

This tutorial shows step by step how to run a batch job (very short NAMD molecular dynamics job) on CSC's Taito supercluster. To do that you'll need a user account on Taito. If you don't have one, please apply for it from our web pages:

<http://research.csc.fi/user-account-application>

- 1) Log on to taito.csc.fi:

```
ssh yourid@taito.csc.fi
```

- 2) Go to the working directory

```
cd $WRKDIR
```

- 3) Create the batch script by opening a file with a file editor

```
nano myscript.sh
```

and paste the following text into the file editor (the method to paste in the ssh-window may depend on your connection. Things you can try: right click and choose paste, press CTRL-Insert(button), mouse middle-button, ... If none of these work, you can create the file on your own computer and copy it to taito.csc.fi with either scp or using the Scientist's User Interface "My files" service.

```
#!/bin/bash
#SBATCH -t 00:10:00
#SBATCH -p test
#SBATCH -J NAMD_test
#SBATCH -o onamd.%j
#SBATCH -e enamd.%j
#SBATCH -n 4
#SBATCH --no-requeue
#SBATCH --mail-type=END
#SBATCH --mail-user=your.name@there.fi
```

```
# change to your email address above
```

```
module load namd-env/2.9r
```

```
# run the job. Note that this differs from program to program.
# have a look for examples on the CSC software pages
# http://research.csc.fi/software
```

```
srun -n 4 namd2 alanin
```

- 4) Replace your.name@there.fi with your own email address
- 5) Save the file

Press CTRL-X

Answer "y"

Accept the name with enter

6) Copy the NAMD input files from to your working directory:

```
cp /appl/chem/namd/example/* .
```

7) Submit the batch job

```
sbatch myscript.sh
```

make note of the <JOBID> that is printed on your screen after the job has been submitted. We will refer to that number with <JOBID> in the text that follows.

Now the job has been submitted and is in the queue waiting to be allocated resources. You can check its status with the following command

```
squeue <JOBID>
```

You can also show the status of all your jobs. Replace the userid in the following command with your CSC username:

```
squeue -u <userid>
```

You should get a number of new files in your directory and when you can't see your job with squeue and you've received an email with some details of your job, it has been completed.

After the job you can check how your job used resources:

```
sacct -l -j <JOBID>
```

To see only the elapsed time, maximum used memory, allocated cores and jobname give:

```
sacct -o elapsed,maxrss,alloc,jobname -j <JOBID>
```

More information on the batch system on Taito in the Taito manual:

<http://research.csc.fi/taito-batch-jobs>

and how to submit jobs for specific applications can be found on the application help pages:

<http://research.csc.fi/software>