HPC Training Series

Course 10 "Introduction to Computational Fluid Dynamics and OpenFOAM, using High Performance Computing"

A virtual HPC environment for familiarization with the SLURM job submission system

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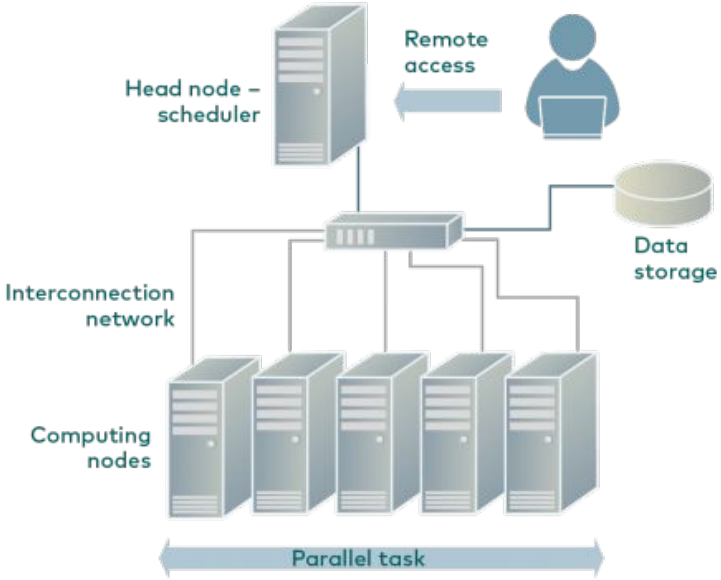
What is HPC?

- High-Performance Computing (HPC) is the ability to perform sophisticated calculations at high speeds.
- An HPC cluster consists of hundreds or thousands of compute servers, so-called nodes. The nodes in each cluster work in parallel with each other.
- HPC solves large problems in science, engineering, or business, that are too complex for a PC. On typical PC it might take e.g. hours, days, weeks to perform the computations, but if you use an HPC Cluster, it might only take minutes, hours, days, respectively.



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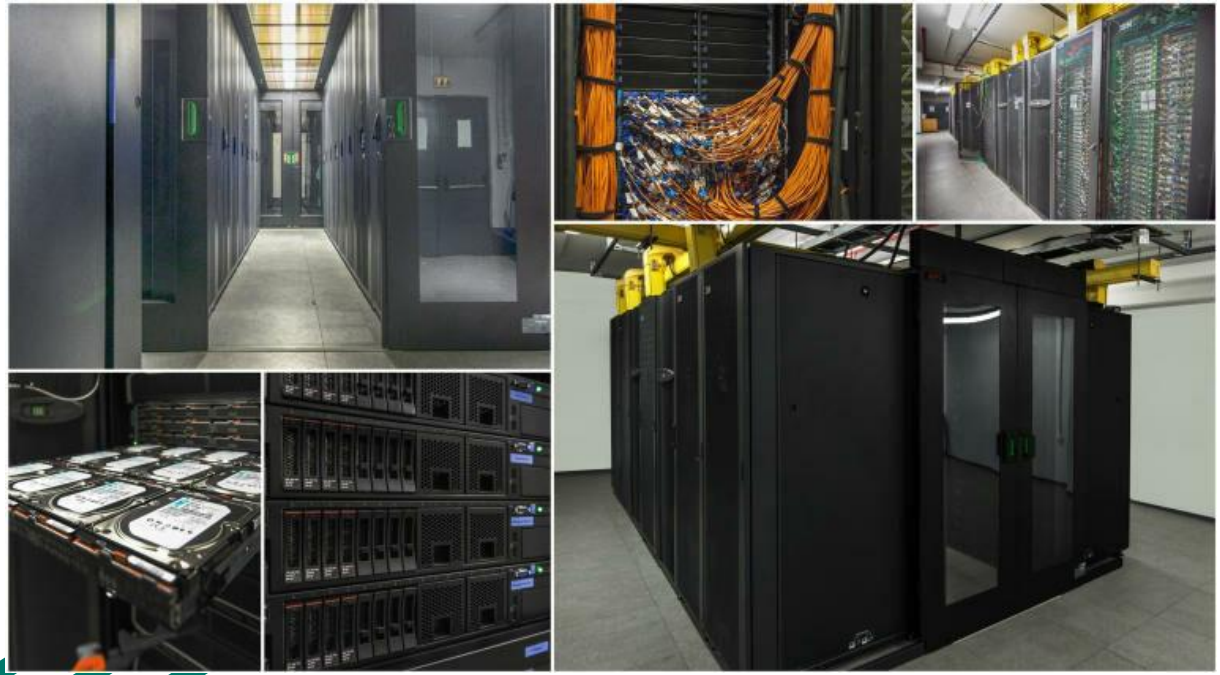
GRNET ARIS HPC Cluster



More info https://www.hpc.grnet.gr

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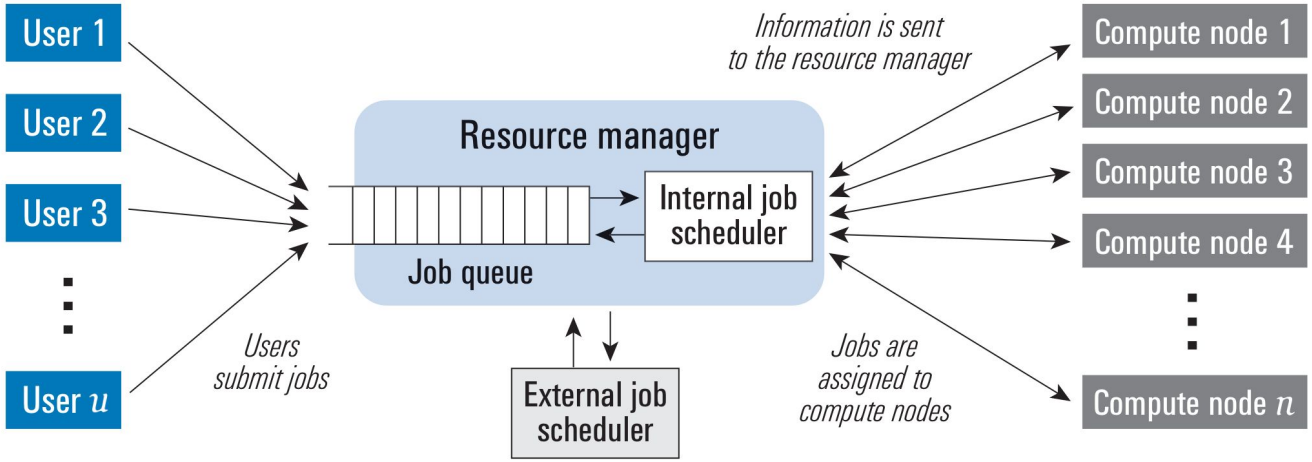
SLURM - Resource and Job Management System



SLURM: software stack that runs on HPC infrastructure and operates resource management, job scheduling and accounting

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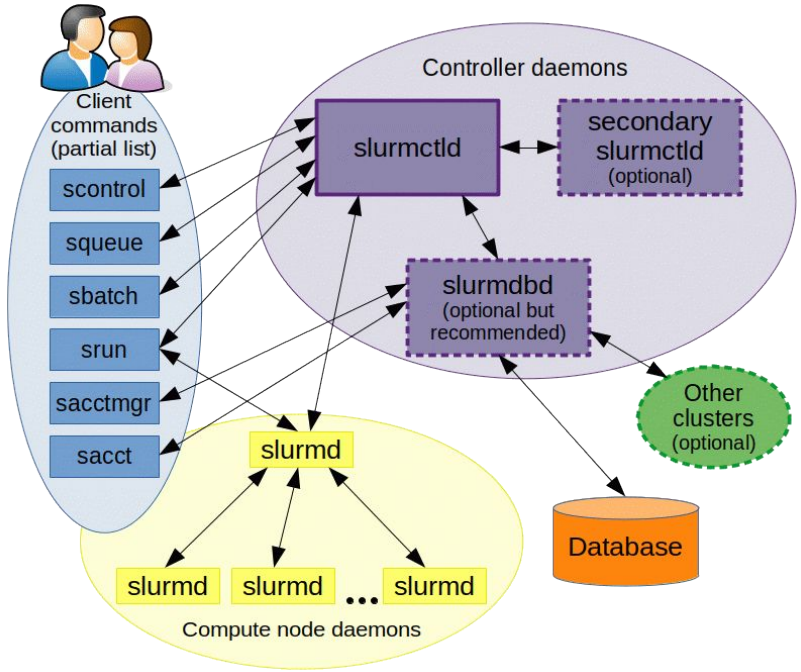
Typical HPC/SLURM infrastructure

- User executes SLURM client commands such as job submissions (sbatch) [Blue area]
- SLURM handles the received jobs and orchestrates operations [Purple area]
- SLURM passes user's jobs to compute nodes [Yellow area]
- User receives job's results back to their working dir



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Tutorial

1. In this tutorial you will deploy a typical HPC infrastructure using the SLURM resource manager under containers
2. Submit a simple MPI program, where each process prints a “Hello world” message
3. View example’s output

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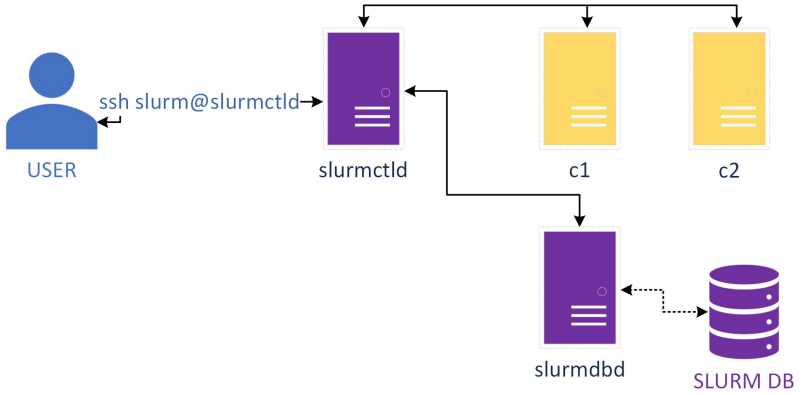
Current HPC/SLURM infrastructure

- 5 containers:
  - 1 MySQL Server instance to store SLURM accounting
  - 1 node as the DB controller
  - 1 login node as the SLURM controller and user's login endpoint
  - 2 compute nodes for calculations
- Each compute node contains 1 CPU of 4 cores
- All 4 nodes operate Debian-based Linux OS



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Prerequisites

For Windows users

- Download **Docker Desktop** from: https://docs.docker.com/desktop/install/windows-install/
- Follow step-by-step instructions here: https://www.linkedin.com/pulse/step-guide-how-install-docker-windows-1011-shashank-abhishek/
- Download gnuplot: https://sourceforge.net/projects/gnuplot/files/gnuplot/6.0.1/
- Download paraview: https://www.paraview.org/download/

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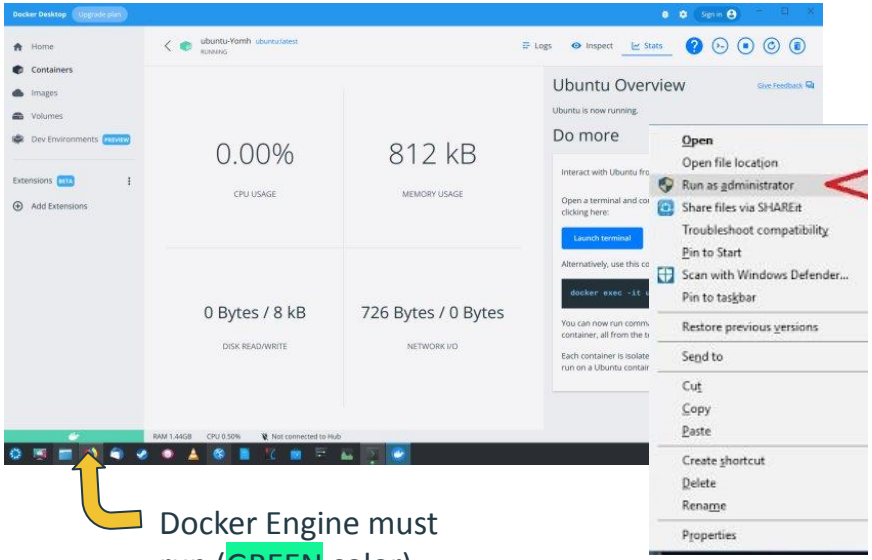
Prerequisites

For Windows users

- Use **default** options in installation
- Your PC must be **restarted**
- If docker engine does not start, you might need to close the Docker Desktop and run it in **administration** mode



Docker Engine must run (GREEN color)

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Steps A-Z

For Windows users

1. Make sure that Docker Desktop is **initiated** (GREEN color)
2. **Download** the Docker recipe to setup the virtual infrastructure of SLURM under containers: https://github.com/nikosT/slurm-docker-cluster/archive/refs/heads/openfoam-pull.zip
3. **Extract** content at some folder e.g. C:\...\slurm-docker-cluster-openfoam-pull
4. Open Windows **PowerShell** (in search button type PowerShell)
5. In Windows PowerShell **terminal** type:

   `cd C:\...\slurm-docker-cluster-openfoam-pull`

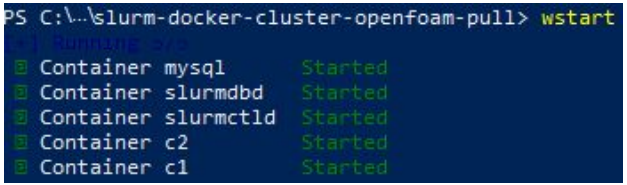
   `powershell -ExecutionPolicy Bypass`

   `. .\alias.ps1` *# load environment*

   `wstart` *# start the virtual cluster (~2.5 GB images' size)*

   When `wstart` is **completed**, you should view this
6. Then, type:

   `ssh slurm@slurmctld` *# access the login node*
7. `cd mpi_hello` *# change dir to the MPI example*
8. `sbatch test.sh` *# submit your first MPI job*
9. `ls` *# view the outputs of your submission*
10. `exit` *# logout from login node*
11. `wstop` *# stop the virtual cluster*



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Steps A-Z

For Linux users

- In terminal type:

```
sudo apt-get install git docker docker.io docker-compose docker-compose-v2 # install docker
sudo apt-get install gnuplot paraview # install visualization s/w
git clone -b openfoam-pull https://github.com/nikosT/slurm-docker-cluster # get docker recipe
cd slurm-docker-cluster # change dir to the appropriate one
chmod -R 777 slurm #set appropriate permissions to the folder
source alias # load environment
wstart # start the virtual cluster (~2.5 GB images' size)
ssh slurm@slurmctld # login control node
cd mpi_hello # change dir to the MPI example
sbatch test.sh # submit your first MPI job
ls # view the outputs of your submission
exit # logout from login node
wstop # stop the virtual cluster
```

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If error occurs

- If an error like this occurs, it is likely due to a previous deployment:

  slurmdbd | ---> Starting the MUNGE Authentication service (munged) …
  slurmdbd | munged: Error: Failed to check keyfile "/etc/munge/munge.key": Permission denied

- You need to remove all associated volumes (check with command: docker volume ls)
  - docker volume rm <volume>
    - etc_munge
    - etc_slurm
    - slurm_jobdir
    - var_lib_mysql
    - var_log_slurm

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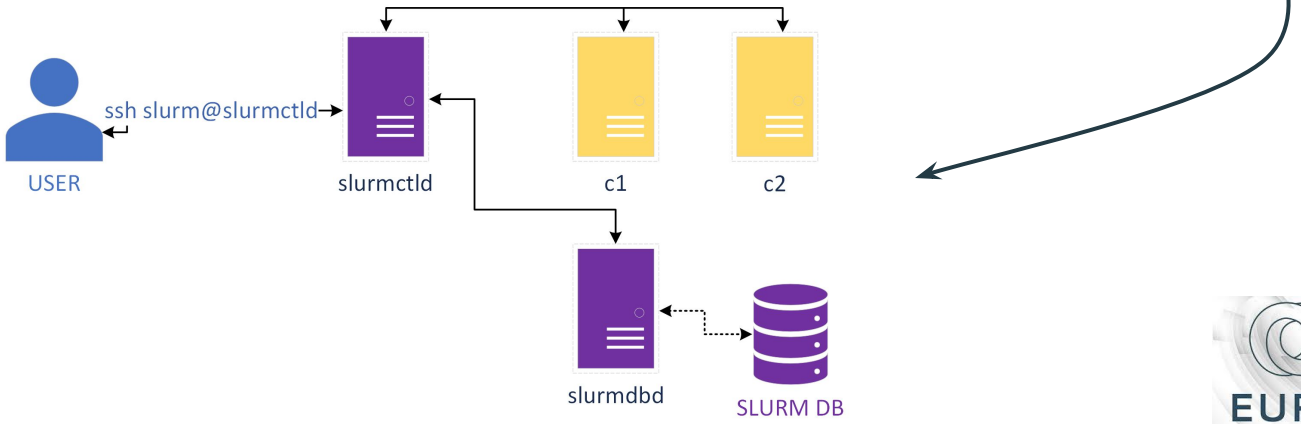
```
Windows PowerShell

Install the latest PowerShell for new features and improvements! https://aka.ms/PSWindows

PS C:\Users\inter\Downloads\slurm-docker-cluster-openfoam-pull\slurm-docker-cluster-openfoam-pull> . .\alias.ps1
PS C:\Users\inter\Downloads\slurm-docker-cluster-openfoam-pull\slurm-docker-cluster-openfoam-pull> wstart
[+] Running 5/5
 ✔Container mysql      Started                                    0.5s
 ✔Container slurmdbd   Started                                    1.0s
 ✔Container slurmctld  Started                                    1.4s
 ✔Container c1         Started                                    1.9s
 ✔Container c2         Started                                    2.1s
PS C:\Users\inter\Downloads\slurm-docker-cluster-openfoam-pull\slurm-docker-cluster-openfoam-pull> wstatus
NAME        IMAGE                                      COMMAND                  SERVICE     CREATED      STATUS          PORTS
c1          intergallactic/slurm-docker-openfoam:21.08   "/usr/local/bin/dock…"   c1          3 days ago   Up 8 seconds    6818/tcp
c2          intergallactic/slurm-docker-openfoam:21.08   "/usr/local/bin/dock…"   c2          3 days ago   Up 8 seconds    6818/tcp
mysql       mariadb:10.10                              "docker-entrypoint.s…"   mysql       3 days ago   Up 10 seconds   3306/tcp
slurmctld   intergallactic/slurm-docker-openfoam:21.08   "/usr/local/bin/dock…"   slurmctld   3 days ago   Up 9 seconds    6817/tcp
slurmdbd    intergallactic/slurm-docker-openfoam:21.08   "/usr/local/bin/dock…"   slurmdbd    3 days ago   Up 9 seconds    6819/tcp
PS C:\Users\inte  Downloads\slurm-docker-cluster-openfoam-pull\slurm-docker-cluster-openfoam-pull>
PS C:\Users\inter\Downloads\slurm-docker-cluster-openfoam-pull\slurm-docker-cluster-openfoam-pull>
```



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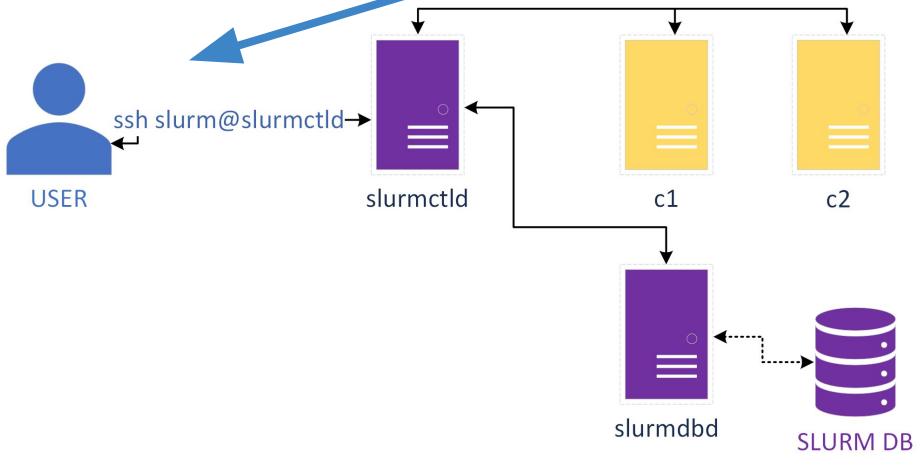
```
PS C:\Users\inter\Downloads\slurm-docker-cluster-openfoam-pull\slurm-docker-cluster-openfoam-pull> ssh slurm@slurmctld
Connected to HPC facility...
bash-4.4$ ls
dummyCase  mpi_hello
bash-4.4$ cd mpi_hello/
```

Inside login node



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Windows PowerShell

```
bash-4.4$ cat test.sh
#!/bin/bash
#SBATCH --job-name=my_mpi_job        # Job name
#SBATCH --output=my_mpi_job_%j.out  # Output file name (%j expands to jobID)
#SBATCH --error=my_mpi_job_%j.err   # Error file name (%j expands to jobID)
#SBATCH --partition=normal          # Partition name
#SBATCH --nodes=2                    # Number of nodes
#SBATCH --ntasks-per-node=2          # Number of tasks per node
#SBATCH --cpus-per-task=1          # Number of tasks per node
#SBATCH --time=00:10:00              # Time limit (HH:MM:SS)

# needed for docker version
export PSM3_HAL=loopback

# Run MPI application
mpirun -np 4 /home/slurm/mpi_hello/mpi_hello

#srun -n 4 /home/slurm/mpi_hello/mpi_hello
bash-4.4$ sbatch test.sh
Submitted batch job 2
bash-4.4$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
                 2    normal my_mpi_j    slurm  R       0:00      2 c[1-2]
bash-4.4$ ls
mpi_hello  mpi_hello.c  my_mpi_job_1.err  my_mpi_job_1.out  my_mpi_job_2.err  my_mpi_job_2.out  test.sh
bash-4.4$ cat my_mpi_job_1.out
Hello from rank 0 of 4 on c1 (pid: 41)
Hello from rank 1 of 4 on c1 (pid: 42)
Hello from rank 2 of 4 on c2 (pid: 34)
Hello from rank 3 of 4 on c2 (pid: 35)
```

Submit job

Check queue

Job output

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SLURM Useful Commands

- sacct is used to report job accounting information
- sbatch is used to submit a job script for later execution
- scancel is used to cancel a pending or running job
- scontrol is the administrative tool used to view/modify SLURM state
- sinfo reports the state of partitions and nodes managed by SLURM
- squeue reports the state of jobs
- srun usually is executed inside the job script to run apps after job submission

More info https://slurm.schedmd.com

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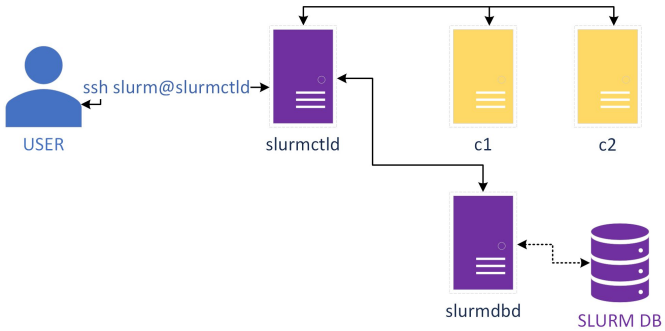
Exercise



Try accessing resources **interactively** in SLURM:

1. Open 2 terminals, change to the slurm-docker-cluster-openfoam-pull directory and load the environment
2. From both terminals access the login node, then:
3. In Terminal #1, type: `localhost` *(what's the node's name and why?)*
4. In Terminal #1, type: `srun --nodes=1 --time=00:10:00 --pty bash` *(what do you think this command does?)*
5. In Terminal #1, type: `localhost` *(what's the node's name and why?)*
6. In Terminal #2, type: `squeue` *(is there any job running?)*
7. In Terminal #1, type: `exit` *(what happened?)*
8. In Terminal #2, type: `squeue` *(is there any job running?)*
9. In Terminal #1, type: `localhost` *(what's the node's name and why?)*

Try to compile it: `cd mpi_hello; mpicc mpi_hello.c -o mpi_hello`

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Thanks!

EuroHPC Joint Undertaking

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