

# Gromacs-2021.3 ( GPU )

## 4. 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

GPU Gromacs-2021.3(GPU 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 laki_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 rms -f md.xtc -s md.tpr -o rmsd.xvg <<< "4 4"
```



```
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 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	

<b>1</b>	<b>em</b>	<b>nvt</b>	<b>npt</b>	<b>md</b>
<b>3</b>	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
Turnaround time	180	451	451	
<b>4</b>	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	
<b>5</b>	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	
<b>6</b>	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	
<b>7</b>	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	
<b>8</b>	em	nvt	npt	md
---	72rtxib	72rtxib	72rtxib	72rtxib



1.8 / / =0.3 / / 83a100ib 4.8 / / =0.3 / /

6. Gromacs "num=4" 4

GPU <http://bbs.keinsci.com/thread-13861-1-1.html>

<https://developer.nvidia.com/blog/creating-faster-molecular-dynamics-simulations-with-gromacs-2020/>

ATOM 50000 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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