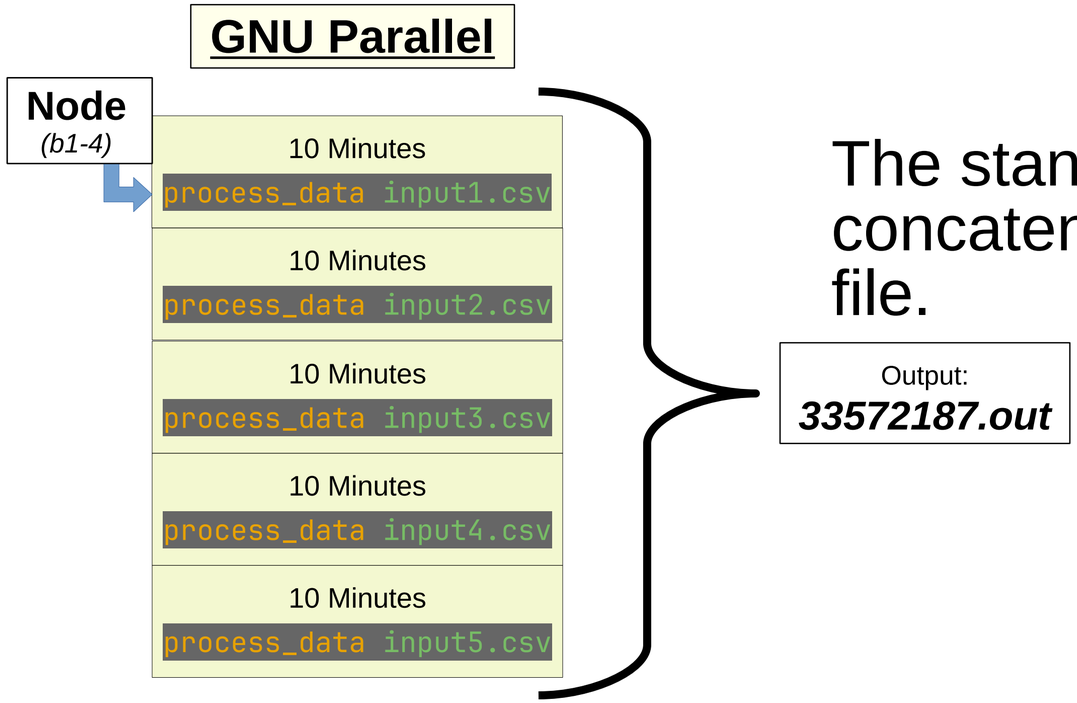


GNU Parallel

GNU Parallel initiates and manages the parallelization on the node itself.

All elements execute within a single job.

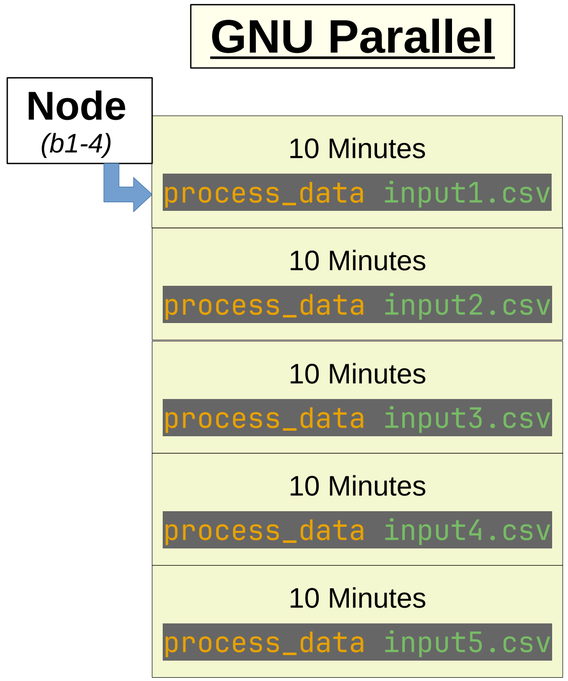
GNU Parallel



GNU Parallel

The standard output of all elements are concatenated into a single Slurm output file.

GNU Parallel



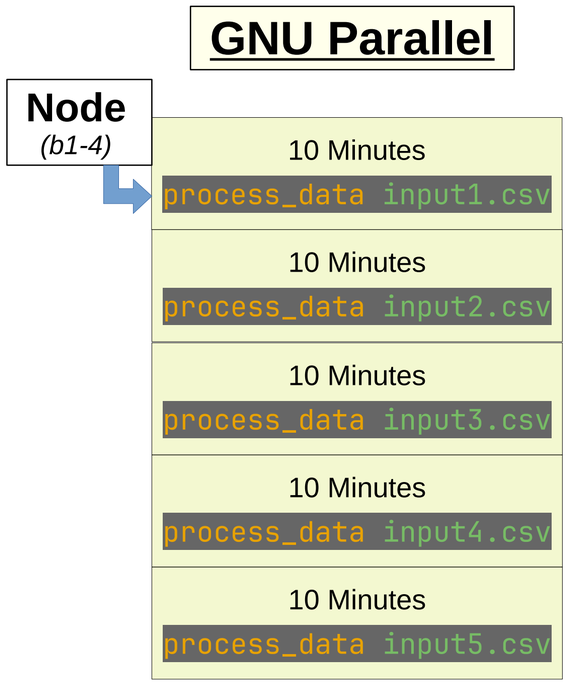
Parallelize a series of commands by prepending the command with `parallel`.

Foundational parameters

Three colons `:::` to pass text as inputs.

Four colons `::::` to pass files as inputs.

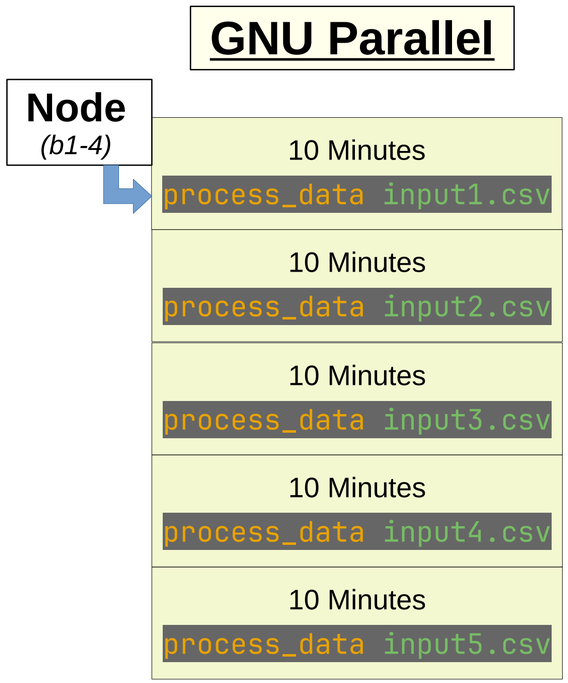
GNU Parallel



Each of the inputs could be specified by name following three colons `:::`.

```
parallel process_data ::: input1.csv input2.csv input3.csv input4.csv input5.csv
```

GNU Parallel



1) Create a file containing the names of all the inputs called `inputs.txt`.

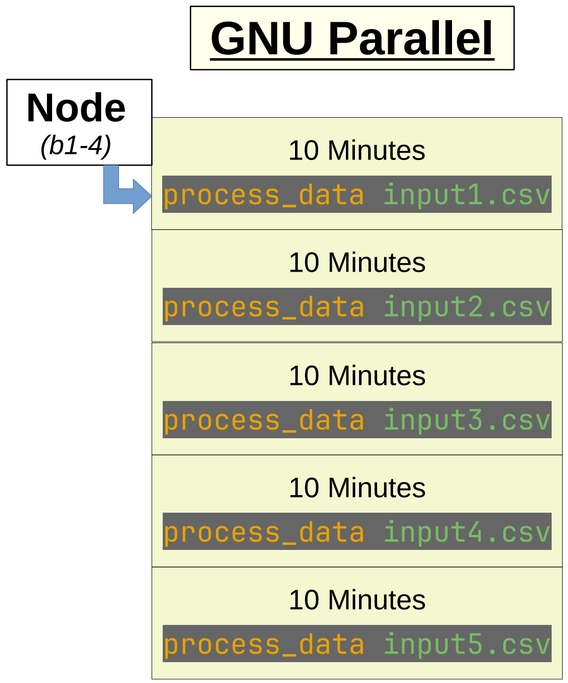
2) Specify the file name following four colons `::::`.

inputs.txt

```
input1.csv
input2.csv
input3.csv
input4.csv
input5.csv
```

```
parallel process_data :::: inputs.txt
```

GNU Parallel

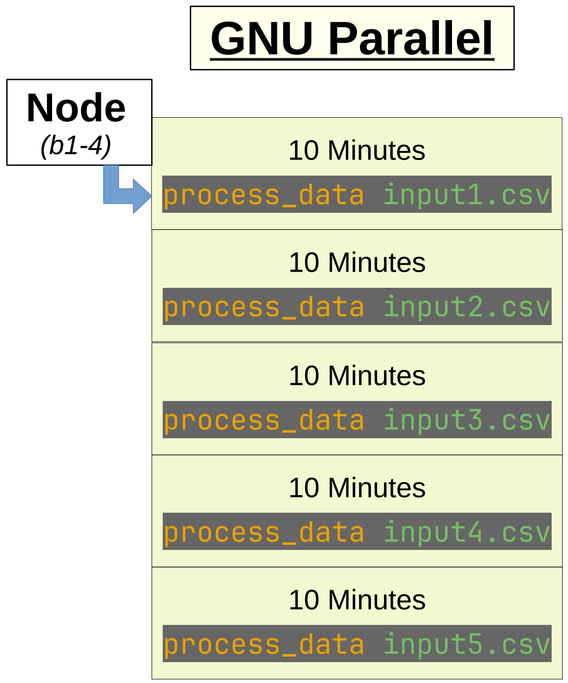



```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --nodes=1
#SBATCH --time=00:15:00
#SBATCH --mem=5G
#SBATCH --ntasks=5

module load parallel/20230722-GCCcore-12.3.0

parallel process_data :::: inputs.txt
```

Request adequate memory and tasks in the Slurm header.

Load the parallel module.

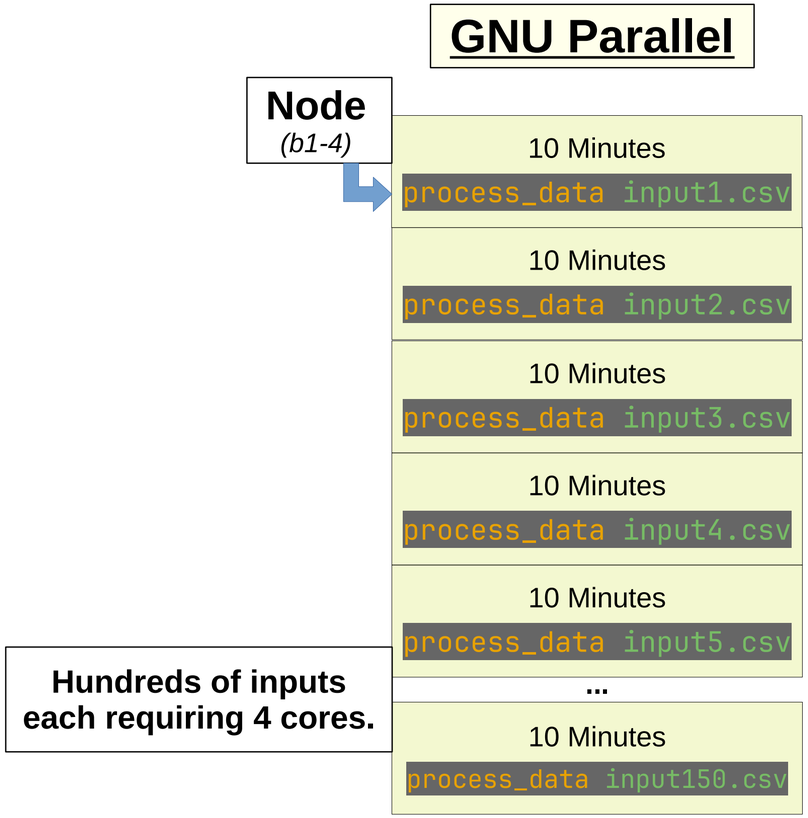
GNU Parallel




```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --nodes=1
#SBATCH --time=00:15:00
#SBATCH --mem=5G
#SBATCH --ntasks=5
#SBATCH --cpus-per-task=4

module load parallel/20230722-GCCcore-12.3.0

parallel process_data :::: inputs.txt
```

Multiple CPU cores can be requested for each job element.

GNU Parallel

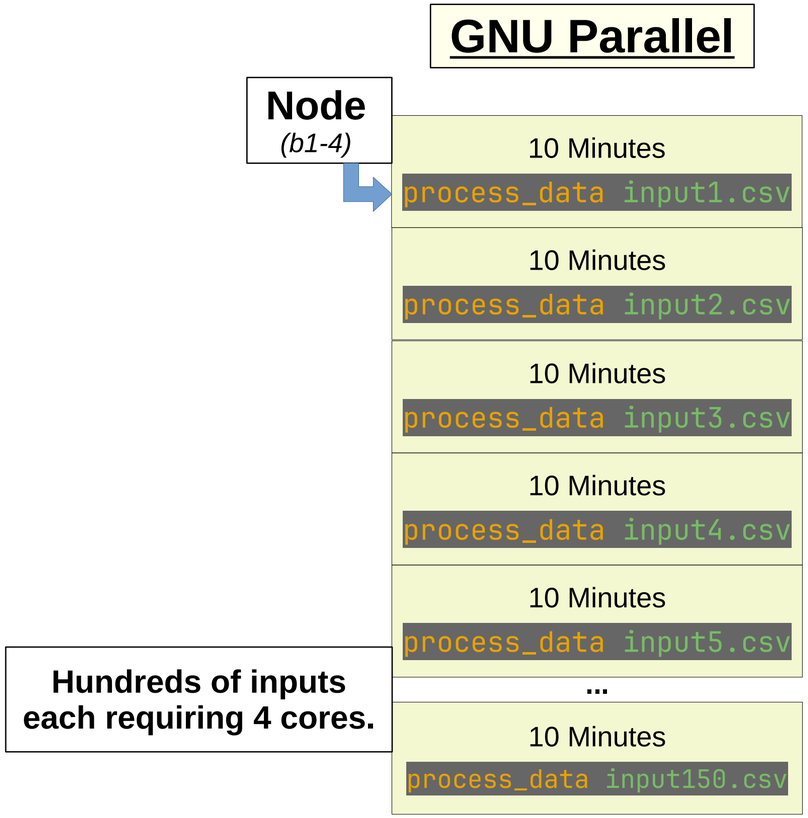



```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --nodes=1
#SBATCH --time=00:15:00
#SBATCH --mem=150G
#SBATCH --ntasks=150
#SBATCH --cpus-per-task=4

module load parallel/20230722-GCCcore-12.3.0

parallel process_data :::: inputs.txt
```

A single node cannot provide this many cores.

150 * 4 = 600 cores

GNU Parallel



Node specifications can be found on the GACRC wiki:
https://wiki.gacrc.uga.edu/wiki/Job_Submission_partitions_on_Sapelo2

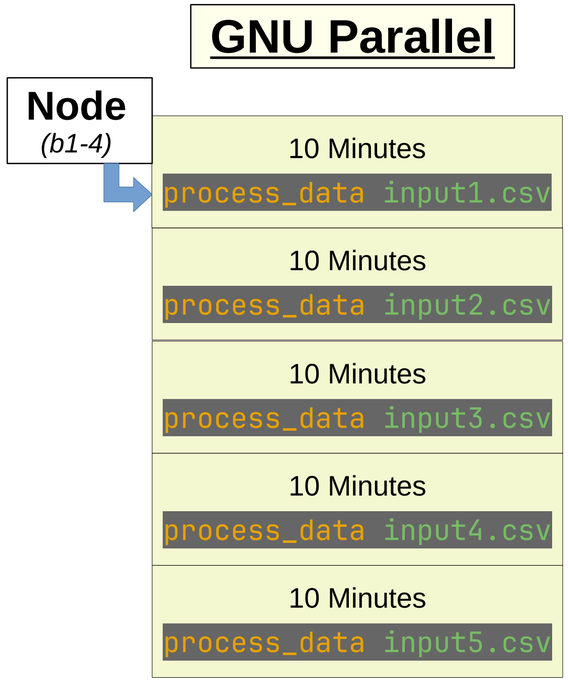
```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --nodes=1
#SBATCH --time=00:15:00
#SBATCH --mem=16G
#SBATCH --ntasks=16
#SBATCH --cpus-per-task=4

module load parallel/20230722-GCCcore-12.3.0

parallel -j 16 process_data :::: inputs.txt
```

Request up to what a node can provide.

16 * 4 = 64 cores

Limit the number of concurrent jobs.

GNU Parallel



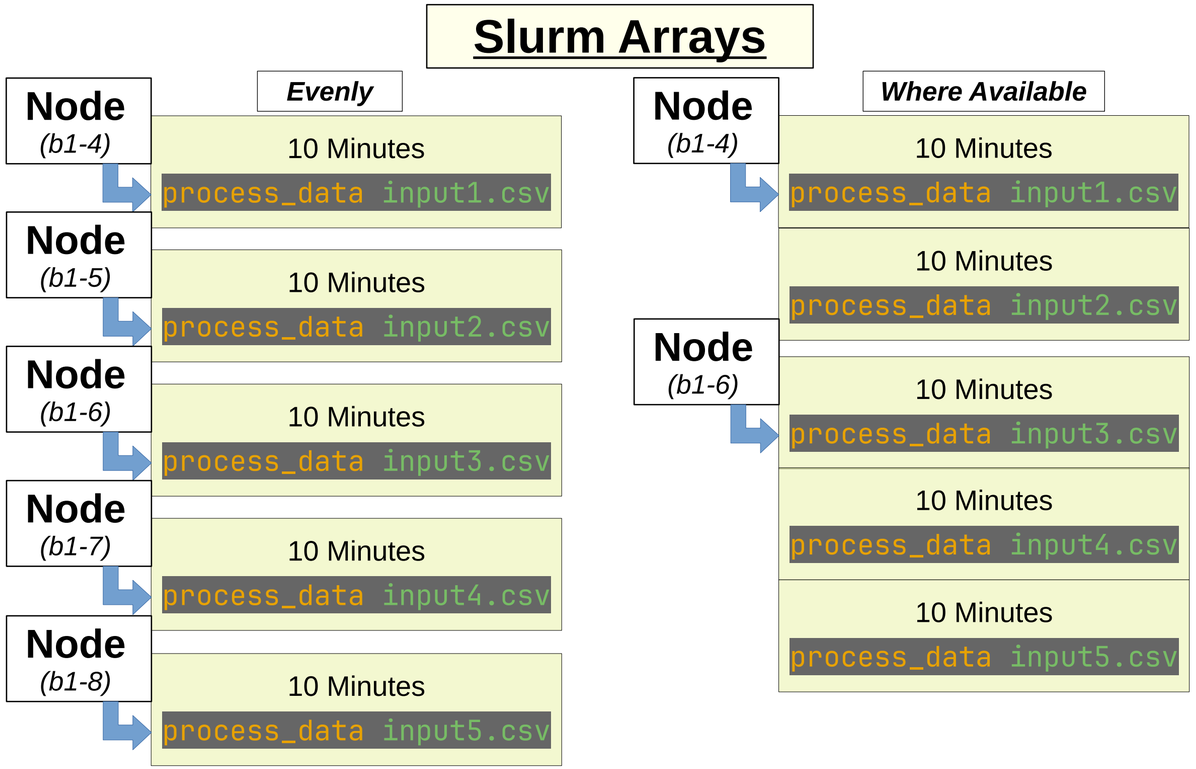
If using GNU Parallel to develop and publish a program, use the `--citation` flag to generate a citation for the project.

```
parallel --citation
```

Slurm Job Arrays

Slurm Arrays

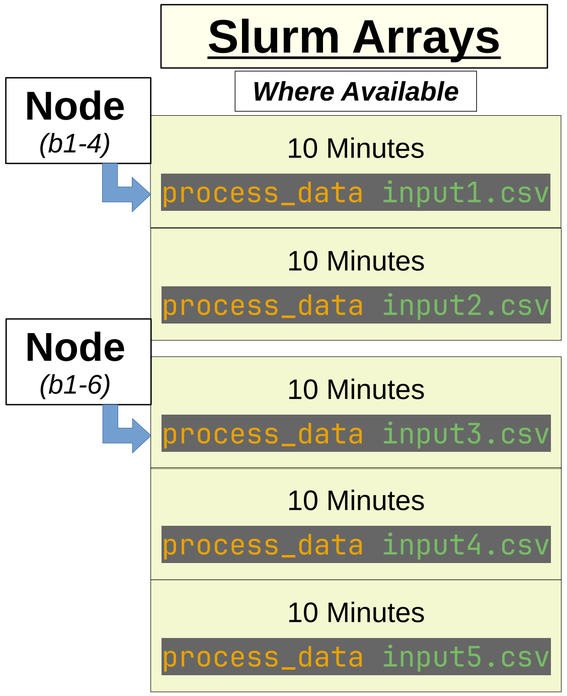
Built-in Slurm functionality that provides a mechanism for submitting and managing collections of similar jobs quickly and easily.



Slurm Job Arrays

Slurm Arrays

By default, Slurm will schedule array job elements wherever available.

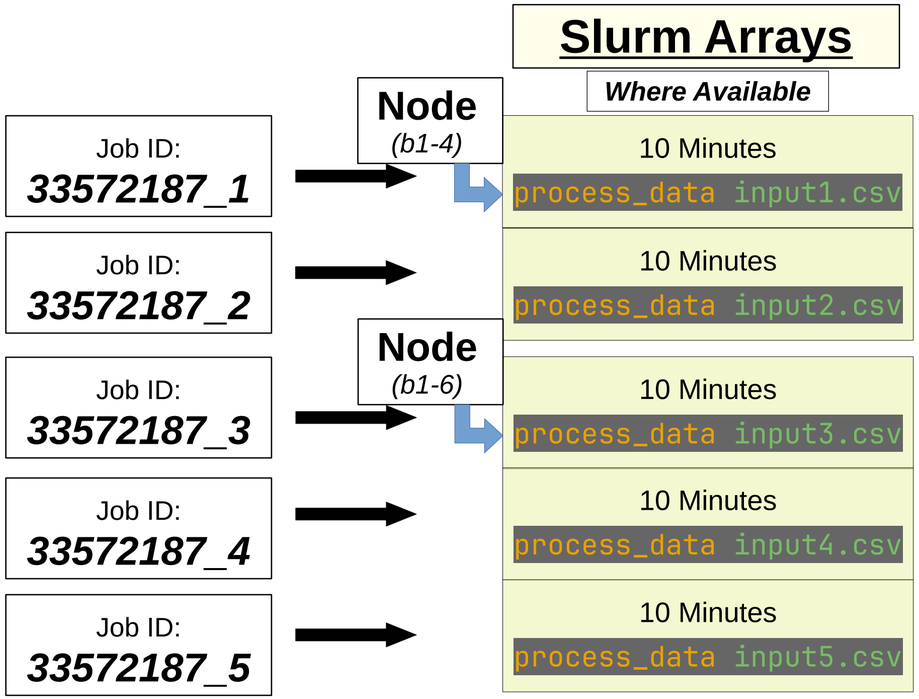


Slurm Job Arrays

Slurm Arrays

The Slurm head node initiates and manages the parallelization.

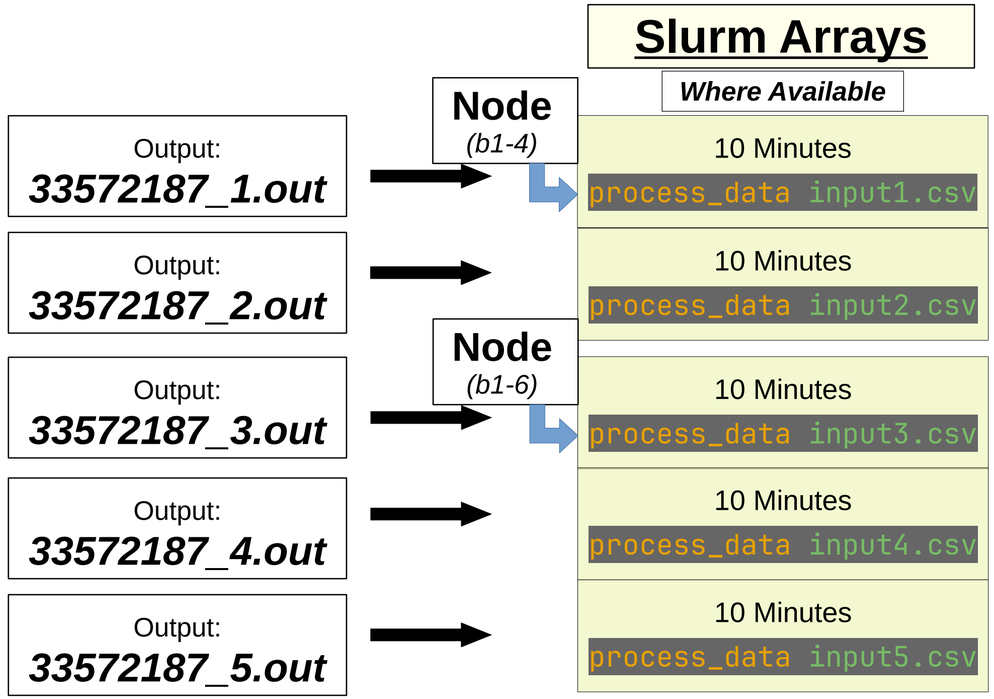
Each element in a Slurm array has its own Job ID.



Slurm Job Arrays

Slurm Arrays

Each job element will produce its own Slurm output file.



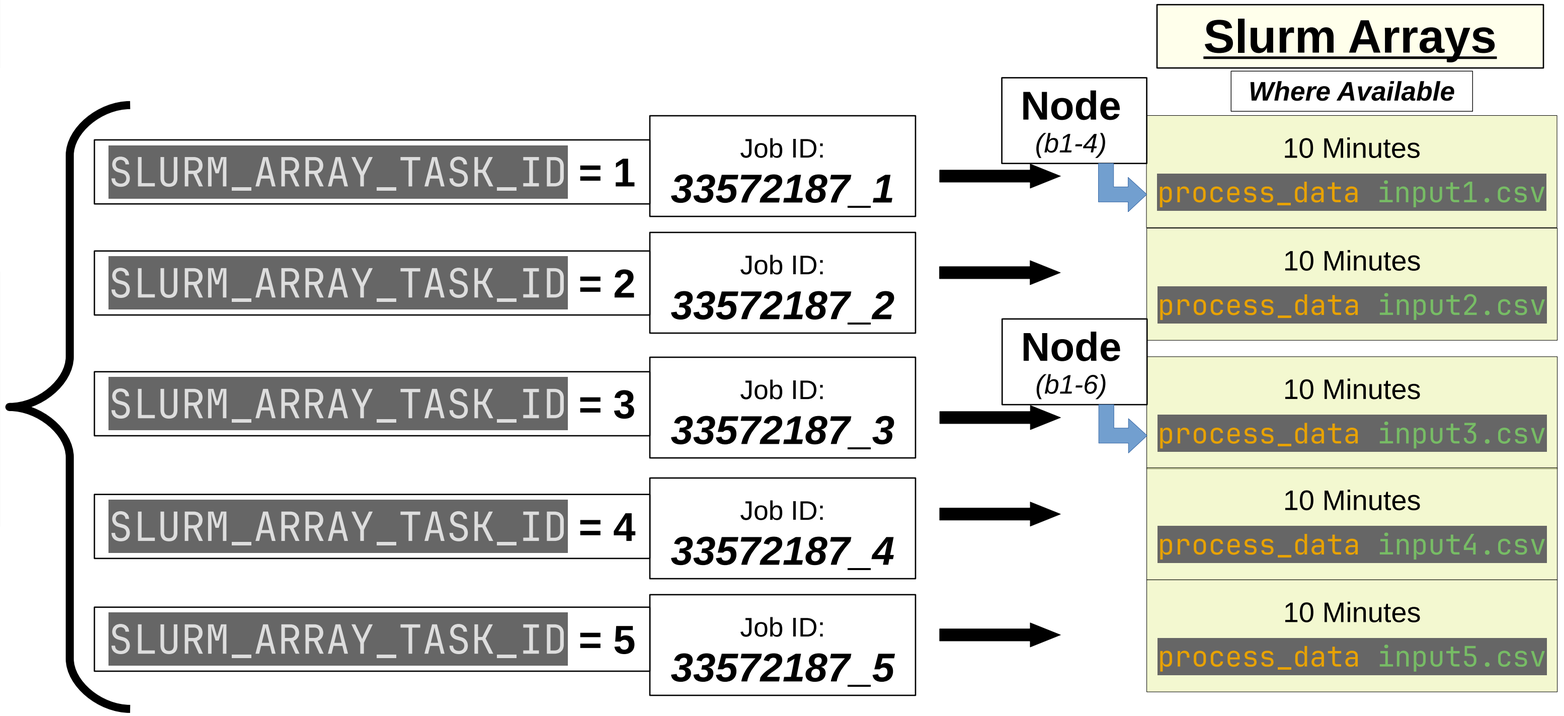
Slurm Job Arrays

Initiated with the Slurm header:

```
#SBATCH --array=START-END
```

Each job element in the array will have its own

`SLURM_ARRAY_TASK_ID`

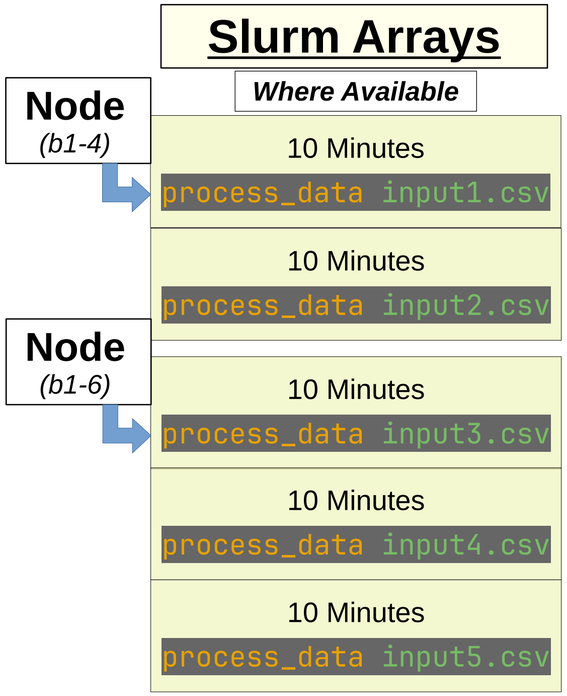


Slurm Job Arrays

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=00:15:00
#SBATCH --mem=1G
#SBATCH --array=1-5

process_data input${SLURM_ARRAY_TASK_ID}.csv
```

Specify a job array in the Slurm header.

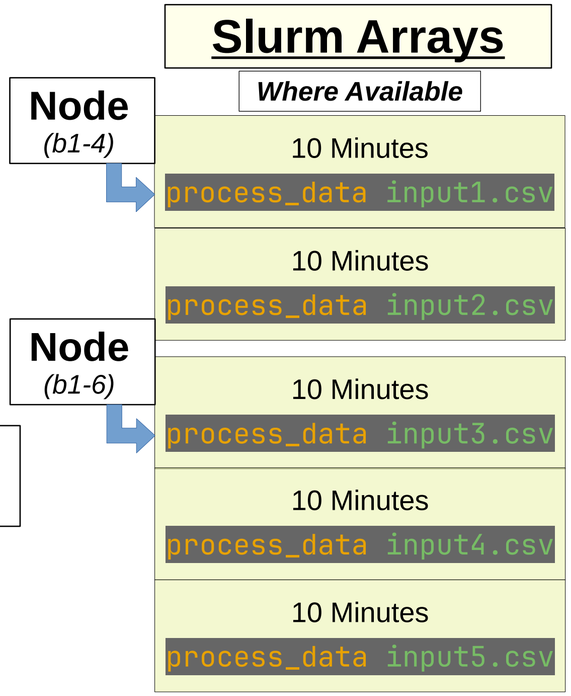
Incorporate the `SLURM_ARRAY_TASK_ID` variable.



Slurm Job Arrays

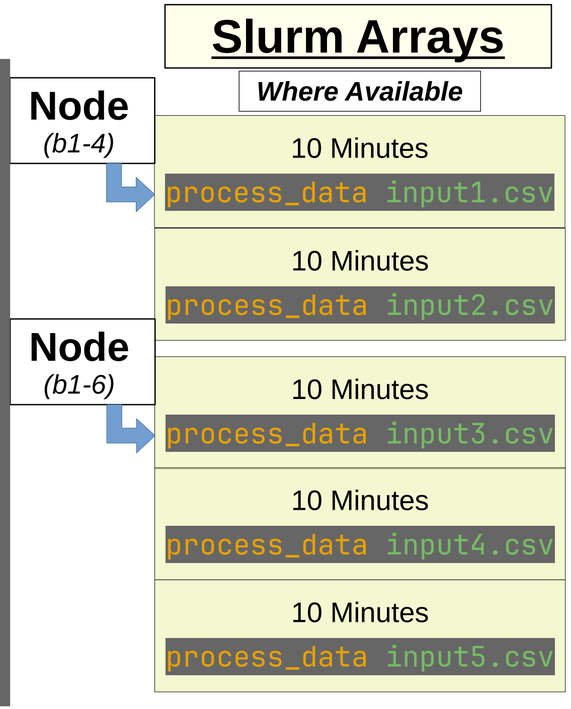
```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=00:15:00
#SBATCH --mem=1G
#SBATCH --cpus-per-task=4
#SBATCH --array=1-5

process_data input${SLURM_ARRAY_TASK_ID}.csv
```

Multiple CPU cores can be requested for each job element.



Slurm Job Arrays

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=test
#SBATCH --ntasks=1
#SBATCH --time=00:15:00
#SBATCH --mem=1G
#SBATCH --cpus-per-task=4
#SBATCH --array=1-5

process_data $(awk "NR==${SLURM_ARRAY_TASK_ID}" inputs.txt)
```



An input file containing the names of all the inputs can be used via `awk`.

Slurm Arrays and GNU Parallel

Slurm Arrays

Can be configured for tasks to execute across multiple nodes.

Parallelization handled through Slurm.

May only be used in non-interactive jobs.

GNU Parallel

All tasks execute on a single node.

Parallelization handled by the GNU Parallel software on the node.

Can be executed interactively.

Practice

./scramble.py

```python
#!/usr/bin/env python

import sys
import time
from pathlib import Path
from random import shuffle

def shuffle_word(word: str) -> str:
    word = list(word)
    shuffle(word)
    return ''.join(word)

def main() -> None:
    shuffled = list()
    with open(sys.argv[1]) as file:
        for line in file.readlines():
            shuffled.append(shuffle_word(line.strip('\n')))

    output_dir = sys.argv[2].split('/')[-1]

    Path(output_dir).mkdir(parents=True, exist_ok=True)

    filename = sys.argv[1].split('/')[-1]
    filename = filename.split('.')[0]

    with open(f'{output_dir}/{filename}.out', 'w') as file:
        for word in shuffled:
            file.write(word + '\n')

    time.sleep(5)
    print(f'"{filename}" shuffled and saved to "{output_dir}/{filename}.out".')

if __name__ ==  "__main__":
    main()
```

Function to shuffle characters

Read input file and shuffle

Create output directory

Write shuffled output

Sorted/input1.txt

```
Orange
Garden
Planet
```

output_dir/input1.out

```
nraOeg
dnearG
eaPltn
```

Practice

./scramble.py

```python
#!/usr/bin/env python

import sys
import time
from pathlib import Path
from random import shuffle

def shuffle_word(word: str) -> str:
    word = list(word)
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def main() -> None:
    shuffled = list()
    with open(sys.argv[1]) as file:
        for line in file.readlines():
            shuffled.append(shuffle_word(line.strip('\n')))

    output_dir = sys.argv[2].split('/')[-1]

    Path(output_dir).mkdir(parents=True, exist_ok=True)

    filename = sys.argv[1].split('/')[-1]
    filename = filename.split('.')[0]

    with open(f'{output_dir}/{filename}.out', 'w') as file:
        for word in shuffled:
            file.write(word + '\n')

    time.sleep(5)
    print(f'"{filename}" shuffled and saved to "{output_dir}/{filename}.out".')

if __name__ ==  "__main__":
    main()
```

Function to shuffle characters

Read input file and shuffle

Create output directory

Write shuffled output

Run script with 10 different input files

```
./scramble.py Sorted/input1.txt sequential_outputs
./scramble.py Sorted/input2.txt sequential_outputs
./scramble.py Sorted/input3.txt sequential_outputs
./scramble.py Sorted/input4.txt sequential_outputs
./scramble.py Sorted/input5.txt sequential_outputs
./scramble.py Sorted/input6.txt sequential_outputs
./scramble.py Sorted/input7.txt sequential_outputs
./scramble.py Sorted/input8.txt sequential_outputs
./scramble.py Sorted/input9.txt sequential_outputs
./scramble.py Sorted/input10.txt sequential_outputs
```

Practice

```
[myid@ss-sub2 ~]$ cd /scratch/$USER
[myid@ss-sub2 myid]$ pwd
/scratch/myid
[myid@ss-sub2 myid]$ cp -r /usr/local/training/parallel/ ./
```

cd to your user's scratch directory

Copy practice files

Practice

```
[myid@ss-sub2 myid]$ tree parallel
parallel
├── Mixed
│   ├── 2BJn5Oak.txt
│   ├── 46XCF1H7.txt
│   ├── TyXa4F8v.txt
│   ├── Us6yfHmH.txt
│   ├── fm5la6TZ.txt
│   ├── luKJRDzy.txt
│   ├── q6U7KWE9.txt
│   ├── sTIYZOsG.txt
│   ├── sc8UMm0F.txt
│   └── yUvcLpln.txt
├── Sorted
│   ├── input1.txt
│   ├── input10.txt
│   ├── input2.txt
│   ├── input3.txt
│   ├── input4.txt
│   ├── input5.txt
│   ├── input6.txt
│   ├── input7.txt
│   ├── input8.txt
│   └── input9.txt
├── full_input.txt
├── scramble.py
└── sub.sh

2 directories, 22 files
```

Input files with numbered names

scramble.py script

Sequential job script

Practice

```
[myid@ss-sub2 myid]$ cd parallel
[myid@ss-sub2 parallel]$ ls
Mixed  Sorted  full_input.txt  scramble.py  sub.sh
```

cd to parallel directory

Practice

```
[myid@ss-sub2 parallel]$ cat sub.sh
#!/usr/bin/env bash
#SBATCH --job-name=Sequential
#SBATCH --ntasks=1
#SBATCH --partition=batch
#SBATCH --mem=1G
#SBATCH --time=00:10:00
#SBATCH --output=standard_outputs/%x_%j.out

cd $SLURM_SUBMIT_DIR

module load Python/3.11.3-GCCcore-12.3.0

./scramble.py Sorted/input1.txt ./sequential_outputs
./scramble.py Sorted/input2.txt ./sequential_outputs
./scramble.py Sorted/input3.txt ./sequential_outputs
./scramble.py Sorted/input4.txt ./sequential_outputs
./scramble.py Sorted/input5.txt ./sequential_outputs
./scramble.py Sorted/input6.txt ./sequential_outputs
./scramble.py Sorted/input7.txt ./sequential_outputs
./scramble.py Sorted/input8.txt ./sequential_outputs
./scramble.py Sorted/input9.txt ./sequential_outputs
./scramble.py Sorted/input10.txt ./sequential_outputs
```

Review provided job submission script

Current approach executes sequentially

Practice

```
[myid@ss-sub2 parallel]$ ls Sorted/* > inputs.txt
[myid@ss-sub2 parallel]$ ls
Mixed  Sorted  full_input.txt  inputs.txt  scramble.py  sub.sh
```

Create list of input files

GNU Parallel Job

inputs.txt

```
Sorted/input1.txt
Sorted/input2.txt
Sorted/input3.txt
Sorted/input4.txt
Sorted/input5.txt
Sorted/input6.txt
Sorted/input7.txt
Sorted/input8.txt
Sorted/input9.txt
Sorted/input10.txt
```

sub_parallel.sh

```
#!/bin/bash
#SBATCH --job-name=Parallel
#SBATCH --nodes=1
#SBATCH --ntasks=10
#SBATCH --partition=batch
#SBATCH --mem=10G
#SBATCH --time=00:10:00
#SBATCH --output=standard_outputs/%x_%j.out

cd $SLURM_SUBMIT_DIR

module load parallel/20230722-GCCcore-12.3.0
module load Python/3.11.3-GCCcore-12.3.0

parallel ./scramble.py {} ./parallel_outputs :::: inputs.txt
```

Slurm Array Job

inputs.txt

```
Sorted/input1.txt
Sorted/input2.txt
Sorted/input3.txt
Sorted/input4.txt
Sorted/input5.txt
Sorted/input6.txt
Sorted/input7.txt
Sorted/input8.txt
Sorted/input9.txt
Sorted/input10.txt
```

sub_array.sh

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name=Array
#SBATCH --ntasks=1
#SBATCH --partition=batch
#SBATCH --mem=1G
#SBATCH --time=00:10:00
#SBATCH --output=standard_outputs/%x_%j.out
#SBATCH --array=1-10

cd $SLURM_SUBMIT_DIR

module load Python/3.11.3-GCCcore-12.3.0

./scramble.py $(awk "NR==${SLURM_ARRAY_TASK_ID}" inputs.txt) ./array_outputs
```