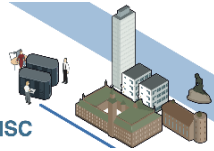


# McStas on the ESS cluster



EUROPEAN  
SPALLATION  
SOURCE

ESS DMSC



1. Get an account on the cluster - and consult [DMSC computing cluster](#) for how to access it!
2. Please **ensure that your simulation runs on your own desktop / laptop first** - and estimate a required runtime to achieve your necessary statistics!
3. When transferring input data to the cluster - please **ensure that all necessary files are present**, i.e. your
  - a. instrument file
  - b. any extra needed components
  - c. any extra c-codes
  - d. any extra datafiles
4. Load the **mpi module of choice**, one of the openmpi ones are recommended:

```
[willend@rln2 ~]$ module load openmpi<tab>

openmpi/3.0_gcc1020 openmpi/3.0_intel17 openmpi/4.0_gcc920
openmpi/3.0_gcc831 openmpi/4.0_gcc1020 openmpi/4.0_intel17
openmpi/3.0_gcc920 openmpi/4.0_gcc831

[willend@rln2 ~]$ module load openmpi/4.0_gcc831
```

**Recommendation is module load openmpi/4.0\_gcc831**

5. Load the **mcstas of choice** using e.g. the below command (which will give you the newest installed mcstas)

```
[willend@rln2 ~]$ module load mcstas/
```

6. **Compile your instrument** at the compile node using a command like

```
[willend@rln2 ~]$ mcrun -c --mpi=1 -n0 BNL_H8.instr
```

or

```
willend@rln2 ~]$ mcrun.pl -c --mpi -n0 BNL_H8.instr
```

You may experience some error output like below, but this can be safely ignored when compiling, since mpi processes are only allowed to run via the slurm scheduler.

```
Error obtaining unique transport key from ORTE (orte_precondition_transports not present in
the environment).
```

```
Local host: rln2.esss.dk
```

```
-----
*** The MPI_Init() function was called before MPI_INIT was invoked.
*** This is disallowed by the MPI standard.
-----
```

```
It looks like MPI_INIT failed for some reason; your parallel process is
likely to abort. There are many reasons that a parallel process can
fail during MPI_INIT; some of which are due to configuration or environment
problems. This failure appears to be an internal failure; here's some
additional information (which may only be relevant to an Open MPI
developer):
```

```

PML add procs failed
--> Returned "Error" (-1) instead of "Success" (0)
-----
*** Your MPI job will now abort.
[r1n2.esss.dk:11016] Abort before MPI_INIT completed successfully; not able to guarantee that all other
processes were killed!

```

7. On the ESS cluster, and optionally also on your own laptop, you can use the `mcsbub_slurm` script to help you generate a batch file for the cluster. It takes a few input arguments:

```

[willend@r1n2 ~]$ mcsbub_slurm --help
Usage: mcsbub_slurm [options] [mcrun params]
-h --help Show this help
-rN --runtime=N Specify maximum runtime (hours) [default 1]
-qQNAME --queue=QNAME Specify wanted SLURM queue [default 'quark']
-e<mail> --email=<mail> Specify address to notify in reg. sim status [default none]
--nodes=NUM Specify wanted number of nodes [default 1]
--name=NAME Specify openPBS job name [default "McSub_<USERNAME>_<TIMESTAMP>"]

Usage: /mnt/lustre/apps/mcstas/2.4.1/bin/mcsbub_slurm [options] [mcrun params]
-h --help Show this help
-rN --runtime=N Specify maximum runtime (hours) [default 1]
-qQNAME --queue=QNAME Specify wanted SLURM queue [default 'express']
--mpimodule=MODULE Specify wanted MPI module [default 'openmpi/3.0_gcc540']
-e<mail> --email=<mail> Specify address to notify in reg. sim status [default none]
--nodes=NUM Specify wanted number of nodes [default 1]
--name=NAME Specify slurm job name [default "McSub_<USERNAME>_<TIMESTAMP>"]

]

```

After running `mcsbub_slurm NAME.batch` is ready for submission using the `sbatch` command

(On McStas installations v. 2.4.1 and newer, the template batchfile writing is also available via File Configuration in mcgui on Linux / Python Preferences on macOS - meta-comma is a shortcut.)

8. To generate a batch file repeating a simulation that worked on your Desktop, use the script "in front" of the `mcrun` command run at your Desktop, e.g.:

```

[willend@r1n2 ~]$ mcsbub_slurm -quark mcrun BNL_H8.instr -nle6 Lambda=2.37

```

9. Having seen the output from 8, you should be able to request a production queue and a longer runtime using the `-q` and `-r` options of the script. (Or simply edit the script output to your taste and need!)
10. It is useful to receive output from the cluster jobs on start/termination etc. - please use the `-e` option for setting a relevant recipient address.

In case of issues with any of the above steps - feel free to contact [support@esss.dk](mailto:support@esss.dk) and [peter.willendrup@esss.se](mailto:peter.willendrup@esss.se)