

Gromacs-2021.3 (GPU)

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Singularity /fs00/software/singularity-images/ngc_gromacs_2021.3.sif

Gromacs em nvt npt md 100%GPU

722080tiib 72rtxib 723090ib

		CPU	(GB)	(GB)	CPU (GHz)	GPU	GPU (GB)	(TFLOPS)
83a100ib	1	64	512	8	2.6	8	40	:82.92 :-----
723090ib	2	48	512	10.7	2.8	8	24	:4.30 :569.28
722080tiib	4	16	128	8.0	3.0	4	11	:3.07 :215.17
72rtxib	3	16	128	8.0	3.0	4	24	:2.30 :195.74

Gromacs-2021.3(GPU) GPU 102808
 464 residues, 9nt DNA, 31709 SOL, 94 NA, 94 CL 50 ns **83a100ib**
250 ns/day **723090ib** **220 ns/day** **722080tiib** **170 ns/day** **72rtxib**
180 ns/day 83a100ib 723090ib 80 NJOBS

/fs00/software/singularity-images/ngc_gromacs_2021.3.sif

em.lsf

```

#BSUB -q 72rtxib
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx grompp -f minim.mdp -c 1aki_solv_ions.gro -p topol.top -o em.tpr
${SINGULARITY} gmx mdrun -nb gpu -ntmpi 2 -deffnm em

```

nvt

```

#BSUB -q 72rtxib
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr
${SINGULARITY} gmx mdrun -nb gpu -ntmpi 2 -deffnm nvt

```

npt

```

#BSUB -q 72rtxib
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr

```

```

$ {SINGULARITY} gmx mdrun -nb gpu -ntmpi 2 -deffnm npt

```

md

```
#BSUB -q 723090ib
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr
${SINGULARITY} gmx mdrun -nb gpu -bonded gpu -update gpu -pme gpu -pmefft gpu -deffnm md_0_1
```

md

```
#BSUB -q 723090ib
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx pdb2gmx -f protein.pdb -o protein_processed.gro -water tip3p -ignh -merge all <<< 4
${SINGULARITY} gmx editconf -f protein_processed.gro -o pro_newbox.gro -c -d 1.0 -bt cubic
${SINGULARITY} gmx solvate -cp pro_newbox.gro -cs spc216.gro -o pro_solv.gro -p topol.top
${SINGULARITY} gmx grompp -f ../MDP/ions.mdp -c pro_solv.gro -p topol.top -o ions.tpr
${SINGULARITY} gmx genion -s ions.tpr -o pro_solv_ions.gro -p topol.top -pname NA -nname CL -neutral <<< 13
${SINGULARITY} gmx grompp -f ../MDP/minim.mdp -c pro_solv_ions.gro -p topol.top -o em.tpr
${SINGULARITY} gmx mdrun -v -deffnm em
${SINGULARITY} gmx energy -f em.edr -o potential.xvg <<< "10 0"
${SINGULARITY} gmx grompp -f ../MDP/nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr
${SINGULARITY} gmx mdrun -deffnm nvt
${SINGULARITY} gmx energy -f nvt.edr -o temperature.xvg <<< "16 0"
${SINGULARITY} gmx grompp -f ../MDP/npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr
${SINGULARITY} gmx mdrun -deffnm npt
${SINGULARITY} gmx energy -f npt.edr -o pressure.xvg <<< "18 0"
${SINGULARITY} gmx grompp -f ../MDP/md.mdp -c npt.gro -t npt.cpt -p topol.top -o md.tpr
${SINGULARITY} gmx mdrun -v -deffnm md
${SINGULARITY} gmx rms -f md.xtc -s md.tpr -o rmsd.xvg <<< "4 4"
```

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GROMACS version: 2021.3-dev-20210818-11266ae-dirty-unknown
Precision: mixed
Memory model: 64 bit
MPI library: thread_mpi
OpenMP support: enabled (GMX_OPENMP_MAX_THREADS = 64)
GPU support: CUDA
SIMD instructions: AVX2_256
FFT library: fftw-3.3.9-sse2-avx-avx2-avx2_128-avx512
CUDA driver: 11.20
CUDA runtime: 11.40

ATOM

ATOM 218234 (401 Protein residues, 68414 SOL, 9 Ion residues)

nsteps = 100000000 ; 200 ns

eScience GPU em nvt npt 1 GPU md
1 GPU

1	em	nvt	npt	md
---	72rtxib	722080tiib	722080tiib	723090ib
CPU time	1168.45	13960.33	42378.71	
Run time	79	1648	5586	117.428 ns/day 0.204 hour/ns
Turnaround time	197	1732	5661	
2	em	nvt	npt	md
---	72rtxib	722080tiib	72rtxib	722080tiib
CPU time	1399.30	15732.66	40568.04	
Run time	93	1905	5236	106.862 ns/day 0.225 hour/ns
Turnaround time	181	1991	5479	
3	em	nvt	npt	md
---	72rtxib	72rtxib	72rtxib	72rtxib
CPU time	1368.11	5422.49	5613.74	
Run time	92	355	366	103.213 ns/day 0.233 hour/ns

<div><div></div><div>1</div></div>	em	nvt	npt	md
Turnaround time	180	451	451	
<div><div></div><div>4</div></div>	em	nvt	npt	md
---	72rtxib	72rtxib	72rtxib	722080tiib
CPU time	1321.15	5441.60	5618.87	
Run time	89	356	369	111.807 ns/day 0.215 hour/ns
Turnaround time	266	440	435	
<div><div></div><div>5</div></div>	em	nvt	npt	md
---	72rtxib	72rtxib	72rtxib	72rtxib
CPU time	1044.17	5422.94	5768.44	
Run time	72	354	380	110.534 ns/day 0.217 hour/ns
Turnaround time	162	440	431	
<div><div></div><div>6</div></div>	em	nvt	npt	md
---	723090ib	723090ib	723090ib	723090ib
CPU time	1569.17	7133.74	6677.25	
Run time	81	326	325	114.362 ns/day 0.210 hour/ns
Turnaround time	75	320	300	
<div><div></div><div>7</div></div>	em	nvt	npt	md
---	723090ib	723090ib	723090ib	722080tiib
CPU time	1970.56	5665.71	6841.73	
Run time	91	253	327	111.409 ns/day 0.215 hour/ns
Turnaround time	123	251	328	
<div><div></div><div>8</div></div>	em	nvt	npt	md
---	72rtxib	72rtxib	72rtxib	72rtxib
CPU time	1234.24	5540.59	5528.91	
Run time	108	363	370	114.570 ns/day 0.209 hour/ns
Turnaround time	85	364	363	

1	em	nvt	npt	md
9	em	nvt	npt	md
---	723090ib	723090ib	723090ib	723090ib
CPU time	2016.10	7633.83	7983.58	
Run time	93	342	361	115.695 ns/day 0.207 hour/ns
Turnaround time	130	377	356	
10	em	nvt	npt	md
---	723090ib	723090ib	723090ib	72rtxib
CPU time	1483.84	7025.65	7034.90	
Run time	68	317	333	102.324 ns/day 0.235 hour/ns
Turnaround time	70	319	316	

- em722080tiib72rtxibRun time88.83 ± 12.4583.25 ± 11.44s;
- nvt722080tiib72rtxib723090ibRun time1776.50 ± 181.73357.00 ± 4.08309.50 ± 39.06 s
- npt722080tiib72rtxib723090ibRun time5411.00 ± 247.49371.25 ± 6.08336.50 ± 16.68 s
- 218234200 nsmd722080tiib72rtxib723090ib110.03 ± 2.75115.83 ± 1.54107.66 ± 5.90 ns/day
- emnvt npt72rtxibmd722080tiib723090ib83a100ibGPU72rtxib1.8 / / =0.45 / / 722080tiib1.2 / / =0.3 / / 723090ib1.8 / / =0.3 / / 83a100ib4.8 / / =0.3 / /
- Gromacs“num=4”4GPUhttp://bbs.keinsci.com/thread-13861-1-1.html

[https://developer.nvidia.com/blog/creating-faster-molecular-dynamics-simulations-with-](https://developer.nvidia.com/blog/creating-faster-molecular-dynamics-simulations-with-gromacs-2020/)

[gromacs-2020/](#)[ATOM 500000](#)[GPU](#)

[Gromacs](#)[Amber](#) GPU

[3090](#) [tesla A100](#) GPU=4 [gromacs](#)

```
gmx mdrun -deffnm $file.pdb.md -ntmpi 4 -ntomp 7 -npme 1 -nb gpu -pme gpu -bonded gpu -pmefft gpu -v
```

Revision #12

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