Molecular Dynamics hands-on exercise on Coarse Grained bilayers

This parallel track will be done according to the instructions from the 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 puhti.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.

The Puhti manual is in here: docs.csc.fi

For the impatient, give these commands before starting the tutorial:

```
module load gromacs-env
module load grace
module load vmd
export OMP_NUM_THREADS=1
cd /scratch/project_2002722
mkdir <your own name>
cd <your own name>
```

Note! Puhti does not have gmx installed, but **`gmx_mpi`**. If you run this tutorial on Puhti, please replace all **`gmx`** → **`gmx_mpi`**. The scripts take care of this automatically, but the interactive command line steps have not been edited in this text. The error will remind you…

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 --time=00:20:00     # 60 minutes on compute time
#SBATCH --partition=small   # small partition i.e. 1-40 cores
#SBATCH --ntasks=10         # we ask for 10 mpi-tasks
#SBATCH --job-name=GMX       #   i.e. cores
#SBATCH --account=project_2002722 # cpu usage billing
#SBATCH --reservation=chem_tue  # for the 2020 school only

module load gromacs-env

srun gmx_mpi mdrun -s topol.tpr -dlb yes
```

For interactive jobs that take longer than a minute, please use the **`sinteractive`** -command available on Puhti. It will allocate you one compute core in an interactive batch job. Use the same account as in the example above. You can have only one job in the interactive partition at a time. Note the usage policy and don't run heavy pre- or post-processing jobs on the login nodes.

Please **don't** use the **`-v`** flag for Gromacs jobs on CSC environment. It slows down your jobs and causes unnecessary file I/O.

More info on interactive jobs at CSC:

- https://docs.csc.fi/computing/running/interactive-usage/

More info on Gromacs at CSC:

- https://docs.csc.fi/apps/gromacs/