GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES
Instituto de Salud Carlos III

Scripting & Parallelization SLURM

Sbatch, JobArray, OpenMP/MPI

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2. Parallelization on our cluster — OpenMP vs MPI (when to use each)
3. From scripts to workflows — building a reproducible pipeline (Nextflow preview)
4. Wrap-up & Q&A

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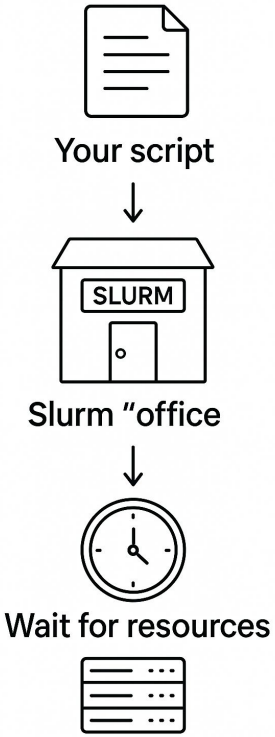
Sbatch File

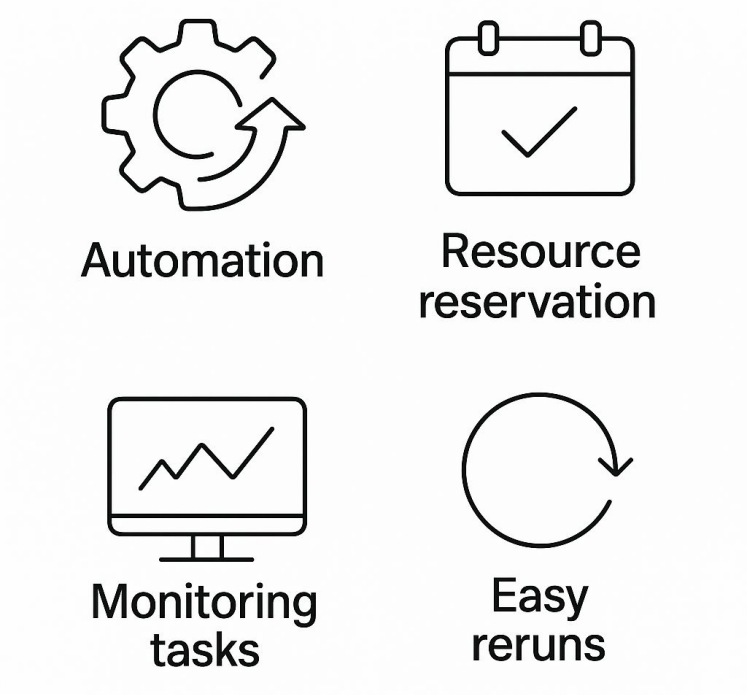
Scripting on the cluster — Slurm: sbatch

What is sbatch?

- Command to submit a job script to Slurm; runs in the background on compute nodes.
- Delegate the work to de cluster:
  - Submit once, let the cluster work
- Example:
  - Your script → Slurm "office" → Wait for resources → Cluster runs it



Scripting on the cluster — Slurm: sbatch



What is for?

- Automation
- Resource reservation
- Monitoring tasks
- Easy reruns

Scripting on the cluster — Slurm: sbatch & job arrays

Set up a sbatch script file

- 1) Create an SBATCH script
- 2) Init with shebang
- 3) Set up slurm directives at the beginning of the script by using “#SBATCH”
- 3) After directives, you can:
  - Load dependencies with ‘module load’
  - Set your commands you want to run

```
#!/bin/bash
#SBATCH --option=value
#SBATCH --option=value
#SBATCH --option=value
# From here on, the commands
command_1
command_2
```

Scripting on the cluster — Slurm: sbatch & job arrays

```
#!/bin/bash
#SBATCH --chdir=/path/to/working/directory   # Folder where the analysis will run
#SBATCH --job-name=my_first_slurm_job        # A recognizable job name
#SBATCH --cpus-per-task=1                    # Number of CPU cores (threads) for this job
#SBATCH --mem=1G                             # RAM to reserve
#SBATCH --time=00:10:00                      # Time limit (HH:MM:SS)
#SBATCH --partition=short_idx                # Queue/partition to run in
#SBATCH --output=slurm-%j.out                # File for standard output
#SBATCH --error=slurm-%j.err                 # File for standard error
# From here on, the commands we want to run:
command_1
command_2
```

Scripting on the cluster — Slurm: sbatch & job arrays

Submit sbatch file and monitor execution

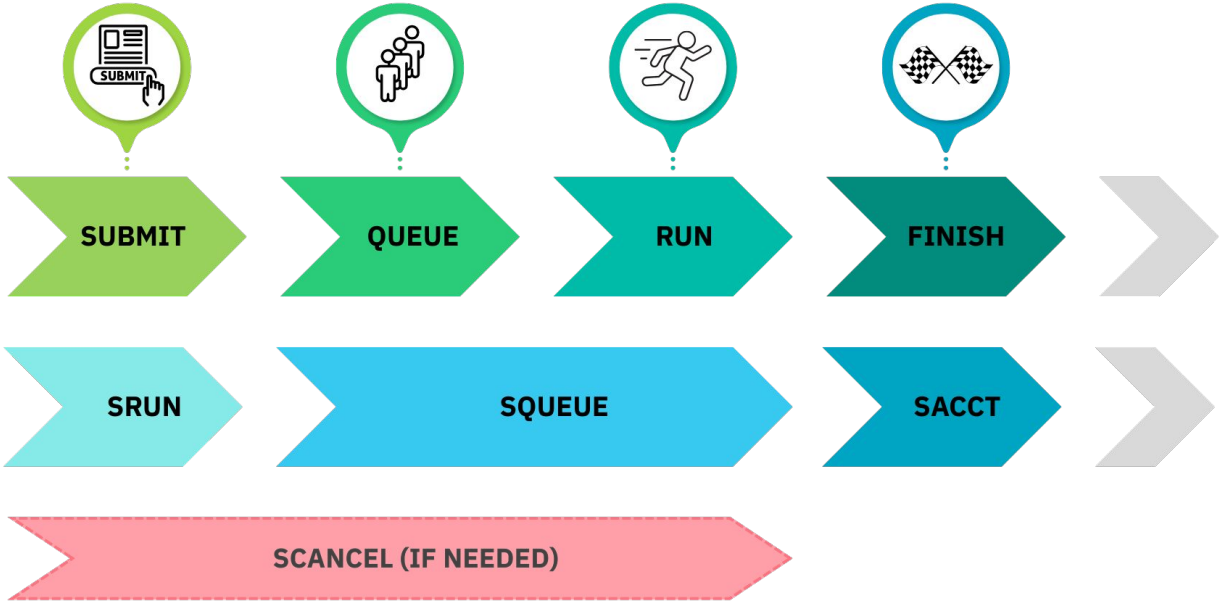
- Submit a job with **sbatch <filename>.sbatch**
  → “Submitted batch job 12345”
- States: PD (Pending) → R (Running) → CG (Completing) → finished
- Monitor while it runs using: **squeue**

Scripting on the cluster — Slurm: sbatch & job arrays

```
# Submit
$ sbatch fastqc_slurm.sbatch
Submitted batch job 12345

# See the queue
$ squeue --me
             JOBID PARTITION     NAME     USER ST   TIME  NODES NODELIST(REASON)
           12345_2 short_idx fastqc_2     dani  R  00:01:12     1 ideafix03
           12345_3 short_idx fastqc_3     dani PD  00:00:00     1 (Resources)
             12344      long   spades     dani CG  01:59:58     1 ideafix07
             12343      long   spades     dani  R  00:10:21     2 ideafix05,ideafix06
             ▲          ▲        ▲         ▲  ▲     ▲        ▲             ▲
             |          |        |         |  |     |        |             └─ Node(s) assigned;
             |          |        |         |  |     |        └─ Number of nodes reserved
             |          |        |         |  |     └─ Elapsed time (HH:MM:SS)
             |          |        |         |  └─ Short state (PD/R/CG/…)
             |          |        |         └─ User
             |          |        └─ Job name (--job-name)
             |          └─ Partition / queue (e.g., short_idx)
             └─ JobID (arrays: JobID_task, e.g., 12345_2)
```

Monitoring and job states



Scripting on the cluster — Slurm: sbatch & job arrays

Bigger asks = longer wait, not faster.

Scripting on the cluster — Slurm: sbatch & job arrays

Output files

- Standard output: Standard outputs of your program

slurm-12345.out

- Standard error: Potential errors you face during execution appear here.

slurm-12345.err

Scripting on the cluster — Slurm: sbatch & job arrays

Good Practices:

- Descriptive --job-name; comment your script.
- Never run heavy jobs on the login node—use sbatch/srun.
- Start small, then scale.
- Version your scripts (Git).

Thank you for your attention

Questions?

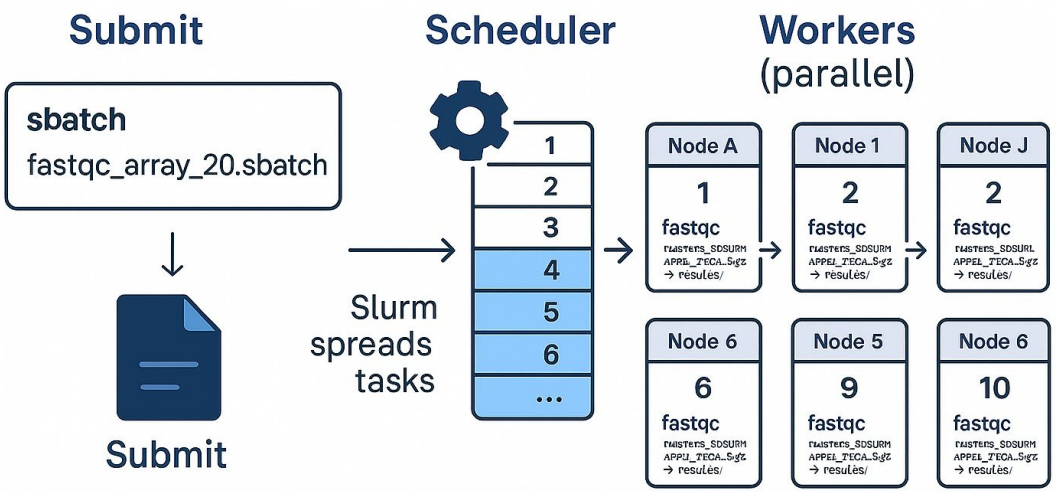
JobArrays

Scripting on the cluster — Slurm: job arrays

What are JobArrays and what are they used for?

- Sbatch script designed to launch many jobs
  - Same operation / multiple inputs
- Instead of creating 50 scripts for 50 samples, you create one script and tell Slurm to run it N times → In Parallel
- If your shell for loop only changes a filename/ID, make it a job array.

SLURM Job Array – How it works



- $SLURM_ARRAY, TASK_ID = task index
- %A = array JobID, %a = task index (used in log file names)

Scripting on the cluster — Slurm: job arrays

Create a JobArray script?

- As simple as using the `--array` inside the sbatch script

```
#!/bin/bash
#SBATCH --chdir=/path/to/project
#SBATCH --job-name=fastqc_array
#SBATCH --partition=short_idx
#SBATCH --array=1-20
#SBATCH --cpus-per-task=1
#SBATCH --mem=5G
#SBATCH --time=00:15:00
#SBATCH --output=fastqc_%A_%a.out # %A: array JobID, %a: task index
#SBATCH --error=fastqc_%A_%a.err

module load fastqc/0.12.1

mkdir fastqc_results
fastqc -o fastqc_results muestra_${SLURM_ARRAY_TASK_ID}.fq.gz
```

Scripting on the cluster — Slurm: job arrays

Monitoring Arrays

```
$ sbatch fastqc_array_20.sbatch
Job Submitted
$ squeue --me
             JOBID PARTITION     NAME       USER ST   TIME  NODES NODELIST(REASON)
          78901_1   short_idx fastqc_array   dani  R   0:41      1 ideafix02
          78901_2   short_idx fastqc_array   dani  R   0:39      1 ideafix03
          78901_3   short_idx fastqc_array   dani  R   0:36      1 ideafix04
          78901_4   short_idx fastqc_array   dani PD   0:00      1 (Resources)
          78901_5   short_idx fastqc_array   dani PD   0:00      1 (Resources)
          78901_6   short_idx fastqc_array   dani PD   0:00      1 (Resources)
          78901_7   short_idx fastqc_array   dani PD   0:00      1 (Priority)
          78901_8   short_idx fastqc_array   dani PD   0:00      1 (Priority)
          78901_9   short_idx fastqc_array   dani PD   0:00      1 (Priority)
         78901_10   short_idx fastqc_array   dani PD   0:00      1 (Priority)
```

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Thank you for your attention

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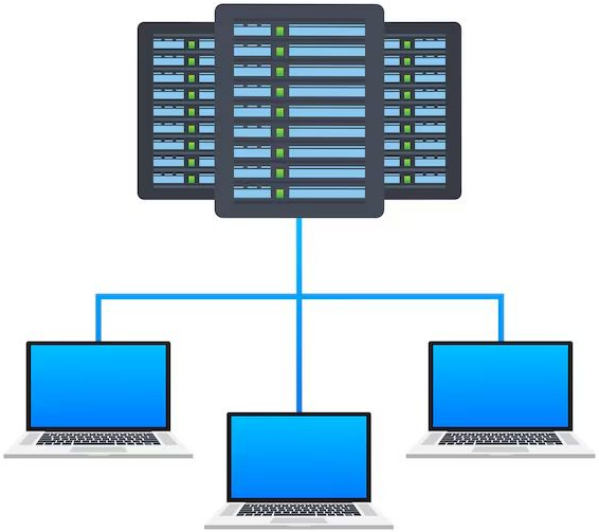
OpenMP v.s. MPI

Parallelization on our cluster — OpenMP vs MPI

Parallel programing -- OpenMP and MPI

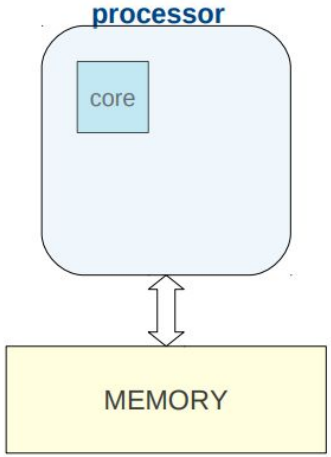
- Parallel programming splits a job into smaller pieces that run at the same time on multiple CPU cores and/or machines.
- We use it to finish faster.
- In HPC, it reduces time-to-results, makes better use of cluster resources, and cuts wall-clock time for analyses.
- The two most used HPC models are **OpenMP** and **MPI**.
- They target different scenarios: OpenMP (shared memory, one node) vs MPI (distributed memory, many nodes).



Parallelization on our cluster — OpenMP vs MPI

Why parallel programming?

Older processor had only one cpu core to execute instructions



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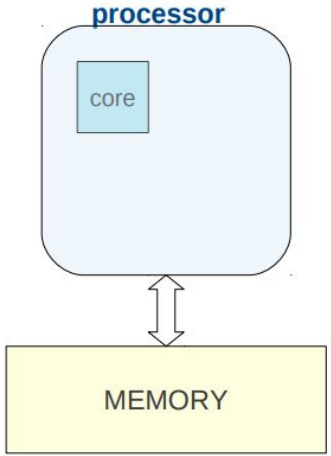
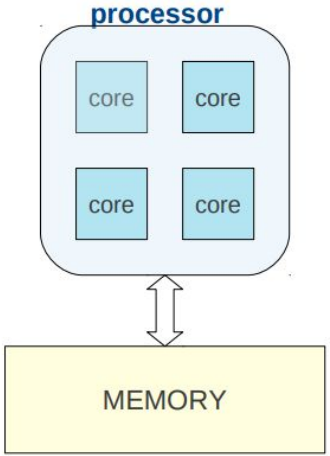


Modern processors have 4 or more independent cpu cores to execute instructions

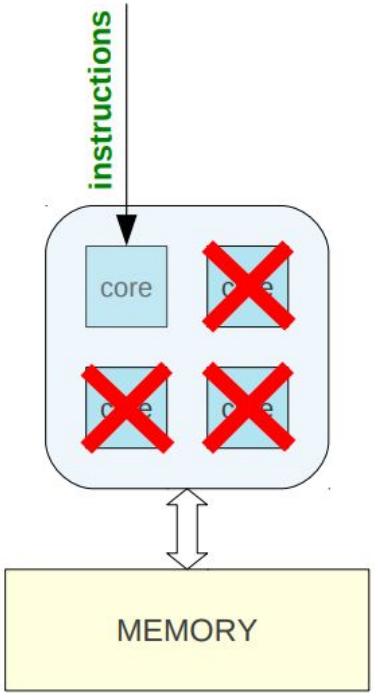


Parallelization on our cluster — OpenMP vs MPI

Why parallel computing?

When you run a sequential program it has an instruction to run a task on 1 core.

Other cores are idle



Parallelization on our cluster — OpenMP vs MPI

Why parallel computing?

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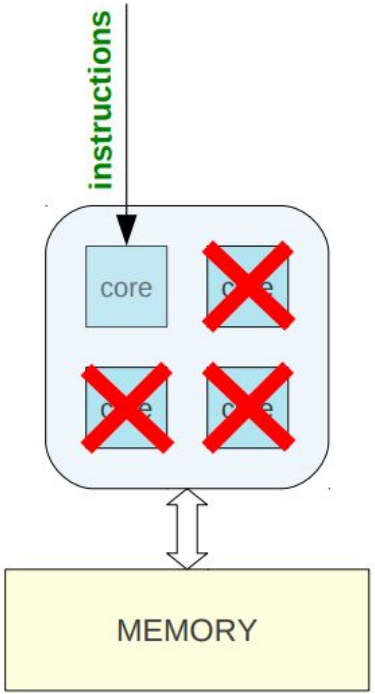
Waste of available resources…



Parallelization on our cluster — OpenMP

OpenMP Essentials

- Shared-memory parallel model
- Lets a program to use **multiple threads** inside a **single process** running **on a node** (usually has >>> CPUs).
- That node shares data in a common RAM

Most bioinformatics tools use the OpenMP model

- **Aligners**
- **Assemblers**
- **Read Processing**
- **Variant Callers**
- **...**

Parallelization on our cluster — MPI

MPI Essentials

- It is designed to run an application using **multiple separate processes**, possibly on **different nodes** of a cluster
- When: multinode scaling & very large memory needs.
- Shares resources by passing messages over the cluster's network → network issues can stop the job

Only a few bioinformatics tools use the MPI model

RAxML

IQ-Tree

Parallelization on our cluster — OpenMP vs MPI

KEY DIFFERENCES				
Technology	**Parallelization level**	**Communication between processes**	**Typical use case**	**Usage (sbatch script)**
OpenMP	Within **one node**	Shared memory: all threads access the same RAM	Align 200 million reads on one node using all its cores	--cpus-per-task (threads) --mem (Ram for the whole process)
MPI	Across **multiple nodes**	Distributed memory: each node has its own RAM; communication by network	Build a very large phylogenetic tree by splitting the work over 4 nodes	--nodes --ntasks --ntasks-per-node

Parallelization on our cluster — OpenMP vs MPI

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Questions?

HANDS-ON