

Gromacs

安装Gromacs GPU加速, 编译Gromacs GPU
2021年 Gromacs GPU
编译Gromacs GPU

1. Gromacs-2018.8

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Gromacs CPU GPU

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

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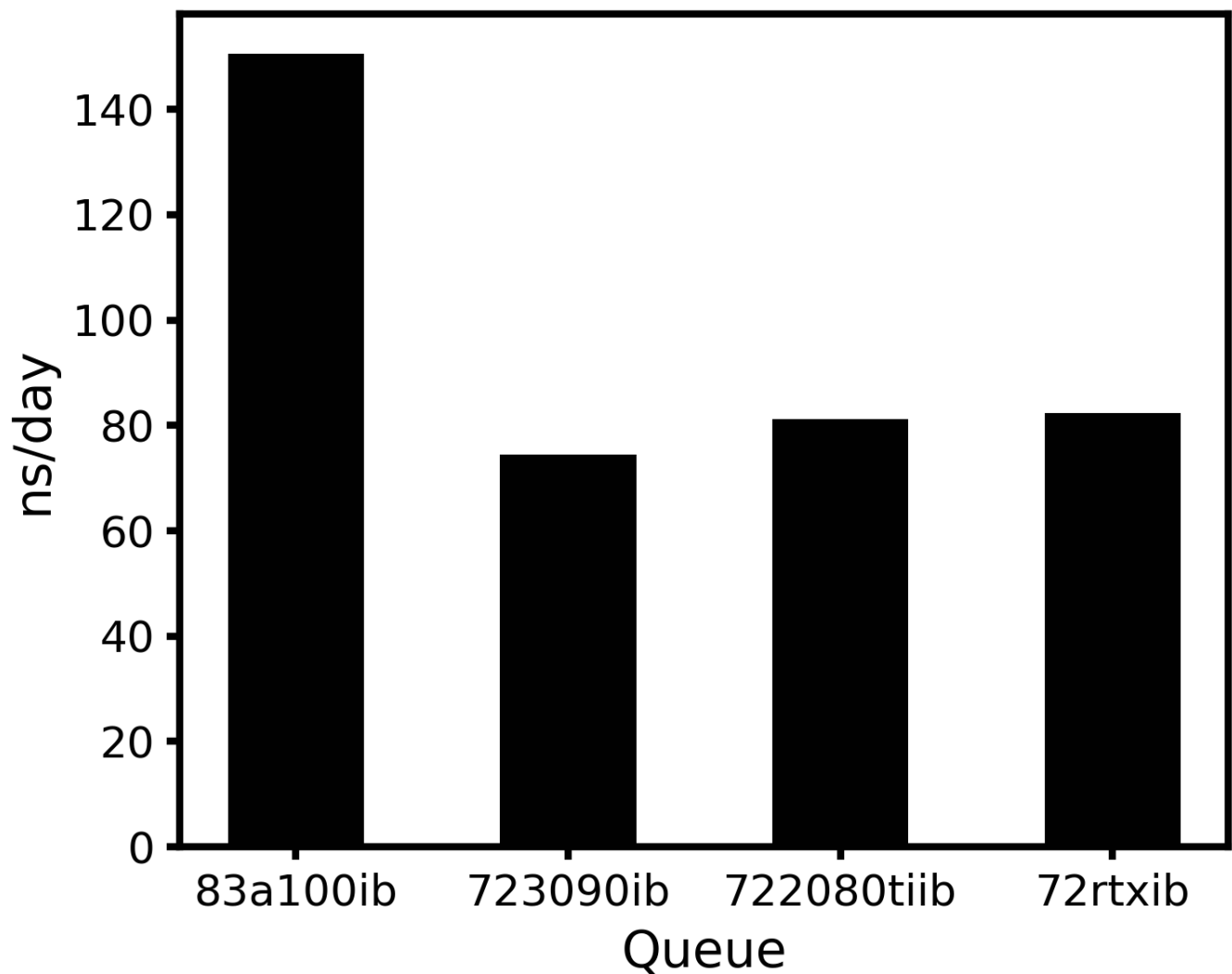
```
GROMACS version: 2018.8
Precision: single
Memory model: 64 bit
MPI library: MPI
OpenMP support: enabled (GMX_OPENMP_MAX_THREADS = 64)
GPU support: CUDA
SIMD instructions: AVX2_256
FFT library: fftw-3.3.7-avx2-avx2_128
CUDA driver: 11.40
CUDA runtime: 10.0
```

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

nsteps = 25000000 ;50 ns

eScience??GPU??? ??GPU??????GPU??????



2. Gromacs-2021.3

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(singularity) gromacs-2021.3. Gromacs

CPU■■■■■■■■■■

GPU

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

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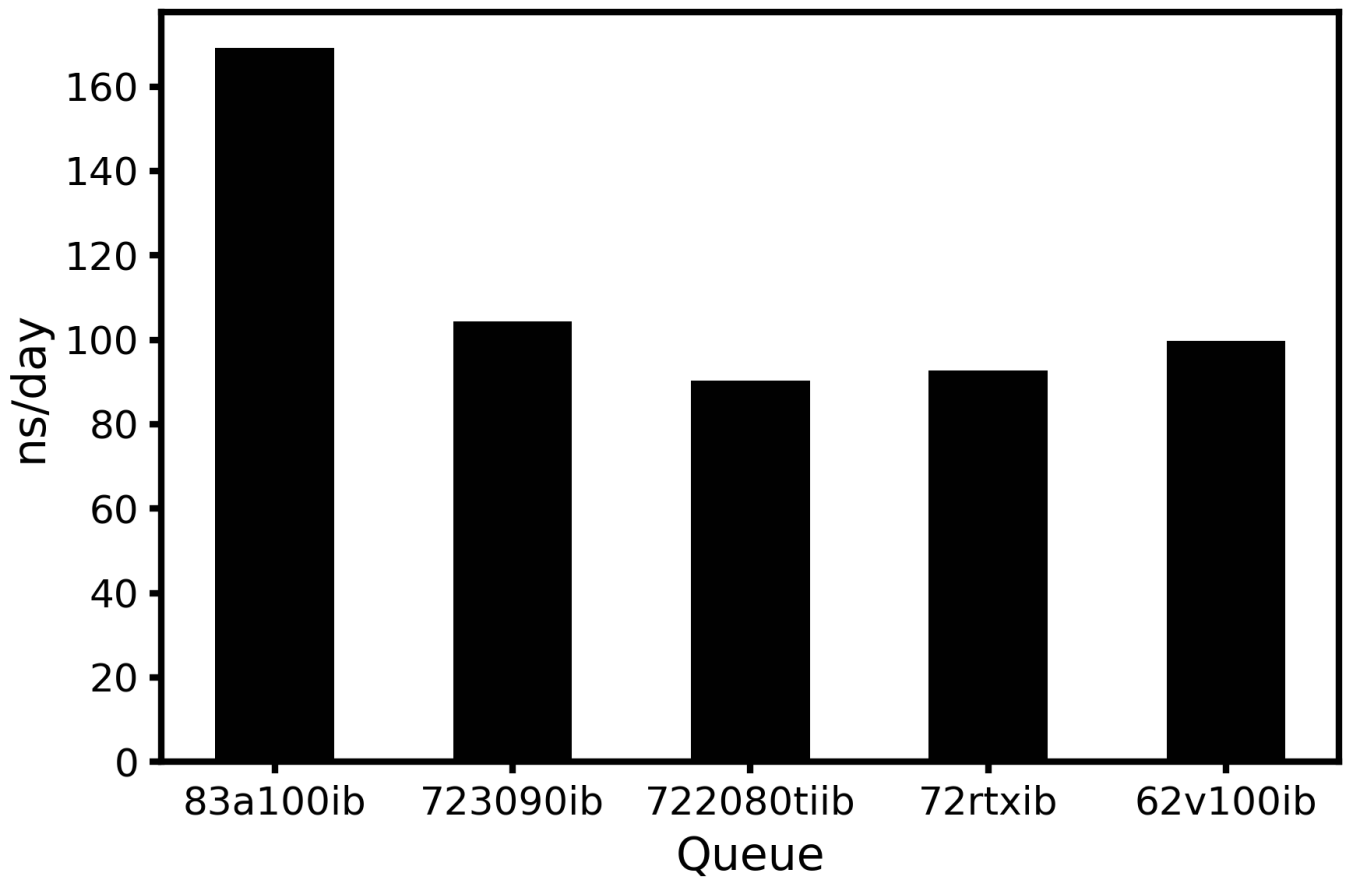
```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx mdrun -nb gpu -deffnm <NAME>
```

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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
```

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



3. Gromacs-2021.3(???????GPU??)

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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"

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

```

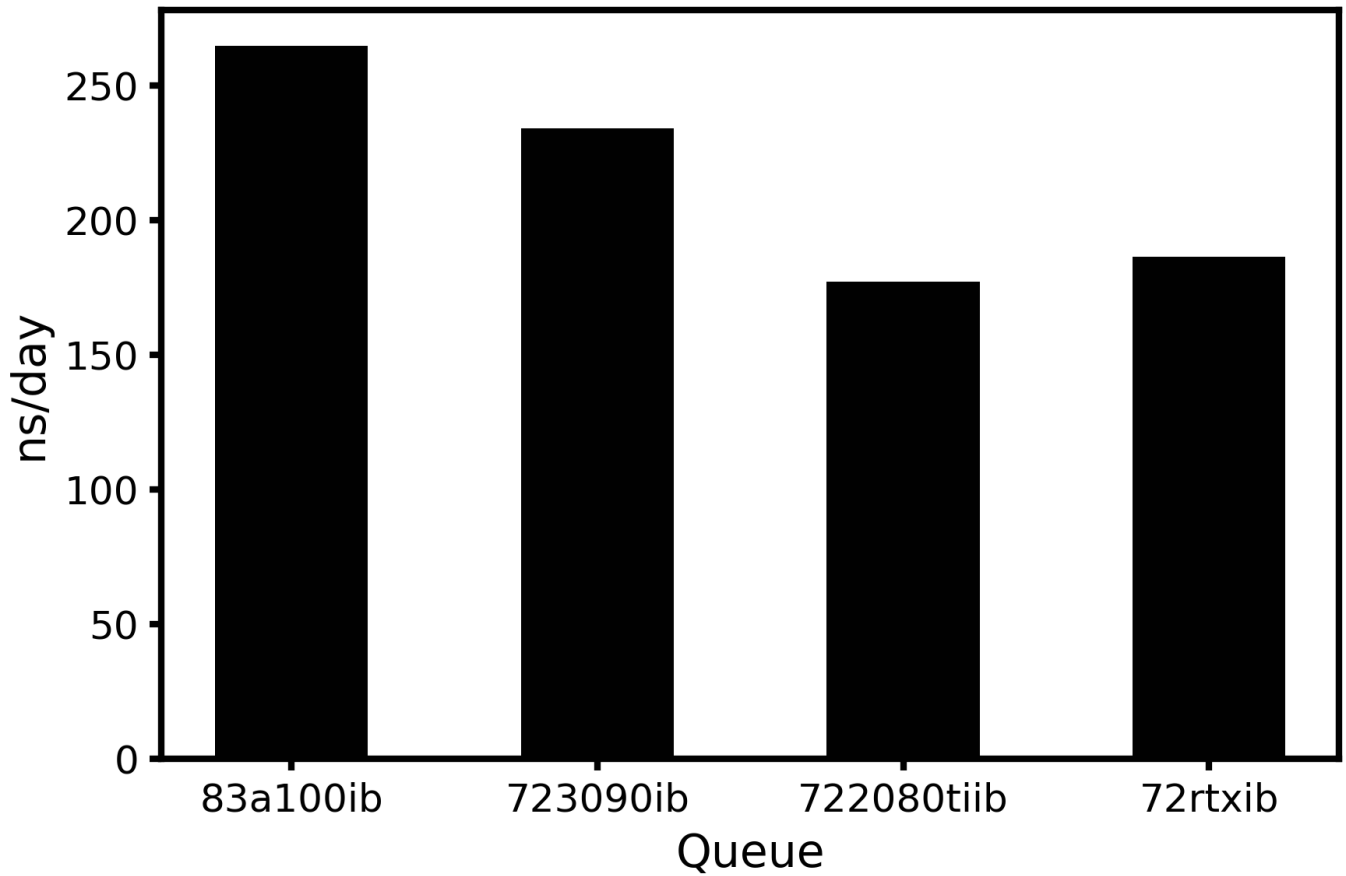
${SINGULARITY} gmx mdrun -nb gpu -bonded gpu -update gpu -pme gpu -pmefft gpu -deffnm <NAME>#
GPU

```




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

eScience□□ GPU□□□ □□ GPU□□□□□ GPU□□□□□



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1.  GPU  CPU 

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