Preparing the Environment

There are lots of litte tweaks we need in order to prepate the environment for running specific software. We will try to describe the ones we use more regularly so it is easier for the users to work with them.

mvapich

Version 2.3.3 compiled wiht Intel 2020

```
module load intel/mvapich2/2.3.3
source $I_MPI_ROOT/intel64/bin/mpivars.sh intel64 -ofi_internal=0
export LD_PRELOAD="libmpi.so"
```

mpich

Version 3.2.2 compiled with Intel 2020

```
module load intel/mpich/3.3.2
export LD_PRELOAD="libmpi.so"
```

OpenMPI 4.0.3

Version 4.0.3 compiled with Intel 2019

```
module load intel/openmpi/4.0.3
export I_MPI_PMI_LIBRARY=/lib64/libpmi.so
```

openfoam

Version 1912 compiled wiht Intel 2020

```
module load intel/openfoami20/1912
source /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1912/build01/OpenFOAM-v1912/etc/bashrc
. /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1912/build01/OpenFOAM-v1912/bin/tools/RunFunctions
```

Version 1906 compiled wiht Intel 2020

```
module load intel/openfoami20/1906
source /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1906/build01/OpenFOAM-v1912/etc/bashrc
. /cvmfs/sw.el7/ar/ix_es2680/i20/openfoami20/1906/build01/OpenFOAM-v1912/bin/tools/RunFunctions
```

gromacs

intel/gromacs/2020.2

```
module load gcc-6.3
source /cvmfs/sw.el7/ar/ix_es2680/i20/gromacs/2020.2/build01/bin/GMXRC.bash
source /cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
module load intel/gromacs/2020.2
```

intel/gromacs/2020.20-i20

```
module load gcc-7.5
source /cvmfs/sw.el7/ar/ix_es2680/i20/gromacs/2020.2/build02/bin/GMXRC.bash#source
/cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
source /cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
module load intel/gromacs/2020.2
```

gromacs-4.6.7

```
module load gromacs-4.6.7
module load gcc63/openmpi/4.0.3
export GMX_MAXBACKUP=-1
mpirun -np 10 mdrun -s  benchMEM.tpr -nsteps 500000 -maxh 3.0 -resethway
```

Version 2020.2 compiled wiht Intel 2020

```
module load gcc-6.3
source /cvmfs/sw.el7/ar/ix_es2680/i20/gromacs/2020.2/build02/bin/GMXRC.bash
source /cvmfs/sw.el7/intel/2020/bin/compilervars.sh intel64
module load intel/gromacs/2020.2
```