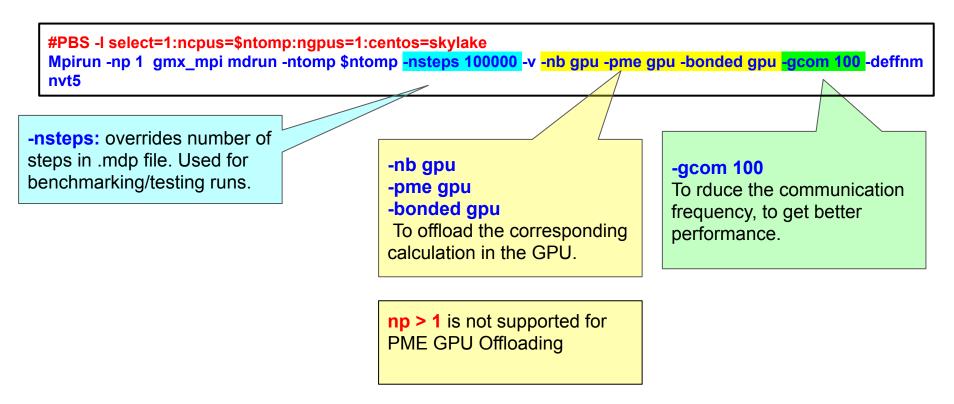
(including PLUMED)

GROMACS Benchmarking in GPU V100

HPC IIT Delhi:Performance GROMACS19 *V100=skylake



^{*}Kutzner et al. used time step fo 2 fs for GROMACS benchmarking, whereas we have used 1 fs.

Kutzner et al. J. Comput. Chem. 2019, 40, 2418-2431.

HPC IIT Delhi:Performance GROMACS19 *V100=skylake

System: 3CLpro ~ 52 K atoms

np	Node [core=20]	gpu*	\$ntomp [5P X core]##	Performance (ns/day)	(GPU+CPU/min)/ (Rs/day)
1	4	1 (V100)	4 (20 P)	77	70P/ 1008 Rs
1	8	1 (V100)	8 (40 P)	89	90P/ 1290 Rs
1	12	1 (V100)	12 (60 P)	93	110P/ 1584 Rs
1	20	1 (V100)	20 (100 P)	95	150P/ 2160 Rs

As in each GPU node 20 processors in CPU

##
EXPORT OMP_NUM_THREADS=\$ntomp

GPU: 50 p/min CPU: 5p/core min 1 Day= 1440 min

#PBS -I select=1:ncpus=\$ntomp:ngpus=1:centos=skylake

Mpirun -np 1 gmx_mpi mdrun -ntomp \$ntomp -nsteps 100000 -v -nb gpu -pme gpu -bonded gpu -gcom 100 -deffnm
nvt5

HPC IIT Delhi:Performance GROMACS19 with PLUMED*V100=skylake

Plumed.dat:

#Add keyword in starting of plumed file to print time consumed in individual CV calculation DEBUG DETAILED_TIMERS

In PBS script

#Add keyword in the PBS submission script. The PLUMED_OMP_THREADS value will be same as OMP_NUM_THREAS value PLUMED_OMP_THREADS=

#PBS -I select=1:ncpus=\$ntomp:ngpus=1:centos=skylake

Mpirun -np 1 gmx_mpi mdrun -ntomp \$ntomp -nsteps 100000 -v -nb gpu -pme gpu -bonded gpu -gcom 100 -deffnm nvt5 -plumed plumed.dat

GROMACS19 with PLUMED: COORDINATION NUMBER CV Optimization

Plumed.dat:

#Add keyword in starting of plumed file to print time consumed in individual CV calculation DEBUG DETAILED_TIMERS

#Coordination Number calculation consumes a lot of time, if calculate for solvent like water. In such cases, to reduce calculation time use neighbour list.

LIGsolv: COORDINATION GROUPA=LIg_heavy GROUPB=OW R_0=0.4 NLIST NL_STRIDE=100 NL_CUTOFF=1.0

#To tunne the value of NL_STRIDE run a setup with printing in COLVAR file

LIGsolv1: COORDINATION GROUPA=Lig_heavy GROUPB=OW R_0=0.4

LIGsolv2: COORDINATION GROUPA=LIg_heavy GROUPB=OW R_0=0.4 NLIST NL_STRIDE=10

NL_CUTOFF=1.0

LIGsolv3: COORDINATION GROUPA=LIg_heavy GROUPB=OW R_0=0.4 NLIST NL_STRIDE=50

NL_CUTOFF=1.0

LIGsolv4: COORDINATION GROUPA=LIg_heavy GROUPB=OW R_0=0.4 NLIST NL_STRIDE=100

NL_CUTOFF=1.0

#Plot and use the NL_STRIDE value giving performance similar to without NLIST case.

GROMACS19 with PLUMED Benchmarking with COORDINATION NUMBER CV

np	Node [core=2 0]	gpu*	\$ntomp [5P X core]##	PLUMED NLIST	Performance (ns/day)	(GPU+CPU/min)/ (Rs/day)
1	20	1 (V100)	20 (20 P)	Without NLIST	7.5	150P/ 2160 Rs
1	20	1 (V100)	20 (20 P)	NLIST STRIDE 10	18	150P/ 2160 Rs
1	20	1 (V100)	20 (20 P)	NLIST STRIDE 50	29	150P/ 2160 Rs
1	20	1 (V100)	20 (20 P)	NLIST STRIDE 100	35.5	150P/ 2160 Rs
1	12	1 (V100)	12 (60 P)	NLIST STRIDE 100	35	110P/ 1584 Rs
1	8	1(V100)	8 (40 P)	NLIST STRIDE 100	34.5	90P/ 1290 Rs

OMP_NUM_THREADS = PLUMED_NUM_THREADS

System: CBL:AVI ~1 lakh atoms