Running simulations in ACEMD + PLUMED

Load conda before doing anything else.

```
eval "$(/opt/miniconda3/bin/conda shell.bash hook)"
```

Then,

```
# License and modules
export ACELLERA_LICENSE_SERVER=28000@tolkien.prib.upf.edu

# PLUMED
PLUMED_KERNEL=/opt/plumed/lib/libplumedKernel.so
```

And run.

```
nohup acemd3 --ncpus 1 --device x > log.txt 2>&1 &
# x according to the number of GPUs
# En Kili: 0,1,2,3
```