

# Gromacs

GPU加速, 并行计算  
2021年 Gromacs GPU  
并行计算

## 1. Gromacs-2018.8

编译

Gromacs CPU 编译 GPU 编译

编译选项

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

编译输出

```
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
```



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

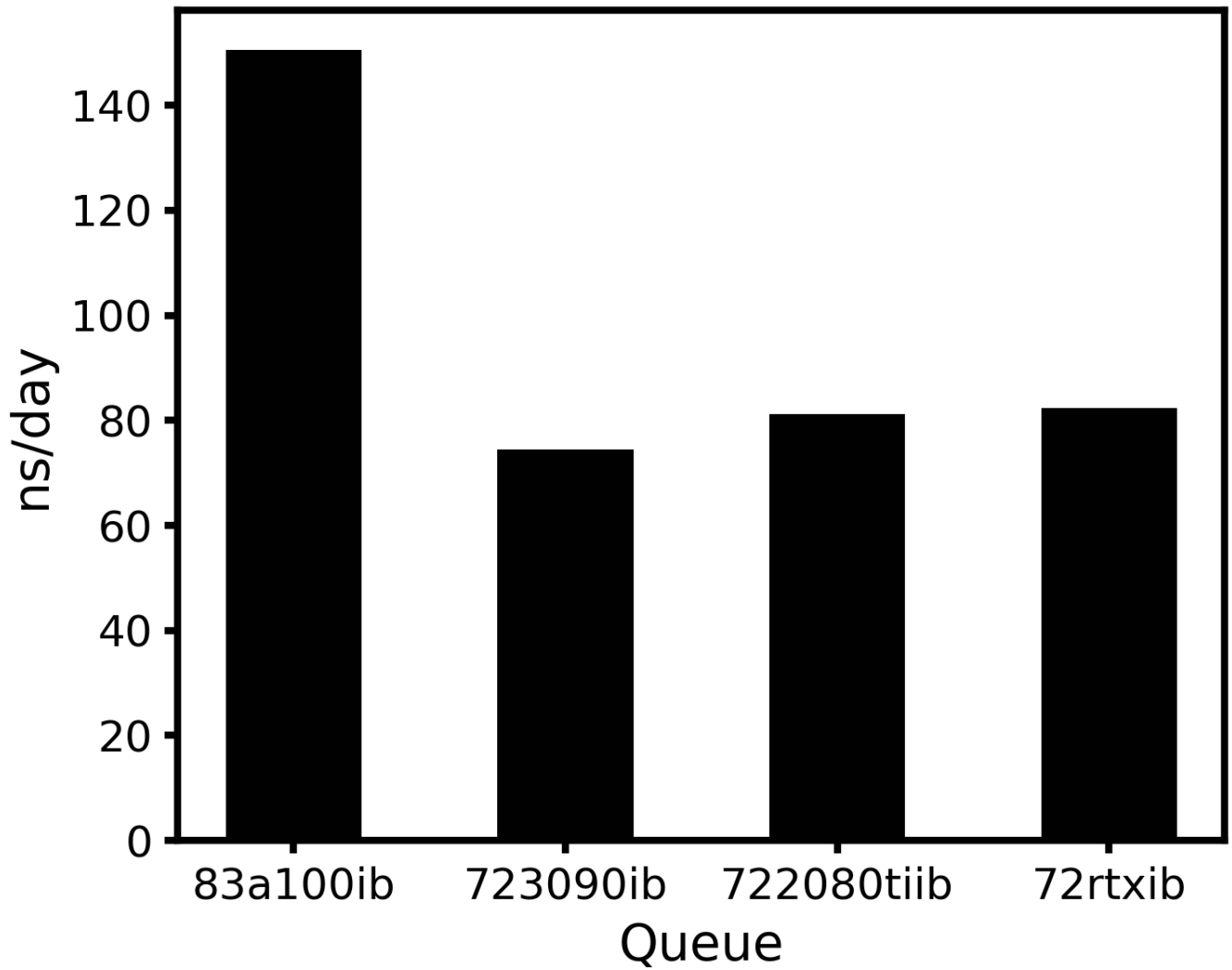
nsteps = 25000000 ;50 ns

eScience

GPU

GPU

GPU



## 2. Gromacs-2021.3



(singularity) gromacs-2021.3. Gromacs CPU

GPU





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



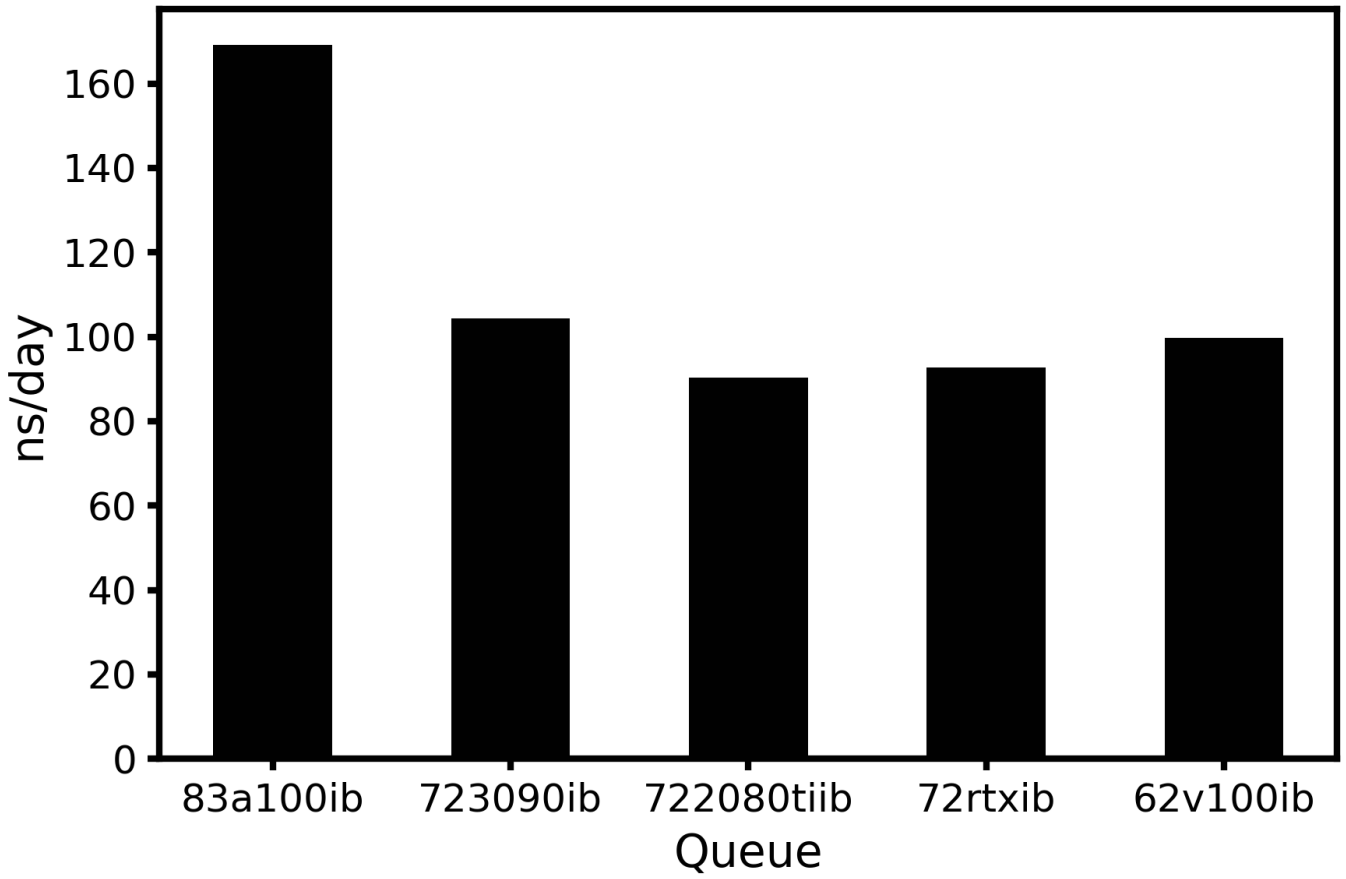
```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx mdrun -nb gpu -deffnm <NAME>
```



```
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

)

2019 GPU 2021

GPU GPU

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



1. GPU GPU+CPU CPU  
GPU GPU



GPU CPU

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

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