EURO
BELGIUM

Advanced Slurm job submission

UCLouvain

Part I. Workflows with Slurm

Part II: Workflows with GNU tools & Slurm

Part III: Heterogeneous jobs

Part IV: Process placement

wide

workflows

Job arrays

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deep

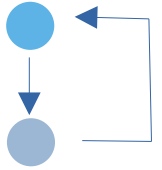
workflows

Job dependencies

Packed jobs

cyclic

workflows



Requeuing

In-job submissions

Job arrays

"Job arrays offer a mechanism for submitting and managing collections of similar jobs quickly and easily"

a.k.a. parametrized jobs

Typical use cases:

- parameter sweep
- file collection processing
- line-in-file processing

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

Job arrays

```
# Submit a job array with index values between 0 and 31
$ sbatch --array=0-31    -N1 tmp



# Submit a job array with index values of 1, 3, 5 and 7
$ sbatch --array=1,3,5,7 -N1 tmp



# Submit a job array with index values between 1 and 7
# with a step size of 2 (i.e. 1, 3, 5 and 7)
$ sbatch --array=1-7:2   -N1 tmp
```

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

Job arrays IDs

```
SLURM_JOB_ID=36
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=1
SLURM_ARRAY_TASK_COUNT=3

SLURM_JOB_ID=37
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=2
SLURM_ARRAY_TASK_COUNT=3
[…]
```

You can address multiple jobs in the array : for instance

`scancel 36_[1-2]`

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

Job array indices

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-9

module load […]

some_program $SLURM_ARRAY_TASK_ID
```

Submits a 10-job array, each job runs `some_program` with a parameter value from 0 to 9. Jobs are independent but can be managed as a whole.

Caveat: integers only

The parameter must be

- integer,
- non-negative,
- one-dimensional,
- bounded.

The parameter cannot be

- categorical,
- real valued,
- multi-dimensional,
- larger than `MaxArraySize`.

Solution: Bash array

Bash array

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-9

module load […]

PARAMS=([…])

some_program ${PARAMS[$SLURM_ARRAY_TASK_ID]}
```

Submits a 10-job array, each job runs `some_program` with a parameter value taken from the `PARAMS` array

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

Bash array : explicit

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-2

module load […]

PARAMS=(red blue green)

some_program ${PARAMS[$SLURM_ARRAY_TASK_ID]}
```

Submits a 3-job array, each job runs `some_program`, once with parameter value `red`, the other `blue` and the final one, `green`

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

Bash array : globbing

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-2

module load […]

PARAMS=(~/data/*.csv) # list of .csv files in data/

some_program “${PARAMS[$SLURM_ARRAY_TASK_ID]}”
```

Submits a 3-job array, each job runs `some_program` with a file matching the `~/data/*.csv` pattern, in alphanumerical order.

https://www.gnu.org/software/bash/manual/bash.html#Filename-Expansion

Bash array : brace expansion

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-9

module load […]

PARAMS=(1.{0..9}) # expands to 1.0 1.1 1.2 … 1.9

some_program ${PARAMS[$SLURM_ARRAY_TASK_ID]}
```

Submits a 10-job array, each job runs `some_program` with a parameter equal to 1.0, 1.1, 1.2, … 1.9.

https://www.gnu.org/software/bash/manual/bash.html#Brace-Expansion

Bash array : brace expansion

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-8

module load […]

PARAMS=({1..3}_{red,green,blue}) # = 1_red 1_green 1_blue 2_red …

some_program ${PARAMS[$SLURM_ARRAY_TASK_ID]/_/ }
```

Submits a 9-job array, each job runs `some_program` with two parameters equal to `1 red`, `1 green`, …, `3 green`, `3 blue`.

https://www.gnu.org/software/bash/manual/bash.html#Brace-Expansion

Bash array : seq

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-9

module load […]

PARAMS=$(seq --format %.3E 1 0.1 2) #= 1.000E+00 1.100E+00 …

some_program ${PARAMS[$SLURM_ARRAY_TASK_ID]}
```

Submits a 10-job array, each job runs `some_program` with a parameter equal to 1.000E+00, 1.100E+00, …, 1.900+E0

https://www.gnu.org/software/bash/manual/bash.html#Brace-Expansion

Bash array : mapfile

```
#! /bin/bash
#
#SBATCH […]
#SBATCH --array=0-9

module load […]

mapfile PARAMS < /path/to/parameterfile # reads file into variable

some_program ${PARAMS[$SLURM_ARRAY_TASK_ID]}
```

Submits a 9-job array, each job runs `some_program` with as parameter one line from the `parameterfile` file.

https://www.gnu.org/software/bash/manual/bash.html

Caveat: nb jobs hardcoded

The `SBATCH` lines are comments in Bash, variable expansion is ignored.

`#SBATCH --array=1-$N`

```
↳ sbatch: error: Batch job submission failed: Invalid job array specification
```

Solutions: CLI option or `stdin` submission

CLI option

```
#! /bin/bash
#
#SBATCH […]

module load […]
echo ${PARAMS[@]}

some_program “${PARAMS[$SLURM_ARRAY_TASK_ID]}”
```

```
$ PARAMS=([…])
$ N=${#PARAMS[@]}
$ sbatch --array=0-$N submit_script.sh
```

Give the argument in the command line rather than in the script

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

`stdin` submission

```
#! /bin/bash
#SBATCH […]
#SBATCH --array=1-$N

module load […]
echo ${PARAMS[@]}

some_program “${PARAMS[$SLURM_ARRAY_TASK_ID]}”
```

```
$ PARAMS=([…])
$ N=${#PARAMS[@]}
$ envsubst '${N}' < submit_script.sh | sbatch
```

Feed the script to `sbatch` through `stdin` rather than as file path

https://www.gnu.org/software/gettext/manual/html_node/envsubst-Invocation.html

Scripted submissions

Submission scripts are not always necessary ; jobs can be submitted directly on the command line.

Typical use cases:

- jobs too different for job arrays
- submission from within a pre-existing script
- only a few jobs

Inline submissions

```
#! /bin/bash
#
#SBATCH --time=[…]
#SBATCH --ntasks=[…]

module load […] OpenMPI

mpirun some_program
```

The script can be replaced with a single call to `sbatch`

```
$ module load […] OpenMPI
$ sbatch --time=[…] --ntasks=[…] --wrap “mpirun some_program”
```

Scripted submissions

```
$ module load OpenMPI
$ for i in 4 8 16 32; do sbatch -n=$i --wrap “mpirun some_program”; done
```

Typical use case: scaling studies

```
#! /bin/bash

for file in ~/data/*.dat
do
compress “$file”
done
```



```
#! /bin/bash

for file in ~/data/*.dat
do
sbatch --wrap “compress \“$file\””
done
```

Typical use case: when you already have a script that works on your laptop without Slurm and want to use it on the cluster.

Job dependencies

"-d, --dependency=<dependency_list>

Defer the start of this job until the specified dependencies have been satisfied completed."

Typical use cases:

1. pre-processing job
2. processing job
3. post-processing job

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

Job dependencies

Possible `dependency_list` items:

```
after:job_id[[+time][:jobid[+time]…]] # after job(s) start (+ time)
afterany:job_id[:jobid…] # after job(s) have terminated
afterburstbuffer:job_id[:jobid…] # after job+bbuffer is done
aftercorr:job_id[:jobid…] # job arrays
afternotok:job_id[:jobid…] # after jobs failed
afterok:job_id[:jobid…] # after jobs completed successfully
singleton
```

Comma-separated list→ AND ; ?-separated list→ OR

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

Job dependencies

Example

```
$ sbatch preprocess.sh
submitted batch job 1

$ sbatch -d afterok:1 process1.sh
submitted batch job 2

$ sbatch -d afterok:1 process2.sh
submitted batch job 3

$ sbatch -d afterok:2:3 postprocess.sh

$ sbatch -d afterany:1:2:3 cleanup.sh

$ sbatch -d afternotok:1?afternotok:2?afternotok:3 cancel.sh
```

Jobs whose dependency will never be satisfied must be dealt with

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

Caveat:IDs unknown until submitted

The dependency jobs must have been submitted before the dependent job and their job IDs be captured.

Solutions: CLI option --parsable

Job dependencies

```
JID=999999 # If jobid does not exist, no dependency is set
for i in {1..4};
do

JID=$(sbatch --parsable --dependency=afterok:$JID submit_script_$i.sh)

done
```

Submits 4 jobs (`submit_script_1.sh` -> `submit_script_4.sh`) chained together with N-1 dependency

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

Packed jobs (serial)

When jobs are small you can pack them into multi-step jobs to ease overhead.

```
#!/bin/bash
#SBATCH […]

for i in {1..4};
do

srun […] some_program $i

done
```

Submits 1 job running 4 steps in series (dependency is implicit)

All steps inherit the full allocation.

Packed jobs (parallel)

When jobs are small you can pack them into multi-step jobs to ease overhead.

```
#!/bin/bash
#SBATCH […]
#SBATCH -n 4 # can be <= 4; srun instances will start when possible
for i in {1..4};
do
srun -n1 -c1 --exact some_program $i &
done
wait
```

Submits 1 job running 4 steps in parallel

Each step gets a subset of the allocation.

Packed jobs (parallel)

When jobs are small you can pack them into multi-step jobs to ease overhead.

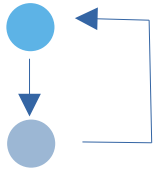
```
#!/bin/bash
#SBATCH […]
#SBATCH -n 4 # can be <= 4; srun instances will start when possible
for i in {1..4};
do
srun -n1 -c1 --exact some_program $i &
done
wait
```

If there are mores steps than the allocation allows, they are queued unless --overlap is specified.

Packed jobs: --exclusive

```
#SLURM change log
* Changes in Slurm 20.11.0rc1
  -- Make --exclusive the default with srun as a step adding --overlap to
reverse behavior.
  -- Add --whole option to srun to allocate all resources on a node in an
allocation.
* Changes in Slurm 20.11.3
  -- Partially revert changes made in 20.11.0 to srun step behavior. […]
This reverts the behavior such that all resources on a node are assigned
to the job step by default.
  -- srun - add a new --exact option, and deprecate the --whole option
(which has been restored as the default behavior).
# and now --exclusive implies --exact
* Changes in Slurm 21.08.0rc1
  -- --cpus-per-task and --threads-per-core now imply --exact.
* Changes in Slurm 21.08.6
  -- Remove implicit --exact when --cpus-per-task is used.
```

Older Slurm versions will prefer `--exclusive`



Job requeuing

A job can requeue itself if it has not finished working

```
#!/bin/bash
#SBATCH […]

SBATCH --append

echo “Restart count: ${SLURM_RESTART_COUNT}“
some_program

if some_condition; do
scontrol requeue $SLURM_JOB_ID
fi
```

Job requeuing

A job can requeue itself if it has not finished working

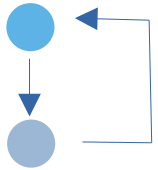
```
#!/bin/bash
#SBATCH […]

SBATCH --append

echo “Restart count: ${SLURM_RESTART_COUNT}“
some_program

if some_condition; do
exit 99
fi
```

```
[dfr@lemaitre3 ~] (StdEnv) $ scontrol show config | grep RequeueExit
RequeueExit             = 99
RequeueExitHold         = 98
```



In-job submission

A job can submit itself again.

```
#!/bin/bash
#SBATCH […]


some_program

if some_condition; do
sbatch $0
fi
```

The same submission script will be used even if modified since.

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Part III: Heterogeneous jobs

Part IV: Process placement

xargs

"xargs reads items from the standard input, […] and executes the command […] with items read from standard input"

Typical use cases:

- execute same command on multiple files
- line-in-file processing
- process each line output from another program

https://en.wikipedia.org/wiki/Xargs

xargs

```
$ find . -name \*.csv -print0 |\
    xargs -I{} -0 sbatch […] --wrap ‘some_program “{}”’
```

Submits one **job** for each CSV file, passed as argument to `some_program`

```
#!/bin/bash
#SBATCH […]

module load […]

find . -name \*.csv -print0 |\
   xargs -P $SLURM_NTASKS -I{} -0 srun --exact […] some_program “{}”
```

Generates one job **step** for each CSV file found (max $SLURM_NTASKS at a time)

https://en.wikipedia.org/wiki/Xargs

xargs

```
$ cat parameters.csv |\
    xargs -I{} sbatch […] --wrap “some_program {}”
```

Submits one **job** for each line in `parameters.csv`

```
#!/bin/bash
#SBATCH […]

module load […]

cat parameters.csv |\
    xargs -P $SLURM_NTASKS -I{} srun --exact […] some_program {}
```

Generates one job **step** for each line in `parameters.csv` (max $SLURM_NTASKS at a time)

https://en.wikipedia.org/wiki/Xargs

envsubst

"standard input is copied to standard output, with references to environment variables of the form $VARIABLE or ${VARIABLE} being replaced with the corresponding values. "

Typical use case:

- when program parameters are in a file rather than on command line

https://www.gnu.org/software/gettext/manual/html_node/envsubst-Invocation.html

envsubst

```
$ cat input.txt
nprocs=$NPROCS
tol=$TOL
MaxIter=$MAXITER

$ export NPROCS=4; export TOL=0.01; export MAXITER=10000

$ envsubst < input.txt
nprocs=4
tol=0.01
MaxIter=100090
```

https://en.wikipedia.org/wiki/Xargs

envsubst

```
$ NPROCLIST=(2 4 8)
$ TOLLIST=(0.01 0.001 0.001)
$ MAXITERLIST=(1000 10000 100000)

$ for i in {0..2}; do
> NPROC=${NPROCLIST[$i]} ; TOL=${TOLLIST[$i]}; MAXITER=${MAXITERLIST[i]}
> envubst < input.txt > input.job$i.txt
> sbatch […] --wrap “some_program input.job$i.txt”
> done
```

Submits one job for each triplet (NPROC, TOL, MAXITER), creating the needed input file from the environment variables.

https://en.wikipedia.org/wiki/Xargs

GNU Parallel

"GNU parallel is a shell tool for executing jobs in parallel using one or more computers. "

Typical use cases:

- for generating parameters (scripted submissions)
- for managing parallel processes (job packing)

https://www.gnu.org/software/parallel/

GNU Parallel

```
$ parallel echo ::: 1 2 3
1
2
3
```

Runs the `echo` command three times in parallel (order of output is random) with each parameter listed after `:::`. Equivalent to

```
$ echo 1 &
$ echo 2 &
$ echo 3 &
```

https://www.gnu.org/software/parallel/

(BEWARE of the version installed by default which can be too old. Look for modules or install by yourself)

GNU Parallel and Slurm

```
$ parallel sbatch […] --wrap “some_program {}” ::: *.csv
```

Submits one **job** for each CSV file found

```
#!/bin/bash
#SBATCH […]

module load […]

parallel -j $SLURM_NTASKS srun --exclusive […] some_program {} ::: *.csv
```

Generates one **job** step for each CSV file found, max $SLURM_NTASK at a time

GNU Make

"GNU Make is a tool which controls the generation of executables and other non-source files of a program from the program's source files."

Typical use case:

- for building software

https://www.gnu.org/software/make/

GNU Make

"GNU Make is a tool which controls the generation of executables and other non-source files of a program from the program's source files. […] Make is not limited to building a package. You can also use Make to control installing or deinstalling a package, generate tags tables for it, or anything else you want to do often enough to make it worth while writing down how to do it."

Highjacked use case:

- for managing processes dependencies (job packing)

https://www.gnu.org/software/make/

GNU Make

```
$ cat Makefile
# comment
target1:  dependencies1 … target2
          commands1
          …

target2:  dependencies2 …
          commands2
          …
```

Running `make` builds the file `target1` by first building file `target2`

https://www.gnu.org/software/make/

GNU Make: //

```
$ make --jobs 4 --output-sync
```

The `-j` or `--jobs` option tells make to execute many recipes simultaneously, while `--output-sync` prevents mingled outputs

https://www.gnu.org/software/make/

GNU Make and Slurm

```
$ cat Makefile
.ONESHELL:
SHELL=srun
.SHELLFLAGS= -n1 -c1 --exact bash -c
[…]
```

```
#!/bin/bash
#SBATCH […]

module load […]

make -j $SLURM_NTASKS
```

Will run every command as a Slurm step, in parallel, honoring dependencies.

http://plindenbaum.blogspot.com/2014/09/parallelizing-gnu-make-4-in-slurm.html

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Heterogeneous job

A job where all processes do not require the same resources. E.g.

- a master/worker setup
- a coupled simulation model

```
#! /bin/bash
#SBATCH --cpus-per-task=2
#SBATCH --mem-per-cpu=1g
#SBATCH --ntasks=1
#SBATCH --partition=main

#SBATCH packjob

#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4g
#SBATCH --ntasks=4
#SBATCH --partition=large

[...]
```

Het. MPMD job

A job where all processes do not require the same resources. E.g.
- a master/worker setup
(No `multi.conf` file)

```
[…]
srun --het-group=0 coordinator.sh &
srun --het-group=1 worker.sh &
wait
```

Distinct steps, distinct MPI world

Het. master/worker job

A job where all processes do not require the same resources. E.g. - a coupled simulation model

```
[…]
srun coordinator.sh : worker.sh
# or
mpirun coordinator.sh : worker.sh
```

Single step, single MPI world

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Process placement

Remember:

How to submit an MPI job >

Specify a number of “tasks” and optionally a number of “nodes”

You want	You ask
N CPUs	`--ntasks=N`

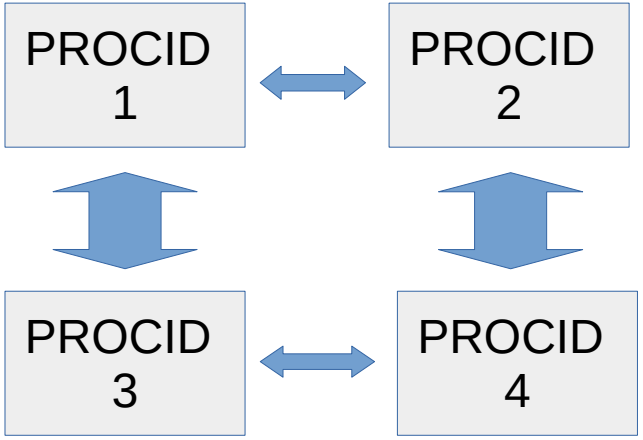
N CPUs spread across distinct nodes	`--ntasks=N --nodes=N`
	or
	`--ntasks=N --ntasks-per-node=1`

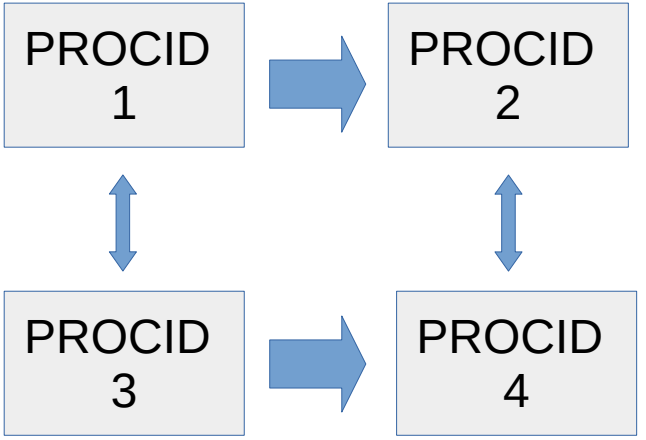
N CPUs spread across distinct nodes and nobody else around	`--nodes=N --exclusive`
N CPUs spread across *N/2* nodes	`--ntasks=N --ntasks-per-node=2`

N CPUs on the same node	`--ntasks=N --ntasks-per-node=N`
	or
	`--ntasks=N --nodes=1`

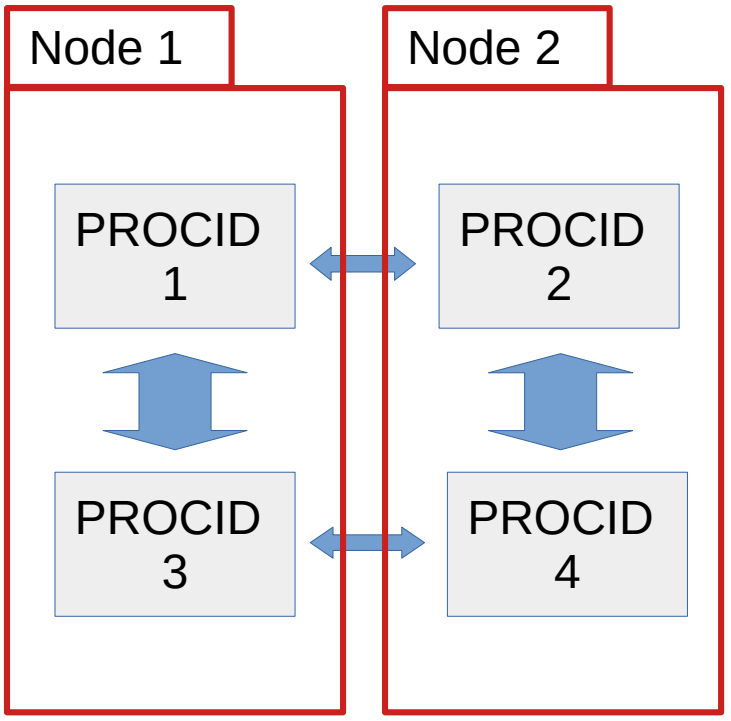
How are ranks distributed?

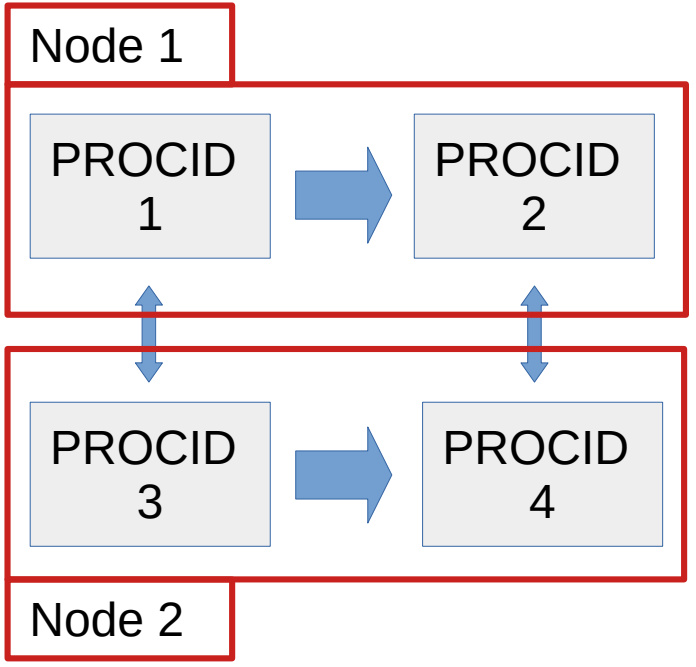
Rank distribution across nodes





Rank distribution across nodes





Rank distribution across nodes

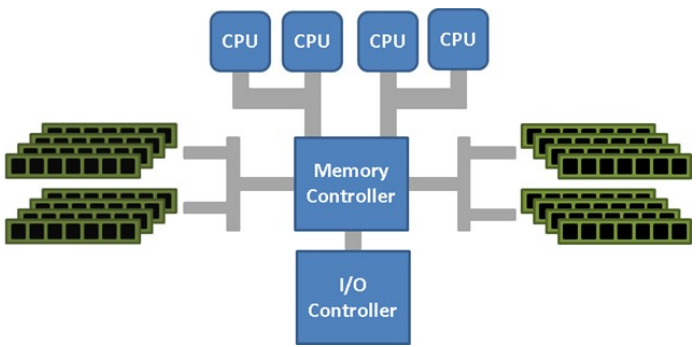
The `-m/--distribution` option controls the strategy for placement

```
$ srun -l -n 4 -N 2 -m block --exclusive  hostname | sort
0: lm3-w014.cluster
1: lm3-w014.cluster
2: lm3-w018.cluster
3: lm3-w018.cluster

$ srun -l -n 4 -N 2 -m cyclic --exclusive  hostname | sort
0: lm3-w014.cluster
1: lm3-w018.cluster
2: lm3-w014.cluster
3: lm3-w018.cluster
```

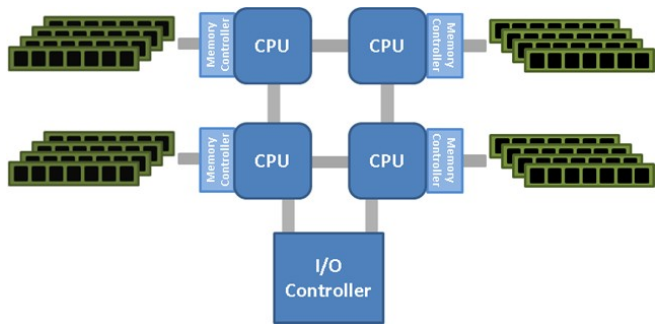
Other options: `arbitrary`, `plane=`*n*

Rank distribution inside the node

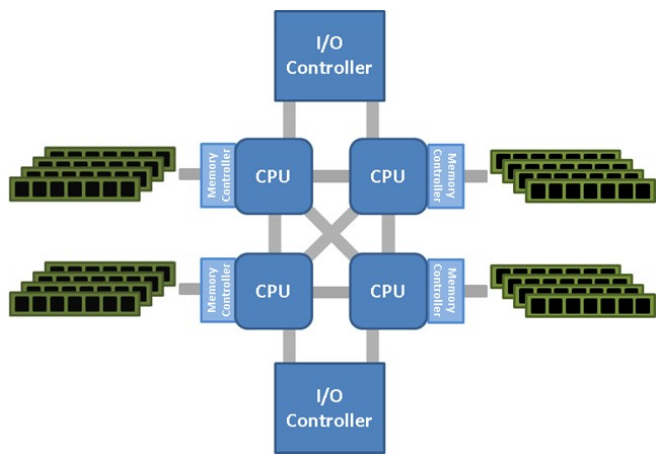
(SMP)



VS.



(NUMA)



https://www.sqlskills.com/blogs/jonathan/understanding-non-uniform-memory-accessarchitectures-numa/

Rank distribution per socket

The -m/--distribution second option controls the strategy for placement on sockets. E.g. on a two-socket node (2x32 cores):

```
$ srun -l -n 4  -c4 -m block:block --exclusive bash -c 'taskset -cp $$'

0: pid 3156907's current affinity list: 0-3
1: pid 3156908's current affinity list: 4-7
2: pid 3156909's current affinity list: 8-11
3: pid 3156910's current affinity list: 12-15

$ srun -l -n 4  -c4 -m block:cyclic --exclusive bash -c 'taskset -cp $$'

0: pid 3156982's current affinity list: 0-3
1: pid 3156983's current affinity list: 32-35
2: pid 3156984's current affinity list: 4-7
3: pid 3156985's current affinity list: 36-39
```

Rank distribution per socket

The -m/--distribution second option controls the strategy for placement on sockets. E.g. on a two-socket node (2x32 cores):

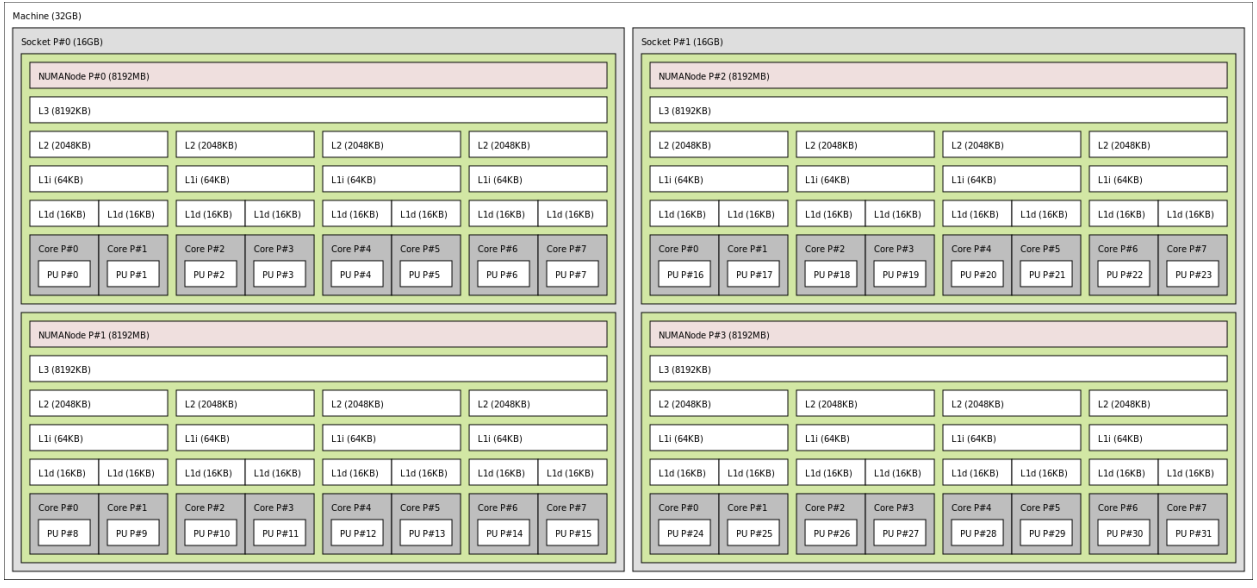
```
$ srun -l -n 4  -c4 -m block:cyclic --exclusive bash -c 'taskset -cp $$'

0: pid 3156982's current affinity list: 0-3
1: pid 3156983's current affinity list: 32-35
2: pid 3156984's current affinity list: 4-7
3: pid 3156985's current affinity list: 36-39

$ srun -l -n 4  -c4 -m block:fcyclic --exclusive bash -c 'taskset -cp $$'

0: pid 3157056's current affinity list: 0,1,32,33
1: pid 3157057's current affinity list: 2,3,34,35
2: pid 3157058's current affinity list: 4,5,36,37
3: pid 3157059's current affinity list: 6,7,38,39
```

Rank distribution per SMT thread

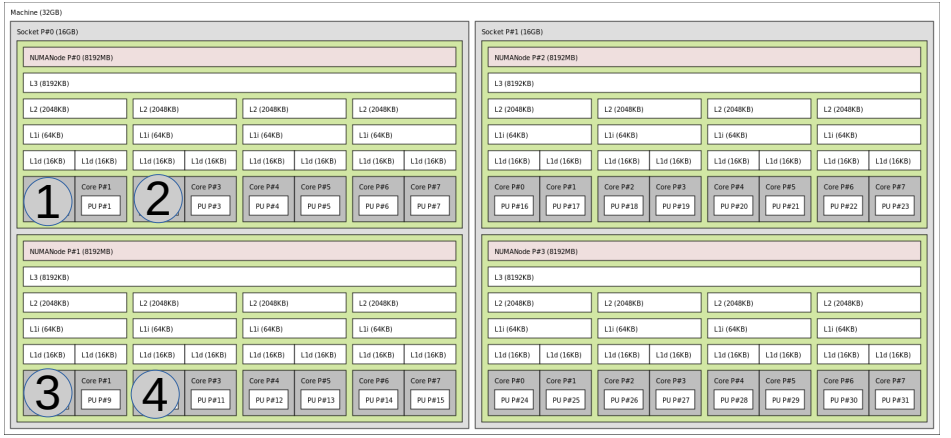
The -m/--distribution third option controls the strategy for placement on cores.

- Can be replaced with `--hint=[no]multithread`

- Unfortunately there are intermediate levels that Slurm does not take into account.



Generic intra-node distribution



	Spread	Packed
Cache size available per process	good	bad
Memory bandwidth available per process	good	bad
Latency to common shared memory	bad	good

Arbitrary intra-node distribution

With the `--cpu-bind=map_cpu:...` option you can specify the (ordered) list of CPUs to distribute the processes on.

```
$  srun -l -n 4  --cpu-bind=map_cpu:3,0,22,12  bash -c 'taskset -cp $$'

0: pid 18258's current affinity list: 3
1: pid 18259's current affinity list: 0
2: pid 18260's current affinity list: 22
3: pid 18261's current affinity list: 12
```

https://slurm.schedmd.com/srun.html#OPT_cpu-bind

Rank distribution helper tool

OpenMPI's utility tool `hwloc-distrib` can be used to build an optimally-spread placement based on the server hardware configuration.

```
$ D=$(hwloc-distrib --single 16 | xargs hwloc-calc --pulist) #128-CPUs node
$ echo $D

0,8,16,24,32,40,48,56,64,72,80,88,96,104,112,120

$  srun -l -n 4  --cpu-bind=map_cpu:$D  bash -c 'taskset -cp $$'

0: pid 18258's current affinity list: 0
1: pid 18259's current affinity list: 8
2: pid 18260's current affinity list: 16
3: pid 18261's current affinity list: 24
[...]
```

https://linux.die.net/man/1/hwloc-distrib

Rank and binary distribution

In case of MPMD job, you might want to distribute executable binaries as well **with `--multi-prog`** or with a launcher script.

```
# multi.conf for --multi-prog

0-3   ./model1.exe
4-7   ./model2.exe
8-11  ./model1.exe
12-15 ./model2.exe

$ hwloc-distrib  4 | xargs -L1 hwloc-calc --pulist \
                   | cut -d, -f 1-4 | paste  -s -d,
0,1,2,3,32,33,34,35,64,65,66,67,96,97,98,99

$ srun -l --cpu-bind=map_cpu:0,1,2,3,32,33,... --multi-prog=multi.conf
```

https://linux.die.net/man/1/hwloc-distrib

Rank and binary distribution

In case of MPMD job, you might want to distribute executable binaries as well with `--multi-prog` or with a **launcher script**.

```
#! /bin/bash

EXE=(./model1.exe ./model2.exe)
PATTERN=(0 0 0 0 1 1 1 1)

INDEX=$((SLURM_PROCID % ${#PATTERN[@]}))
exec ${EXE[${PATTERN[INDEX]}]}


$ srun -l –cpu-bind=map_cpu:0,1,2,3,32,33,... helper.sh
```

Part I. Workflows with Slurm

Part II: Workflows with GNU tools

Part III: Heterogeneous jobs

Part IV: Process placement