Advanced Molecular Dynamics hands-on exercise Coarse Grained bilayers

This parallel track will be done according to the instructions fromthe Martini group online in here:

http://cgmartini.nl/index.php/tutorials-general-introduction-gmx5/bilayers-gmx5

The hands-ons are planned to be done on taito.csc.fi with either your own CSC account or on the training accounts. Of course, it's possible to do these on any platform with a compatible version of Gromacs installed.

An example batch job script for simulations that take longer (adapt as needed, note the advance_reservation which will guarantee resources during the Spring School):

```
#!/bin/bash -l
#SBATCH -t 00:60:00 # 60 minutes on compute time
#SBATCH -p serial   # serial partition i.e. 1-24 cores
#SBATCH -n 10       # we ask for 10 mpi-tasks i.e. cores
#SBATCH -J GMX
#SBATCH -o ogmx.%j
#SBATCH -e egmx.%j
#SBATCH --reservation=chem_tue  # for the 2019 school only

export OMP_NUM_THREADS=1

module load gromacs-env/2018.6

srun mdrun_mpi -s topol.tpr -dlb yes
```

alternative with thread parallelization

```
#!/bin/bash -l
#SBATCH -t 00:60:00 # 60 minutes on compute time
#SBATCH -p serial   # serial partition i.e. 1-24 cores
#SBATCH -n 1        # we ask for 1 task
#SBATCH --cpus-per-task=10 # 10 threas
#SBATCH -J GMX
#SBATCH -o ogmx.%j
#SBATCH -e egmx.%j
#SBATCH --reservation=chem_tue  # for the 2019 school only
```

```
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

module load gromacs-env/2018.6

srun gmx mdrun -nt $SLURM_CPUS_PER_TASK -s topol.tpr -dlb yes
```

Note, for interactive jobs that require some computing power, please log i taito-shell.csc.fi instead of taito.csc.fi (login nodes). Batch jobs can be submitted also from there.