

# Gromacs-2021.3 (???? GPU??)

## 4. Gromacs-2021.3 (????GPU??)

???

```
 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<br>:----- |
| 723090ib   | 2 | 48  | 512  | 10.7 | 2.8       | 8   | 24       | :4.30<br>:569.28 |
| 722080tiib | 4 | 16  | 128  | 8.0  | 3.0       | 4   | 11       | :3.07<br>:215.17 |
| 72rtxib    | 3 | 16  | 128  | 8.0  | 3.0       | 4   | 24       | :2.30<br>: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
```

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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 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 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<br>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<br>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<br>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<br>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<br>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<br>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<br>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<br>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<br>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<br>0.235 hour/ns |
| Turnaround time | 70       | 319      | 316      |                                 |

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1. 722080tiib 72rtxib Run time 88.83 ± 12.45 83.25 ± 11.44s;
2. nvt 722080tiib 72rtxib 723090ib Run time 1776.50 ± 181.73 357.00 ± 4.08 309.50 ± 39.06 s
3. npt 722080tiib 72rtxib 723090ib Run time 5411.00 ± 247.49 371.25 ± 6.08 336.50 ± 16.68 s
4. 218234 200 ns md 722080tiib 72rtxib 723090ib 110.03 ± 2.75 115.83 ± 1.54 107.66 ± 5.90 ns/day
5. em nvt npt 72rtxib md 722080tiib 723090ib 83a100ib GPU 72rtxib 1.8 / / =0.45 / / 722080tiib 1.2 / / =0.3 / / 723090ib 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-](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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