

# Gromacs

如何安装GPU, 如何安装2021GromacsGPU

## 1. Gromacs-2018.8

1.1

GromacsCPUGPU

1.1.1

```
gcc/7.4.0
cmake/3.16.3
ips/2017u2
fftw/3.3.7-iccifort-17.0.6-avx2
cuda/10.0.130
```

1.1.2

```
GROMACS version: 2018.8
Precision: single
Memory model: 64 bit
MPI library: MPI
OpenMP support: enabled (GMX_OPENMP_MAX_THREADS = 64)
GPU support: CUDA
SIMD instructions: AVX2_256
FFT library: fftw-3.3.7-avx2-avx2_128
CUDA driver: 11.40
CUDA runtime: 10.0
```

1.1.3

```
nsteps      = 25000000    ;50 ns
```

Queue	ns/day
83a100ib	150
723090ib	75
722080tiib	82
72rtxib	83

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/fs00/software/singularity-images/ngc\_gromacs\_2021.3.sif



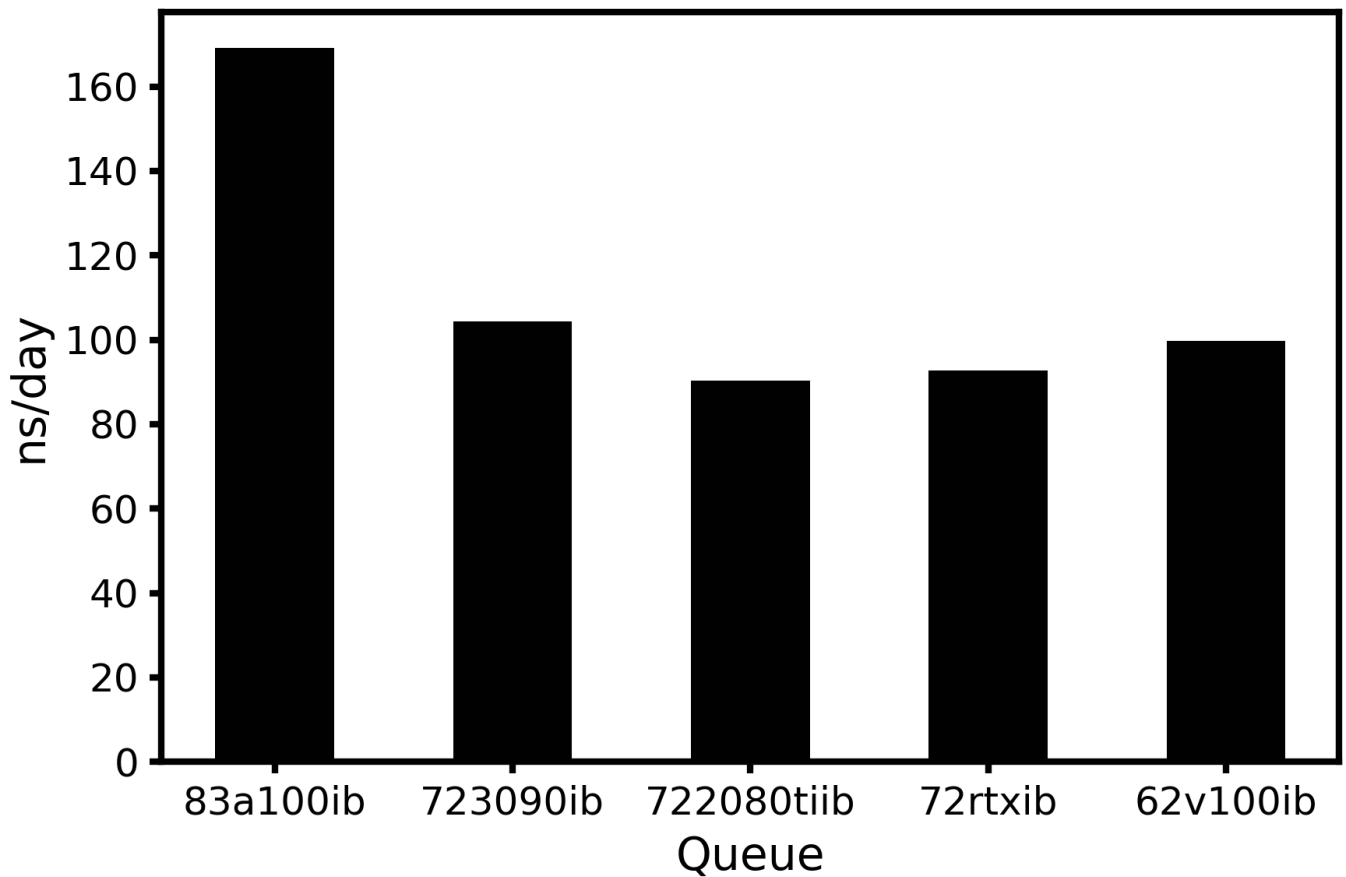
```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
module load singularity/latest
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx mdrun -nb gpu -deffnm <NAME>
```



```
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 102808(464 residues, 9nt DNA, 31709 SOL, 94 NA, 94 CL)
nsteps    = 25000000    ;50 ns
```



### 3. Gromacs-2021.3(□□□□□GPU□□)

103

A horizontal timeline bar divided into three equal segments for the years 2019, 2020, and 2021. Each year segment contains a series of 12 small squares representing months. The word 'GPU' is written in the center of each year's segment, indicating that GPU usage was present throughout the entire period from 2019 to 2021.

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/fs00/software/singularity-images/ngc\_gromacs\_2021.3.sif

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```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
module load singularity/latest
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC" # [|||||]CPU[|||||]
```

```
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
```

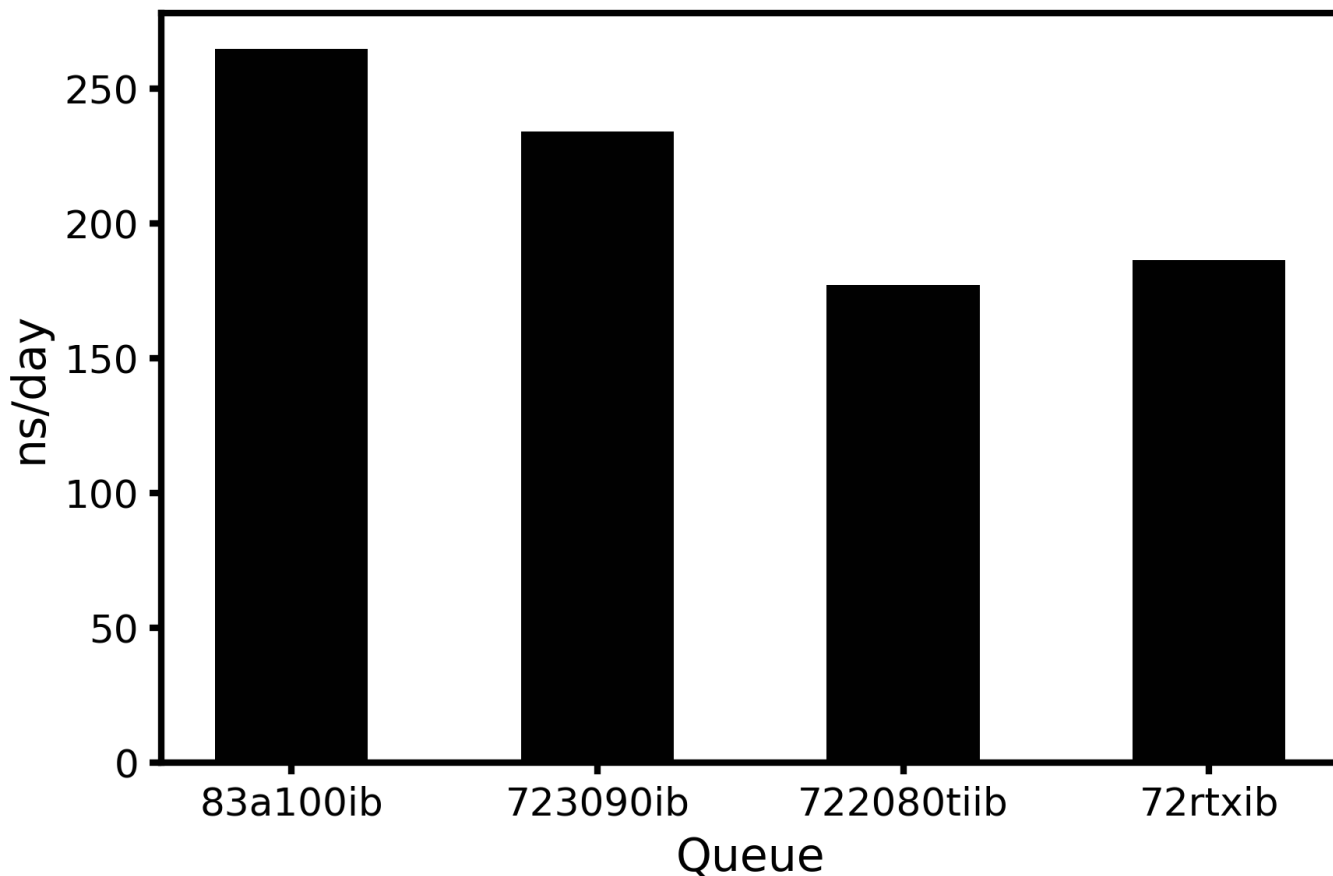
```
${SINGULARITY} gmx mdrun -nb gpu -bonded gpu -update gpu -pme gpu -pmefft gpu -deffnm <NAME>.# ██████
```



ATOM 102808(464 residues, 9nt DNA, 31709 SOL, 94 NA, 94 CL)

nsteps = 25000000 ;50 ns

eScience██GPU██ GPU████GPU████



1. █GPU████GPU+CPU████████████████████CPU████████████████████GPU████████████████████



██GPU████CPU██

Queue	CPU Core
72rtxib	4
722080tiib	4
723090ib	6
62v100ib	5
83a100ib	8

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Revision #23

Created 16 November 2021 15:18:31 by Yao Ge

Updated 3 January 2023 10:54:50 by Yao Ge