

Manage jobs

Submitting and managing jobs in the Cirrus HPC and HTC clusters

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Start here

Cluster specific information

INCD provides access to several HPC computing clusters. The policies, limits and characteristics of these HPC clusters can be different, always check where you are running and whether the manuals and/or instructions are the correct ones.

INCD-Lisbon cluster

- This cluster uses the Slurm batch system. The documentation for the Slurm batch system is [\[click here\]](#)

ISEC-Coimbra cluster

- This cluster uses the Slurm batch system. The documentation for the Slurm batch system is [\[click here\]](#)

INCD-Minho cluster

- This cluster uses the Slurm batch system. The documentation for the Slurm batch system is [\[click here\]](#)

Queues information

List of Queues

INCD-Lisbon cluster (cirrus.a.incd.pt)

Name	Jobs max elapsed time	access	Memory	Max #cores[1]	Comments
gpu	72h	everyone	2 GB/Core	16	queue for GPU resources
hpc	72h	everyone	8 GB/Core	64	default queue
fct	72h	reserved (require use of QOS)	8 GB/Core	96	queue for FCT grant users

[1] Maximum number of cores a user can request

[2] Access based on evaluation and upon request

Manage slurm jobs

How to handle jobs management using slurm batch system. Used at Minho and ISEC and Lisbon data center

Slurm

Slurm's architecture

Slurm is made of a slurmd daemon running on each compute node and a central slurmctld daemon running on a management node.

Node

In slurm a node is a compute resource, usually defined by particular consumable resources, i.e. cores, memory, etc...

Partitions

A partition (or queue) is a set of nodes with usually common characteristics and/or limits. Partitions group nodes into logical sets. Nodes are shareable between partitions.

Jobs

Jobs are allocations of consumable resources from the nodes and assigned to a user under the specified conditions.

Job Steps

A job step is a single task within a job. Each job can have multiple tasks (steps) even parallel ones.

Common user commands:

- [**sacct**](#): report job accounting information about running or completed jobs.
- [**salloc**](#): allocate resources for a job in real time. Typically used to allocate resources and spawn a shell. Then the shell is used to execute commands to launch parallel tasks.
- [**sbatch**](#): submit a job script for later execution. The script typically contains the tasks plus and the environment definitions needed to execute the job.
- [**scancel**](#): cancel a pending or running job or job step.
- [**sinfo**](#): overview of the resources (node and partitions).

- [squeue](#): used to report the state of running and pending jobs.
- [srun](#): submit a job for execution or initiate job steps in real time. The srun allows users to request consumable resources.

Jobs information

List all current jobs for a user:

```
squeue -u <username>
```

List all running jobs for a user:

```
squeue -u <username> -t RUNNING
```

List all pending jobs for a user:

```
squeue -u <username> -t PENDING
```

List all current jobs in the shared partition for a user:

```
squeue -u <username> -p shared
```

List detailed information for a job (useful for troubleshooting):

```
scontrol show jobid -dd <jobid>
```

List status info for a currently running job:

```
sstat --format=AveCPU,AvePages,AveRSS,AveVMSize,JobID -j <jobid> --allsteps
```

Additional information for complet jobs (not available during the run):

```
sacct -j <jobid> --format=JobID,JobName,MaxRSS,Elapsed
```

To view information for all jobs of a user:

```
sacct -u <username> --format=JobID,JobName,MaxRSS,Elapsed
```


My first slurm job

Examples

Submit a simple MPI job

- On this example we run a small MPI application doing the following steps:
 - Create a submission file
 - Submit the job to the default partition
 - Execute a simple MPI code
 - Check the status of the job
 - Read the output
- Download source code

```
wget --no-check-certificate https://wiki.incd.pt/attachments/71 -O cpi.c
```

- Create a submission file

```
vi my_first_slurm_job.sh
```

- Edit the file

```
#!/bin/bash

#SBATCH --job-name=MyFirstSlurmJob
#SBATCH --time=0:10:0
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16

# Be sure to request the correct partition to avoid the job to be held in the queue, furthermore
# On CIRRUS-B (Minho) choose for example HPC_4_Days
# On CIRRUS-A (Lisbon) choose for example hpc
#SBATCH --partition=hpc
```

```
# Used to guarantee that the environment does not have any other loaded module
module purge

# Load software modules. Please check session software for the details
module load gcc63/openmpi/4.0.3

# Prepare
src='cpi.c'
exe="./cpi.$SLURM_JOB_ID"

# Compile application
echo "=== Compiling ==="
mpicc -o $exe $src

# Run application. Please note that the number of cores used by MPI are assigned in the SBATCH directives.
echo "=== Running ==="
if [ -e $exe ]; then
    chmod u+x $exe
    mpiexec -np $SLURM_NTASKS $exe
    rm -f $exe
fi

echo "Finished with job $SLURM_JOBID"
```

- Submit the job

```
sbatch my_first_slurm_job.sh
```

- Check status of the job

```
$ squeue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
1171	HPC_4_Days	MyFirstS	username	PD	0:00	1	wn075

- Check further details about your job (very long output)

```
scontrol show job 1171
```

- Read the output of the job:

If name is not specified slurm will create by default a file with the output of your run

slurm-{job_id}.out

e.g. slurm-1171.out

- Cancel your job

```
$ scancel 1171
```

MPI examples:

Hellow World:

```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
    // Initialize the MPI environment
    MPI_Init(NULL, NULL);

    // Get the number of processes
    int world_size;
    MPI_Comm_size(MPI_COMM_WORLD, &world_size);

    // Get the rank of the process
    int world_rank;
    MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);

    // Get the name of the processor
    char processor_name[MPI_MAX_PROCESSOR_NAME];
    int name_len;
    MPI_Get_processor_name(processor_name, &name_len);

    // Print off a hello world message
    printf("Hello world from processor %s, rank %d out of %d processors\n",
        processor_name, world_rank, world_size);

    // Finalize the MPI environment.
    MPI_Finalize();
}
```

```
}
```

PI calculation

```
/* -*- Mode: C; c-basic-offset:4 ; -*- */
/*
 * (C) 2001 by Argonne National Laboratory.
 * See COPYRIGHT in top-level directory.
 */

#include "mpi.h"
#include <stdio.h>
#include <math.h>

int main(int argc, char *argv[])
{
    long int    n, i;
    int    myid, numprocs;
    double PI25DT = 3.141592653589793238462643;
    double mypi, pi, h, sum, x;
    double startwtime = 0.0, endwtime;
    int    namelen;
    char    processor_name[MPI_MAX_PROCESSOR_NAME];

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD, &myid);
    MPI_Get_processor_name(processor_name, &namelen);

    n = 100000000000; /* default # of rectangles */
    if (myid == 0) {
        startwtime = MPI_Wtime();
    }

    MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);

    h = 1.0 / (double) n;
    sum = 0.0;

    /* A slightly better approach starts from large i and works back */
```

```

    for (i = myid + 1; i <= n; i += numprocs)
    {
        x = h * ((double)i - 0.5);
        sum += 4.0 / (1.0 + x*x);
    }
    mypi = h * sum;

    MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);

    if (myid == 0) {
        endwtime = MPI_Wtime();
        printf("pi=%.16f, error=%.16f, ncores %d, wall clock time = %f\n", pi, fabs(pi - PI25DT), numprocs, endwtime-
startwtime);
        fflush(stdout);
    }

    MPI_Finalize();
    return 0;
}

```

overview of the resources offered

`sinfo` : overview of the resources offered by the cluster

By default, `sinfo` lists the available partitions name(s), availability, time limit, number of nodes, their **state** and the nodelist. A partition is a set of compute nodes.

The command `sinfo` by default

```
$ sinfo
```

PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST
all*	up	infinite	5	down*	wn[075,096,105,110,146]
all*	up	infinite	6	drain	wn[077,091,101,117,143,148]
all*	up	infinite	2	mix	wn[079,097]
all*	up	infinite	33	alloc	wn[081-089,092-095,099-100,104,108,112,115,118,124,135-139,144-145,151,155-158]
all*	up	infinite	40	idle	wn[071-073,076,080,090,098,102-103,106-107,109,111,113-114,116,120-123,125-128,130-134,140-142,147,149-150,152-154,159-160]
all*	up	infinite	4	down	wn[074,078,119,129]
debug	up	infinite	8	idle	wn[060-063,065-067,069]
debug	up	infinite	3	down	wn[064,068,070]

The command `sinfo --Node` provides the list of nodes and their actual state individually.

```
$ sinfo -Node
```

NODELIST	NODES	PARTITION	STATE
wn071	1	all*	alloc
wn072	1	all*	drain

```
wn073      1  all* alloc
wn074      1  all* down
wn075      1  all* down*
wn076      1  all* alloc
```

The command `sinfo --summarize` provides the node state in the form "available/idle/other/total"

```
$ sinfo --summarize

PARTITION AVAIL  TIMELIMIT  NODES(A/I/O/T)  NODELIST
all*      up  infinite    36/7/47/90  wn[071-160]
debug     up  infinite     2/6/3/11  wn[060-070]
```

The command `sinfo --long` provides additional information than `sinfo`. Informations about the OverSubscribe (OVERSUBS), All the queues are defined as OVERSUBS=NO, none of the partitions(queues) allow requestes over the limit of the consumable resources.

```
$ sinfo --long

PARTITION AVAIL  TIMELIMIT  JOB_SIZE ROOT OVERSUBS   GROUPS  NODES    STATE NODELIST
all*      up  infinite 1-infinite  no    NO    all    5    down* wn[075,096,105,110,146]
all*      up  infinite 1-infinite  no    NO    all   38   drained wn[072-073,076-077,080,090-091,098,101-
103,106-107,109,113-114,116-117,120-123,125-128,130,133-134,136,140-141,143,147-148,150,152,159]
all*      up  infinite 1-infinite  no    NO    all    4    mixed wn[079,094,097,137]
all*      up  infinite 1-infinite  no    NO    all   32   allocated wn[071,081-089,092-093,095,099-
100,104,108,112,115,118,124,131-132,135,138-139,144,151,155-158]
all*      up  infinite 1-infinite  no    NO    all    7    idle  wn[111,142,145,149,153-154,160]
```

With `sinfo` you can also filter the nodes/partitions for specific situation, in this example we requested to list the nodes either idle or down

```
$sinfo --states=idle,down

PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
all*      up  infinite    5  down* wn[075,096,105,110,146]
all*      up  infinite    8  idle  wn[113,116,121-122,126,140-141,143]
```

```
all*      up  infinite    4  down wn[074,078,119,129]
debug     up  infinite    7  idle wn[060-063,065-067]
debug     up  infinite    3  down wn[064,068,070]
```

“ For more detailed information, please see manual [man sinfo](#)

states:

- **mix** : consumable resources partially allocated
- **idle** : available to requests consumable resources
- **drain** : unavailable for use per system administrator request
- **drng** : currently executing a job, but will not be allocated to additional jobs. The node will be changed to state DRAINED when the last job on it completes
- **alloc** : consumable resources fully allocated
- **down** : unavailable for use. Slurm can automatically place nodes in this state if some failure occurs.

show job accounting data

`sacct:` displays accounting data for all jobs and job steps in the Slurm job accounting log or Slurm database

If you use the command without any paremeters it will show you the currently running jobs accounting data.

```
$ sacct
```

JobID	JobName	Partition	Account	AllocCPUS	State	ExitCode
1127	omp-bkp-o+	debug	incd	16	RUNNING	0:0
1128	omp-bkp-o+	debug	incd	16	RUNNING	0:0
1128.0	a.out	incd	16	RUNNING	0:0	
1129	omp-bkp-o+	debug	incd	16	RUNNING	0:0
1129.0	a.out	incd	16	RUNNING	0:0	
1130	omp-bkp-o+	debug	incd	16	RUNNING	0:0
1156	run_zacar+	HPC_4_Days	root	1	RUNNING	0:0

You can specify the job which data you would like to view by using the `-j` flag.

```
$ sacct -j 1156
```

JobID	JobName	Partition	Account	AllocCPUS	State	ExitCode
1156	run_zacar+	HPC_4_Days	root	1	RUNNING	0:0

You can list jobs by user, by adding the `-u` flag and choosing the user.

```
$ sacct -u jprmachado
```

JobID	JobName	Partition	Account	AllocCPUS	State	ExitCode
1127	omp-bkp-o+	debug	incd	16	RUNNING	0:0
1128	omp-bkp-o+	debug	incd	16	RUNNING	0:0

```

1128.0      a.out      incd      16  RUNNING    0:0
1129      omp-bkp-o+   debug    incd      16  RUNNING    0:0
1129.0      a.out      incd      16  RUNNING    0:0
1130      omp-bkp-o+   debug    incd      16  RUNNING    0:0

```

You can also filter or create your own custom reports by using the `--format` flag and choosing what data to show.

```

$ sacct --
format=User,JobID,Jobname,partition,state,time,start,end,elapsed,MaxRss,MaxVMSize,nnodes,ncpus,nodelist

  User   JobID  JobName Partition  State Timelimit      Start      End  Elapsed  MaxRSS
MaxVMSize NNodes  NCPUS   NodeList
-----
jprmacha+ 1127      omp-bkp-o+   debug  RUNNING 20-20:00:+ 2019-11-20T11:44:28      Unknown 9-
04:00:00          1    16      wn018
jprmacha+ 1128      omp-bkp-o+   debug  RUNNING 20-20:00:+ 2019-11-20T11:46:43      Unknown 9-
03:57:45          1    16      wn019
      1128.0      a.out      RUNNING      2019-11-20T11:46:43      Unknown 9-
03:57:45          1    16      wn019
jprmacha+ 1129      omp-bkp-o+   debug  RUNNING 20-20:00:+ 2019-11-20T11:51:30      Unknown 9-
03:52:58          1    16      wn020
      1129.0      a.out      RUNNING      2019-11-20T11:51:31      Unknown 9-
03:52:57          1    16      wn020
jprmacha+ 1130      omp-bkp-o+   debug  RUNNING 20-20:00:+ 2019-11-20T11:52:37      Unknown 9-
03:51:51          1    16      wn012
      root 1156      run_zacar+ HPC_4_Days  RUNNING 8-00:00:00 2019-11-27T13:40:02      Unknown 2-
02:04:26          1    1      wn035

```

There is also the possibility to filter you custom report by user and date, you just have to add the `-u` and `--start` flags.

```

$ sacct --
format=User,JobID,Jobname,partition,state,time,start,end,elapsed,MaxRss,MaxVMSize,nnodes,ncpus,nodelist -u
zbenta --start 2019-11-28

  User   JobID  JobName Partition  State Timelimit      Start      End  Elapsed  MaxRSS
MaxVMSize NNodes  NCPUS   NodeList

```

```

-----
zbenta 1163      clover32  stage2  TIMEOUT  04:00:00 2019-11-28T13:22:31 2019-11-28T17:22:46
04:00:15          8      128  wn[022-029]
      1163.batch  batch      CANCELLED      2019-11-28T13:22:31 2019-11-28T17:22:47
04:00:16  40152K  186176K  1      16      wn022
      1163.0      orted      FAILED      2019-11-28T13:22:35 2019-11-28T17:22:46  04:00:11
38104K  254748K  7      7  wn[023-029]

```

You can also use the flags to give you a report during a specific time interval, just use the `--start` and `--end` flags.

```

$ sacct --
format=User,JobID,Jobname,partition,state,time,start,end,elapsed,MaxRss,MaxVMSize,nnodes,ncpus,nodelist -u
zbenta --start 2019-10-07 --end 2019-10-11

```

User	JobID	JobName	Partition	State	Timelimit	Start	End	Elapsed	MaxRSS
MaxVMSize	NNodes	NCPUS	NodeList						
zbenta 15	Run_PRISM	debug	FAILED	365-00:00+	2019-10-07T11:05:58	2019-10-07T11:06:09			
00:00:11	2	32	wn[018-019]						
15.batch	batch	FAILED	2019-10-07T11:05:58	2019-10-07T11:06:09					
00:00:11	1	16	wn018						
15.0	orted	COMPLETED	2019-10-07T11:06:02	2019-10-07T11:06:07					
00:00:05	1	1	wn019						
zbenta 20	Run_PRISM	debug	CANCELLED+	UNLIMITED	2019-10-08T11:42:01	2019-10-08T12:12:03	00:30:02		
	2	32	wn[018-019]						
20.batch	batch	CANCELLED	2019-10-08T11:42:01	2019-10-08T12:12:05	00:30:04				
2626556K	186140K	1	16	wn018					
20.0	orted	FAILED	2019-10-08T11:42:05	2019-10-08T12:12:08	00:30:03				
2594880K	292116K	1	1	wn019					
zbenta 28	Run_PRISM	debug	FAILED	UNLIMITED	2019-10-11T14:33:06	2019-10-11T14:33:06			
00:00:00	2	32	wn[003,015]						
28.batch	batch	FAILED	2019-10-11T14:33:06	2019-10-11T14:33:06					
00:00:00	1	16	wn003						

“**For more detailed information, please see the manual `man sacct` **

stop or cancel jobs

scancel : used to signal jobs or job steps that are under the control of Slurm

The command `scancel` is used to signal or **cancel jobs, job arrays** or **job steps** . A job or job step can only be signaled by the **owner** of that job or user root. If an attempt is made by an unauthorized user to signal a job or job step, an error message will be printed and the job will not be signaled.

```
$ scancel <jobid>
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
33416	all	Hexadeca	fcruz	R	3:26:11	2	wn[131-132]
33434	debug	OFBuild	lmendes	R	1:50:42	1	wn069
33437	all	FE ngalamba	R	58:07	1	wn094	
33439	all	FE ngalamba	R	29:43	1	wn097	
33440	all	FE ngalamba	R	29:13	1	wn137	
33441	all	FE ngalamba	R	13:43	1	wn126	
33442	all	FE ngalamba	R	1:58	1	wn071	
33443	all	FE ngalamba	R	1:41	1	wn071	
33445	all	FE ngalamba	R	0:12	1	wn079	

You can all your jobs (running and pending)

```
$ scancel --user <username>
```

You may also only cancel all your jobs in a specific element, i.e. state, partition...

```
$ scancel --state PENDING --user <username>
```

\$ Job can be also canceled using the job name

```
$ scancel --name <jobname>
```

“ For more detailed information, please see `man scancel`

Show jobs information in queue

`squeue`: view information about jobs located in the Slurm scheduling queue.

`gsqueue`: squeue alias formatted to show specific jobs information

general usage

If you use the command without any paremeters it will show you the currently running jobs in the queue.

```
$ squeue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
1127	debug	omp-bkp-	jprmacha	R	9-04:38:00	1	wn018
1128	debug	omp-bkp-	jprmacha	R	9-04:35:45	1	wn019
1129	debug	omp-bkp-	jprmacha	R	9-04:30:58	1	wn020
1130	debug	omp-bkp-	jprmacha	R	9-04:29:51	1	wn012
1156	HPC_4_Day	run_zaca	root	R	2-02:42:26	1	wn035

view jobs from a specific user

You can filter by user, using the `--user` flag

```
$ squeue --user root
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
1156	HPC_4_Day	run_zaca	root	R	2-02:44:28	1	wn035

view particular jobs

You can also filter by job id, using the `-j` flag.

```
$ squeue -j 1127
```

```
JOBID PARTITION  NAME    USER ST    TIME  NODES NODELIST(REASON)
1127   debug omp-bkp- jrmacha R 9-04:41:26    1 wn018
```

it is possible to provide multiple job id's separated by comma.

format the command output

The user may provide the output fields with format option "-O", for example showing the number of requested cpus:

```
$ squeue -o "%.7i %.9P %.8j %.8u %.2t %.10M %.6D %C %N" -u jmartins
JOBID PARTITION  NAME    USER ST    TIME  NODES CPUS NODELIST
192427  debug  cpi.sh jmartins R    0:06    1  64 hpc047
```

gqueue alias

The user interfaces have an alias for the **squeue** comand called **gqueue** with some useful fields

```
$ gqueue
JOBID PARTITION NAME    USER  ST TIME    NODES CPUS TRES_PER_NODE  NODELIST
184472 gpu      gpu-job gpuuser R 18:34:54 1    1  gpu          hpc058
```

“ **For more detailed information, please see the manual `man squeue` **

How to run parallel job's with srun

srun : Used to submit/initiate job or job step

Typically, srun is invoked from a SLURM job script but alternatively, srun can be run directly from the command, in which case srun will first create a resource allocation for running the parallel job (the salloc is implicit)

```
srun -N 1 -c 16 -p HPC_4_Days --time=1:00:00 --pty /bin/bash
```

This command will request 16 cores (-c) of one Node (-N) for 1h00 in the partition (-p) HPC_4_Days. Please note that this is subject to Nodes availability, if no Nodes are available your request will be put in the queue waiting for resources.

The srun may also be executed inside a shell script.

```
#!/bin/bash

#SBATCH -N 3
#SBATCH -p HPC_4_Days

echo Starting job $SLURM_JOB_ID
echo SLURM assigned me these nodes
srun -l hostname
```

This batch job will result in the following output:

```
Starting job 51057
SLURM assigned me these nodes
0: wn054.b.incd.pt
1: wn055.b.incd.pt
2: wn057.b.incd.pt
```

The 3 allocated nodes are released after the `srun` finish.

By default `srun` will use the `pmi2`, but you may consult the full list of the available mpi types.

```
$ srun --mpi=list
```

```
srun: MPI types are...
```

```
srun: pmi2
```

```
srun: openmpi
```

```
srun: none
```

To use a different mpi type e.g. `srun --mpi=openmpi`

“ For more detailed information, please see `man srun`

Preparing the Environment

There are lots of little tweaks we need in order to prepare the environment for running specific software. We will try to describe the ones we use more regularly so it is easier for the users to work with them.

mvapich

Version 2.3.3 compiled with Intel 2020

```
module load intel/mvapich2/2.3.3
source $I_MPI_ROOT/intel64/bin/mpivars.sh intel64 -ofi_internal=0
export LD_PRELOAD="libmpi.so"
```

mpich

Version 3.2.2 compiled with Intel 2020

```
module load intel/mpich/3.3.2
export LD_PRELOAD="libmpi.so"
```

OpenMPI 4.0.3

Version 4.0.3 compiled with Intel 2019

```
module load intel/openmpi/4.0.3
export I_MPI_PMI_LIBRARY=/lib64/libpmi.so
```

openfoam

Version 1912 compiled wiht Intel 2020

```
module load intel/openfoami20/1912
source /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1912/build01/OpenFOAM-v1912/etc/bashrc
. /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1912/build01/OpenFOAM-v1912/bin/tools/RunFunctions
```

Version 1906 compiled wiht Intel 2020

```
module load intel/openfoami20/1906
source /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1906/build01/OpenFOAM-v1912/etc/bashrc
. /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1906/build01/OpenFOAM-v1912/bin/tools/RunFunctions
```

gromacs

intel/gromacs/2020.2

```
module load gcc-6.3
source /cvmfs/sw.el7/ar/ix_es2680/i20/gromacs/2020.2/build01/bin/GMXRC.bash
source /cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
module load intel/gromacs/2020.2
```

intel/gromacs/2020.20-i20

```
module load gcc-7.5
source /cvmfs/sw.el7/ar/ix_es2680/i20/gromacs/2020.2/build02/bin/GMXRC.bash#source
/cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
source /cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
module load intel/gromacs/2020.2
```

gromacs-4.6.7

```
module load gromacs-4.6.7
module load gcc63/openmpi/4.0.3
export GMX_MAXBACKUP=-1
mpirun -np 10 mdrun -s benchMEM.tpr -nsteps 500000 -maxh 3.0 -resethway
```

Version 2020.2 compiled wiht Intel 2020

```
module load gcc-6.3
```

```
source /cvmfs/sw.el7/ar/ix_es2680/i20/gromacs/2020.2/build02/bin/GMXRC.bash
```

```
source /cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
```

```
module load intel/gromacs/2020.2
```

Interactive Sessions

Slurm allow interactive sessions into the workernodes, using ssh, but within a valid job allocation, normal ssh are disabled. The interactive session can be created on the scope of normal partitions but those jobs will have the same priority as a regular job.

There is a limitation of 1 job and 1 task per node on partitions **hpc** and **gpu**, we would like to encourage users to close sessions as soon as possible to give all a good chance to use the resources.

“ The *FCT* grant users should use the partition *fct* instead in the examples bellow.

Starting srun Session

The most simple way to start an interactive session is:

```
[user@cirrus01 ~]$ srun -p hpc --job-name "my_interactive" --pty bash -i
srun: job 72791 queued and waiting for resources
srun: job 72791 has been allocated resources
[user@hpc059 ~]$
```

You will have an ssh session on a worker node were other users are running jobs or interactive sessions as well, try not bother them with unsolicited interactions, and exit the session when you are finished.

“ The *FCT* call users should target the *partition* **fct** and the *QOS* associate to the user, e.g. "***srun -p fct -q cpcaXXXX2020 ...***", where XXXX is the call ID.

The **srun** command have the same restrictions as a normal *job* and will be aborted or refused to run when the system limits are exceeded. If you run the **squeue** you will see your interactive job listed as any other job:

```
[user@hpc059 ~]$ squeue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
72818	hpc	my_inter	user	R	2:03	1	hpc059

Starting salloc Session

The **salloc** is setup to behave like the **srun** command, for example:

```
[user@cirrus01 ~]$ salloc -p hpc --job-name "my_interactive"
```

```
salloc: Pending job allocation 72818
```

```
salloc: job 72818 queued and waiting for resources
```

```
salloc: job 72818 has been allocated resources
```

```
salloc: Granted job allocation 72818
```

```
salloc: Waiting for resource configuration
```

```
salloc: Nodes hpc059 are ready for job
```

```
[user@hpc059 ~]$
```

“ Once again the *FCT* call users should target the *partition* **fct** and the *QOS* associate to the user

Job pipeline using slurm dependencies

Some times we need to launch a list of jobs that execute in sequence, one after another. In those cases we will use the **--dependency sbatch** option, check the manual page for more details, we will only present a simple example.

Simple example

Suppose we need to submit the script **my_first_job.sh** and then **my_second_job.sh** that should run after the first one:

```
[user@cirrus01 ~]$ sbatch my_first_job.sh
Submitted batch job 1843928

[user@cirrus01 ~]$ sbatch --dependency=after:1843928 my_second_job.sh
Submitted batch job 1843921

[user@cirrus01 ~]$ squeue
JOBID PARTITION      NAME USER ST TIME NODES NODELIST(REASON)
1843928    hpc  my_first_job.sh user  R 0:11    1 hpc046
1843921    hpc  my_second_job.sh user  PD 0:00    1 hpc047
```

In this case the second job will run even if the first job fails for some reason. The pending job will execute when the first finish his execution.

Tipical example

On a real case we may need the ensure that a good termination of the first job, for example, the first job may produce some output file needed as input for the second job:


```
[user@cirrus01 ~]$ sbatch my_first_job.sh
```

```
Submitted batch job 1843922
```

```
[user@cirrus01 ~]$ sbatch --dependency=afterok:1843922 my_second_job.sh
```

```
Submitted batch job 1843923
```

The ***afterok*** parameter states that the second job would start only if the previous job terminate with no errors.

Complex cases

Check the ***sbatch*** manual page for more details:

```
[user@cirrus01 ~]$ man sbatch
```

search for the ***-d***, ***--dependency=<dependency_list>*** options explanation.

Use of user QOS for CPU jobs

In order to use QOS you will to have an assigned user QOS. In the following example the user will submit a job to the fct partition using an specific created cpca097822021.

```
#!/bin/bash
#SBATCH --job-name=prod01
#SBATCH --time=0:10:0
#SBATCH --partition=fct
#SBATCH --qos=cpca097822021
#SBATCH --output=%x.o%j
#SBATCH --error=%x.o%j
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16

### Prepare the environment
module purge
module load gcc83/openmpi/4.1.1 cuda-11.2

echo hostname
```

Not all queues allow QOS please follow guidance provided by INCD team when assigning the QOS.

GPU user guide

How to Run a Job with a GPU

Let's run the gravitational N-body simulation found on the CUDA toolkit samples on a GPU. This example is suited for a standard *INCD* user eligible to use the ***hpc*** and ***gpu*** partitions.

“ The ***fct*** partition and included resources is meant for users with a *FCT* grant and although the request of GPUs is made on the same way, they have specific instructions to follow found at [FCT Calls](#)

“ The GPU's are only available at CIRRUS-A infrastructure on Lisbon.

Login on the user interface cirrus.ncg.ingrid.pt

```
$ ssh -l user cirrus.ncg.ingrid.pt  
[user@cirrus01 ~]$ _
```

Prepare your working directory

Prepare your environment on a specific directory in order to protect from inter job interferences and create a submission batch script: *** only works for Cuda 10.2

```
[user@cirrus01 ~]$ mkdir myworkdir  
[user@cirrus01 ~]$ cd myworkdir  
[user@cirrus01 ~]$ cat nbody.sh  
#!/bin/bash  
  
#SBATCH --partition=gpu  
#SBATCH --gres=gpu  
#SBATCH --mem=8192MB
```

```
COMMON=/usr/local/cuda/samples/common
SAMPLE=/usr/local/cuda/samples/5_Simulations/nbody

[ -d ../common ] || cp -r $COMMON ..
[ -d nbody ] || cp -r $SAMPLE .

module load cuda
cd nbody
make clean
make

if [ -e nbody ]; then
  chmod u+x nbody
  ./nbody -benchmark -numbodies=2560000
fi
```

In this example we copy the n-body CUDA toolkit sample simulation to the working directory, load cuda environment, build the simulation and run it.

Requesting the partition

Standard *INCD* users at *CIRRUS-A* have access to the **gpu** partition providing NVIDIA Tesla-T4 GPUs. In order to access these GPUs request the **gpu** partition with directive:

```
#SBATCH --partition=gpu
```

The partition **ft** provide several types of NVIDIA: T4 and V100S (please check current resources available page). As a general rule and depending on the application, the types of GPUs available on the cluster are similar but the Tesla-V100S perform the same work in half the time when compared with the Tesla-T4. Nevertheless, if you request a Tesla-V100S you may have to wait for resource availability until you have a free Tesla-T4 ready to go.

If you only want a free GPU allocated for your job then the **#SBATCH --grep=gpu*** form would be the best choice.

Requesting the Tesla-T4 GPU

We request the allocation of one GPU NVIDIA Tesla-T4 through the option:

```
#SBATCH --gres=gpu:t4
```

Standard *INCD* users can access only NVIDIA Tesla-T4 GPUs, so we can simplify the request:

```
#SBATCH --gres=gpu
```

this way we ask for a GPU of any type, the same is valid on partitions with more than one type of GPU if we do not care about the type of allocated GPU to our job.

Requesting memory

Ensure enough memory for your simulation, follow the tips on *Determining Memory Requirements*(*page_to_be*) page.

On our example 8GB is sufficient to run the simulation:

```
#SBATCH --mem=8192M
```

Submit the simulation

```
[user@cirrus01 ~]$ sbatch nbody.sh  
Submitted batch job 1176
```

Monitor your job

You can use the **squeue** command line tool

```
[user@cirrus01 ~]$ gqueue  
JOBID PARTITION NAME    USER  ST STATIME    NODES CPUS TRES_PER_NODE NODELIST  
1176 gpu      nbody.sh user5  R RUN0-00:02:33 1    1  gpu:t4      hpc058
```

or use the command **sacct**, the job is completed when the *State* field mark is *COMPLETED*.

```
[user@cirrus01 ~]$ gacct  
JobID  JobName Partition Account AllocCPUS   ReqGRES   AllocGRES   State ExitCode  
-----  
1170   nbody.sh    fct      hpc       2  gpu:v100s:1    gpu:1 COMPLETED  0:0  
1171   nbody.sh    fct      hpc       2   gpu:t4:1      gpu:1 COMPLETED  0:0  
1175   teste.sh    fct      hpc       1                   COMPLETED  0:0  
1176   nbody.sh    gpu      hpc       1    gpu:1        gpu:1 COMPLETED  0:0
```

if the state is different from *COMPLETED* or *RUNNING* then check your simulation or request help through the email address **helpdesk@incd.pt** providing the *JOBID*, the submission script, the relevant slurm output files, e.g. *slurm-1176.out*, or other remarks you think it may be helpful

Check the results at job completion

```
[user@cirrus01 ~]$ ls -l
-rw-r-----+ 1 user hpc 268 Oct 22 13:56 gpu.sh
drwxr-x---+ 3 user hpc 4096 Oct 20 18:09 nbody
-rw-r-----+ 1 user hpc 611 Oct 22 13:41 slurm-1176.out
```

```
[user@cirrus01 ~]$ cat slurm-1176.out
```

...

> Windowed mode

> Simulation data stored in video memory

> Single precision floating point simulation

> 1 Devices used for simulation

GPU Device 0: "Turing" with compute capability 7.5

> Compute 7.5 CUDA device: [Tesla T4]

number of bodies = 2560000

2560000 bodies, total time for 10 iterations: 308586.156 ms

= 212.375 billion interactions per second

= 4247.501 single-precision GFLOP/s at 20 flops per interaction

Use QOS to run GPU jobs

- This page is dedicated to users who want to run GPU's and have a QOS.

GPU JOB submission using QOS

- In this example we will use the attributed QOS=gpu097822021 to be used for GPU and submit a job for the V100 Nvidia.

```
#!/bin/bash
#SBATCH --job-name=prod01
#SBATCH --partition=gpu
#SBATCH --qos=gpu097822021
#SBATCH --gres=gpu:v100s
#SBATCH --output=%x.o%j
#SBATCH --error=%x.o%j

### Prepare the environment
module purge
module load gcc83/openmpi/4.1.1 cuda-11.2

echo hostname
```


Deep Learning Example

The INCD-Lisbon facility provide a few GPU, check the [Comput Node Specs](#) page.

Login on the submit node

Login on the cluster submission node, check the [How to Access](#) page for more information:

```
$ ssh -l <username> cirrus8.a.incd.pt
[username@cirrus01 ~]$ _
```

Alternatives to run the Deep Learning example

We have alternatives to run the *Deep Learning* example, or any other python based script:

1. prepare a user python virtual environment on home directory and launch a batch job;

The next three sections shows how to run the example for each method.

1) Run a Deep Learning job using a prepared CVMFS python virtual environment

Instead of preparing an user python virtual environment we can use the environment already available on the system, named **python/3.10.13**, check it with the command

```
[username@cirrus08 ~]$ module avail
----- /cvmfs/sw.el8/modules/hpc/main -----
...
intel/oneapi/2023  python/3.8          udocker/alphafold/2.3.2
julia/1.6.7        python/3.10.13 (D)
...
```

“ We will find other **python** version, namely version **3.7** and **3.8**, this version do not contain the **tensorflow** module due to **python** version incompatibility.

We will change the submit script **dl.sh** to the following:

```
[username@cirrus08 dl]$ vi dl.sh
#!/bin/bash
#SBATCH -p gpu
#SBATCH --gres=gpu
#SBATCH --mem=64G

module load python/3.10.7
python run.py

[username@cirrus08 dl]$ ls -l
-rwxr-----+ 1 username usergroup 124 Feb 26 16:44 dl.sh
-rw-r-----+ 1 username usergroup 1417 Feb 26 16:46 run.py
```

Submit the Job

```
[username@cirrus08 dl]$ sbatch dl.sh
Submitted batch job 15135448
```

JOBID	PARTITION	NAME	USER	ST TIME	NODES	CPUS	TRES_PER_NODE	NODELIST
15290034	gpu	dl.sh	jpina	PD 0:00	1	1	gres/gpu	

Check Job results

On completion check results on standard output and error files:

```
[username@cirrus08 dl]$ ls -l
-rwxr-----+ 1 username usergroup 124 Feb 26 16:44 dl.sh
-rw-r-----+ 1 username usergroup 1417 Feb 26 16:46 run.py
-rw-r-----+ 1 username usergroup 18000 Feb 26 18:51 slurm-15135448.out
```

and proceed as in the previous example.

How to selected a GPU

Select any GPU

- On this example we choose one GPU with at least 8192 MB memory.

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gres=gpu
#SBATCH --mem=8192MB

COMMON=/usr/local/cuda/samples/common
SAMPLE=/usr/local/cuda/samples/5_Simulations/nbody

[ -d ../common ] || cp -r $COMMON ..
[ -d nbody ] || cp -r $SAMPLE .

module load cuda
cd nbody
make clean
make

if [ -e nbody ]; then
  chmod u+x nbody
  ./nbody -benchmark -numbodies=2560000
fi
```

Select a specific GPU: V100s

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gres=gpu:v100s
```

```
COMMON=/usr/local/cuda/samples/common
SAMPLE=/usr/local/cuda/samples/5_Simulations/nbody
```

```
[ -d ../common ] || cp -r $COMMON ..
[ -d nbody ] || cp -r $SAMPLE .
```

```
module load cuda
cd nbody
make clean
make
```

```
if [ -e nbody ]; then
  chmod u+x nbody
  ./nbody -benchmark -numbodies=2560000
fi
```

GPU list

You can find the full GPU list per cluster [here](#)

Troubleshooting information

My jobs need to run longer than the queues permit

- At INCD the **default** max elapsed time for the queues is 72h. The values for all queues can be consulted [here](#)
- In case you cannot parallelize your job (split one single job into multiple parallel jobs) you can use job dependencies. In this case you create a chain of jobs on which N+1 jobs depends on the previous one N. Check this [link](#)

“ **NOTE** There is a special queue available for very long jobs. This queue is restricted and available only in very special circumstances. If you have this type of requirement please contact the [INCD support helpdesk](#)

UDocker Containers

Availability of udocker containers directly on *CVMFS* read-only filesystem in order to speedup their use and improve reproducibility, reliability and avoid interferences between calls, we will try to optimize compilations when ever possible. This containers can be used directly or run an user command through a wrapper script.

The container technology is a conveniente way to provide stable software environments or to install them on situations where the configuration is complex or impossible. For example, the *tensorflow* framework is normally very hard to install on CentOS 7.x systems as found on our worknodes.

Available containers on CVMFS

Environment	Target Arch.	Arch. Optimizations	Container SO	Applications
udoker/tensorflow/cp u/2.4.1	Epyc_7552, Epyc_7501	AVX AVX2 FMA	Ubuntu 18.04	tensorflow-2.4.1 keras-2.43 pandas- 1.1.5 madminer-0.8.0 numpy-1.19.5 scipy- 1.5.4
udocker/tensorflow/g pu/2.4.1	Epyc_7552, NVidia_Tesla	AVX AVX2 FMA	Ubuntu 18.04	CUDA-11.2 tensorflow-2.4.1 keras-2.43 pandas- 1.1.5 madminer-0.8.0 numpy-1.19.5 scipy- 1.5.4

How to use the udocker containers

“ The containers are meant to be run on workernodes, they will not work on the login servers, launch a batch job or start an [interactive session](#). Note also that the *gpu* partition is the only one providing GPU devices.

Load environment

Load the appropriate environment, for exemple *udocker/tensorflow/gpu/2.4.1*:

```
$ module load udocker/tensorflow/gpu/2.4.1
```

This will configure the *udocker* environment and made available the wrapper *u_wrapper* used to start the container. When the container is started through the wrapper the */tmp* and the user working directory is imported into the container.

Execute a command

Now we can run any command using the wrapper, for example:

```
$ u_wrapper nvidia-smi -L
*****
*                                     *
*   STARTING 2bcfad7b-1750-3fb8-9fb1-74acdf4e869e   *
*                                     *
*****
executing: bash
GPU 0: Tesla T4 (UUID: GPU-8cce58c9-f3f7-839c-50f9-63e21f042152)
GPU 1: Tesla T4 (UUID: GPU-1f698e19-a902-2e73-0a54-44e02fa9c8ee)
```

Execute an interactive shell

We can run an interactive shell, as long we acquire an interactive allocation:

```
$ u_wrapper bash -i
*****
*                                     *
*   STARTING 2bcfad7b-1750-3fb8-9fb1-74acdf4e869e   *
*                                     *
*****
executing: bash

_____
_ /_____ /_ /_____ _
_ / _ \ _ \ _ / _ \ _ / _ \ _ \ | / /
_ / / _ / / ( _ ) / / / _ _ / / / _ / / /
/ / \ / / / / _ \ / / / / / \ / _ \ / /
```


You are running this container as user with ID 5800002 and group 5800000, which should map to the ID and group for your user on the Docker host. Great!

tf-docker ~ >

Example of a complete job script

We will run a [Deep Learning](#) example.

Get the python script [run.py](#) and create a submit script as follow:

```
$ cat dl.sh
#!/bin/bash
#SBATCH -p gpu
#SBATCH --gres=gpu
#SBATCH --mem=45G
module load udocker/tensorflow/gpu/2.4.1
u_wrapper python run.py
```

Next, launch the script and wait for completion, once it start to run it should be very fast, about 10 seconds.

```
$ sbatch dl.sh
Submitted batch job 1435321

$ squeue
JOBID PARTITION  NAME   USER ST  TIME  NODES NODELIST(REASON)
1435321    gpu    dl.sh username R   0:01    1 hpc062

$ ls -l
-rwxr-----+ 1 username usergroup  409 May 25 21:06 dl.sh
-rw-r-----+ 1 username usergroup 1417 May 25 20:49 run.py
-rw-r-----+ 1 username usergroup 17034 May 25 21:06 slurm-1435321.out
```

The output file should be something like the file [slurm-1435321.out](#).

Monitoring

Useful commands to monitor jobs or consumption

- ```
[root@cirrus08 ~]$ report --user fabiananeves
```

- On this example the user fabiananeves consumed 50920 mins of the cpca582052022 total consumed for the period 2023-12-01T00:00:00 - 2023-12-06T12:59:59.
- On the second line you have the total QOS consumed 157722 mins (red bar) and in brackets you have the QOS atributed (cpu=1800000). The blue bar show the difference between the total and the consumed.

# Quality of Service (QOS)

Quality of Service (QoS) is used to limit the characteristics that a job can have.

## Default QOS per partition

For every partition (fct, gpu, etc), there is a Quality of Service with different defined parameters like MaxJobs, MaxSubmitJobs. These parameters act on all the jobs submitted by all users on that partition. To see the default QOS for a specific partition run the below scontrol command:

### fct partition

```
[jpina@cirrus02 ~]$ scontrol show partition fct
PartitionName=fct
 AllowGroups=ALL
 AllowAccounts=fct1,cpca27902020,cpca59032020,cpca3952082021,cpca3949842021,cpca4021052021,cpca3969692021,cpca097952021,cpca4076702021,biosim,cpca4209172021,cpca4081432021,cpca4011972021,dsaipa00832020,cpca098302021,cpca097822021,cpca097522021,cpca096232021,cpca097312021,cpca097642021,cpca230372022,cpca262792022,cpca158802022,cpca158802023,cpca56132020,cpca156102022,cpca158542022,cpca280462022,cpca096232021,cpca159122022 DenyQos=normal,low,medium,high
 AllocNodes=ALL Default=NO QoS=N/A
 DefaultTime=NONE DisableRootJobs=NO ExclusiveUser=NO GraceTime=0 Hidden=NO
 MaxNodes=UNLIMITED MaxTime=4-00:00:00 MinNodes=0 LLN=NO MaxCPUsPerNode=90
 Nodes=hpc06[0-3]
 PriorityJobFactor=1 PriorityTier=1 RootOnly=NO ReqResv=NO OverSubscribe=NO
 OverTimeLimit=NONE PreemptMode=OFF
 State=UP TotalCPUs=384 TotalNodes=4 SelectTypeParameters=NONE
 JobDefaults=(null)
 DefMemPerCPU=5000 MaxMemPerNode=UNLIMITED
```

### gpu partition

```
[jpina@cirrus02 ~]$ scontrol show partition gpu
PartitionName=gpu
 AllowGroups=ALL
 AllowAccounts=aeon,biomeng,biosim,cbmr,ccmar,cedis,centec,cerberos,chlabb,cicco,ciimar,cncb,comics,cosmo
```

```
s,csys,dei,eeisel,eworm,dosimetry,fcneuro,fctunlrequinte,fculbioisi,fculce3c,fculdi,fculfisica,fculgfm,fculibeb,feno
,hpc,ibb,ibet,ihmt,inl,inov,ipfn,insa,istcsociologia,ispa,istcftp,lapmet,lasige,lnec,lnecprd,localmaxs,mcfeup,neur
o,nlx,nps,scipion,seatox,solarb,spac,t3atlas,t3cms,ua,uaberta,uait,uaquimica,ubim,uc,uccibit,uedi,ulcefisa,ulibeb
,ulusofona,um,unlims,unlitqb,xtal,yeastgenomics,cpca27902020,cpca59032020,fct1,cpca4209172021,cpca2627
92022,cpca56132020,cpca158542022,cpca280462022,cpca097822021,cpca159122022
AllowQos=normal,gpu3952082021,gpu4021052021,gpu4209172021,gpu262792022,gpu158802022,gpu158002
022,gpu158542022,gpu280462022,fct1,gpu159122022,gpu097822021
AllocNodes=ALL Default=NO QoS=N/A
DefaultTime=NONE DisableRootJobs=NO ExclusiveUser=NO GraceTime=0 Hidden=NO
MaxNodes=1 MaxTime=4-00:00:00 MinNodes=0 LLN=NO MaxCPUsPerNode=2
Nodes=hpc06[0-3]
PriorityJobFactor=1000 PriorityTier=1000 RootOnly=NO ReqResv=NO OverSubscribe=NO
OverTimeLimit=NONE PreemptMode=OFF
State=UP TotalCPUs=384 TotalNodes=4 SelectTypeParameters=NONE
JobDefaults=(null)
DefMemPerCPU=5000 MaxMemPerNode=UNLIMITED
```

## hpc partition

```
[jpina@cirrus02 ~]$ scontrol show partition hpc
PartitionName=hpc
AllowGroups=ALL
AllowAccounts=aeon,biomeng,biosim,cbmr,ccmar,cedis,centec,cerberos,chlabb,cicco,ciimar,cncb,comics,cosmo
s,csys,dei,dosimetry,eeisel,eworm,fcneuro,fctunlrequinte,fculbioisi,fculce3c,fculdi,fculfisica,fculgfm,fculibeb,feno
,hpc,ibb,ibet,ihmt,inl,inov,ipfn,insa,istcsociologia,ispa,istcftp,lapmet,lasige,lnec,lnecprd,localmaxs,mcfeup,neur
o,nlx,nps,scipion,seatox,solarb,spac,t3atlas,t3cms,ua,uaberta,uait,uaquimica,ubim,uc,uccibit,uedi,ulcefisa,ulibeb
,ulusofona,um,unlims,unlitqb,xtal,yeastgenomics AllowQos=normal
AllocNodes=ALL Default=YES QoS=N/A
DefaultTime=NONE DisableRootJobs=NO ExclusiveUser=NO GraceTime=0 Hidden=NO
MaxNodes=UNLIMITED MaxTime=4-00:00:00 MinNodes=0 LLN=NO MaxCPUsPerNode=UNLIMITED
Nodes=hpc04[6-8]
PriorityJobFactor=1 PriorityTier=1 RootOnly=NO ReqResv=NO OverSubscribe=NO
OverTimeLimit=NONE PreemptMode=OFF
State=UP TotalCPUs=192 TotalNodes=3 SelectTypeParameters=NONE
JobDefaults=(null)
DefMemPerCPU=8000 MaxMemPerNode=UNLIMITED
```

## User QOS

By default there are no user QOS attributed. All user QOS attributed by INCD team are unique to specific users. The following command shows how to check the QOS you belong to:

```
[martinsj@cirrus02 ~]$ sacctmgr show user fmartins withassoc -p
User|Def
Acct|Admin|Cluster|Account|Partition|Share|Priority|MaxJobs|MaxNodes|MaxCPUs|MaxSubmit|MaxWall|MaxCPUMi
ns|QOS|Def QOS|
fmartins|biosim|None|production|cpca097522021||1|||||||cpca097522021,gpu097522021,normal||
fmartins|biosim|None|production|cpca097822021||1|||||||cpca097822021,gpu097822021,normal||
fmartins|biosim|None|production|biosim||1|||||||cpca71402020,incdbiosim21,normal||
```