

Gromacs

编译Gromacs 2018.8 GPU加速，并安装相关依赖库

1. Gromacs-2018.8

编译

Gromacs 2018.8 CPU加速 GPU加速

编译

```
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

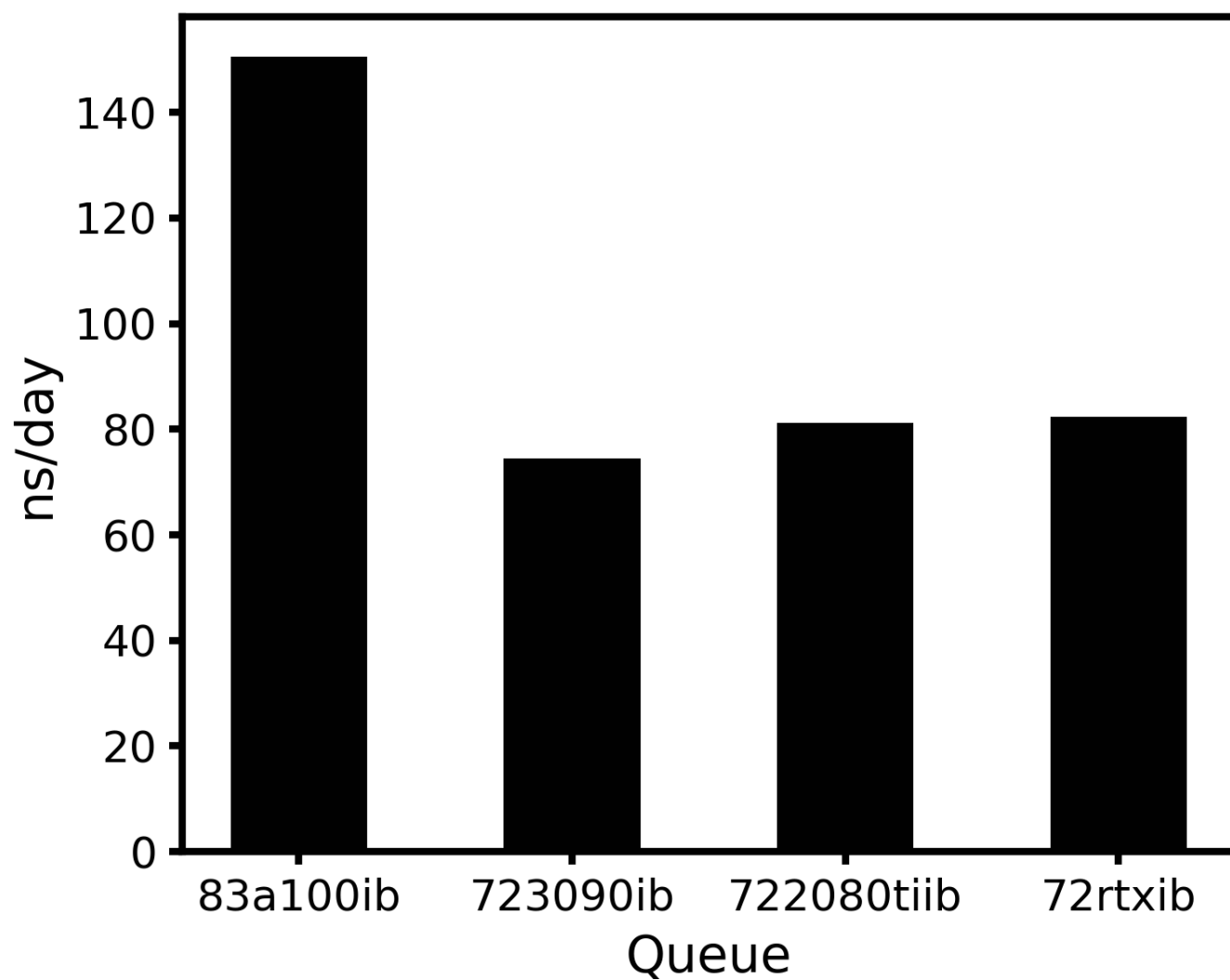
```
GROMACS version: 2018.8
Precision: single
Memory model: 64 bit
MPI library: MPI
OpenMP support: enabled (GMX_OPENMP_MAX_THREADS = 64)
GPU support: CUDA
SIMD instructions: AVX2_256
FFT library: fftw-3.3.7-avx2-avx2_128
CUDA driver: 11.40
CUDA runtime: 10.0
```



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
```



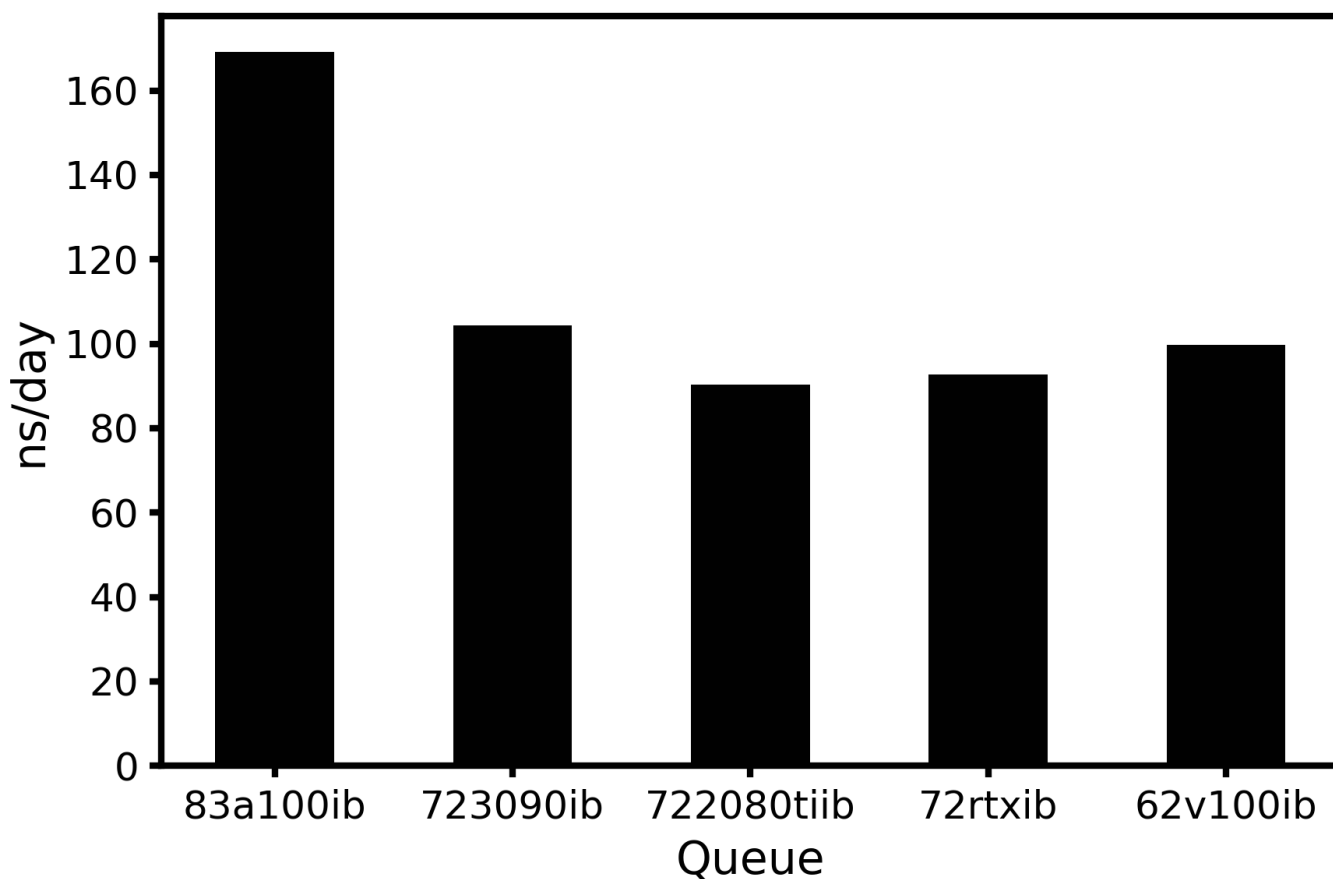
```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx mdrun -nb gpu -deffnm <NAME>
```



```
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

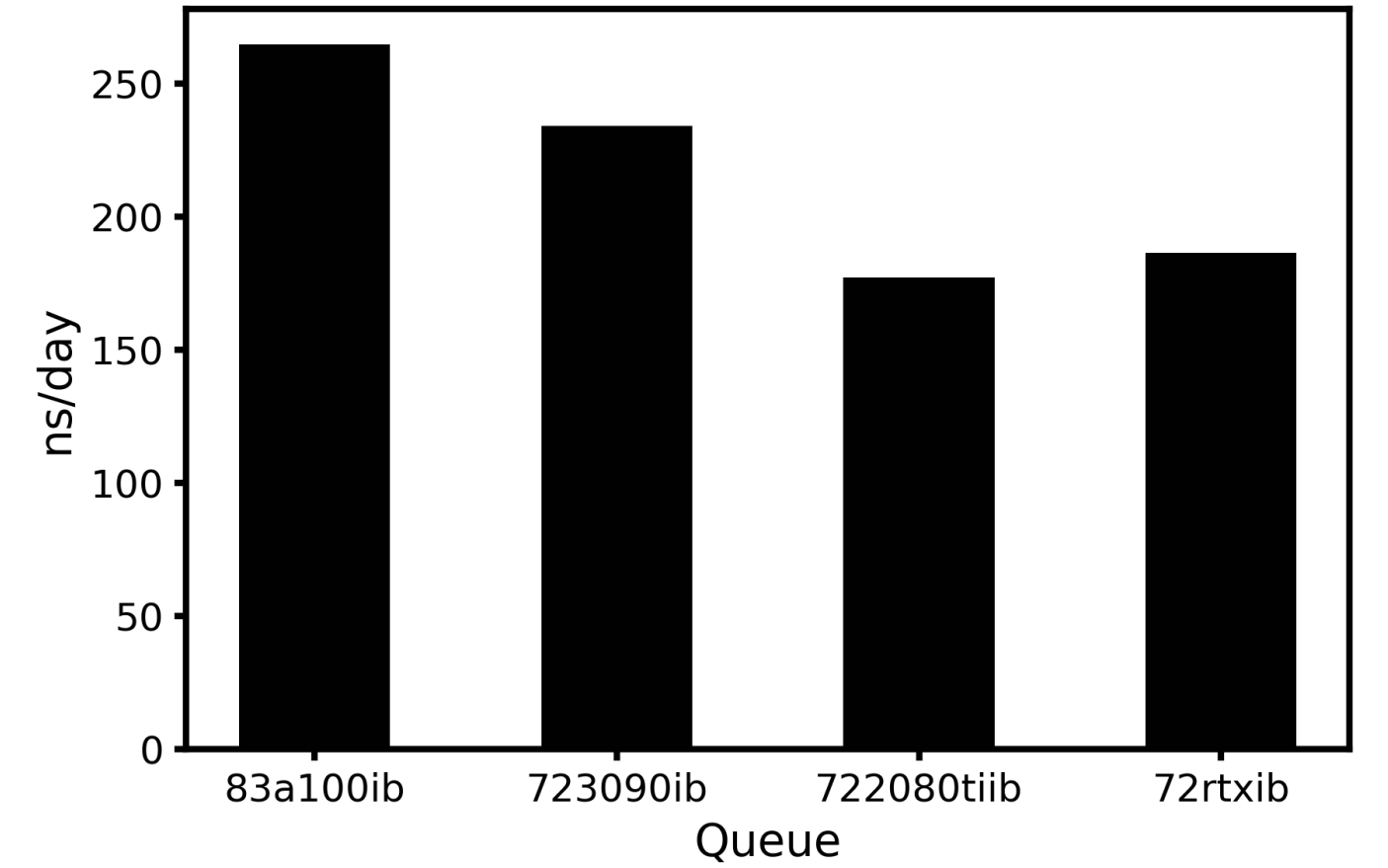
  

```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_gromacs_2021.3.sif"
${SINGULARITY} gmx mdrun -nb gpu -bonded gpu -update gpu -pme gpu -pmefft gpu -deffnm <NAME>
GPU
```



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

eScience GPU GPU GPU GPU GPU GPU



1. GPU GPU+CPU CPU
 GPU GPU



GPU CPU

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