Gromacs

□□□□□□□ GPU□□ ，□□□□□□□□□□□□□□□
2021□□□ Gromacs□□□ GPU
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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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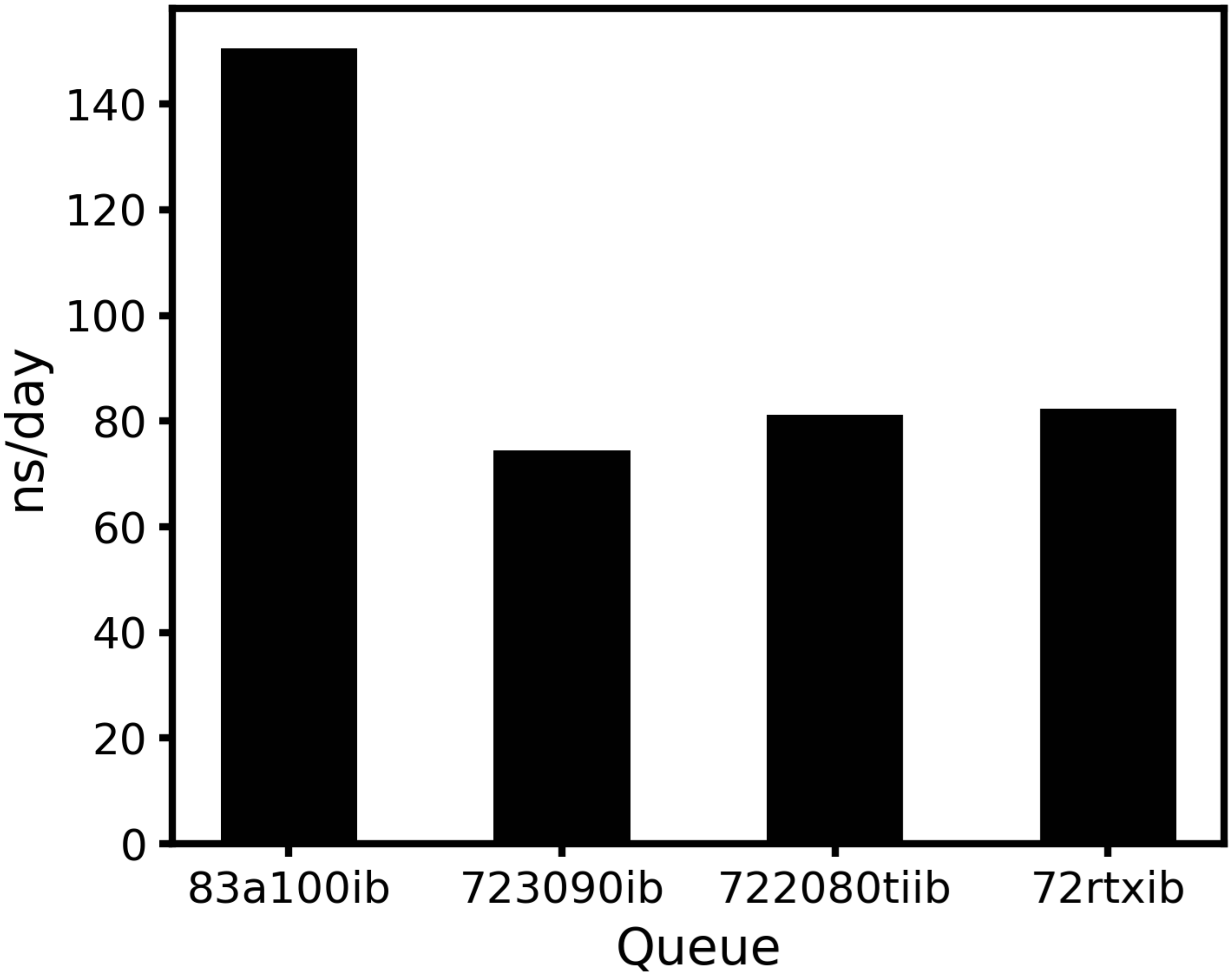
```
ATOM  102808(464 residues, 9nt DNA, 31709 SOL, 94 NA, 94 CL)
nsteps      = 25000000     ;50 ns
```

eSience??GPU??? ??GPU??????GPU?????



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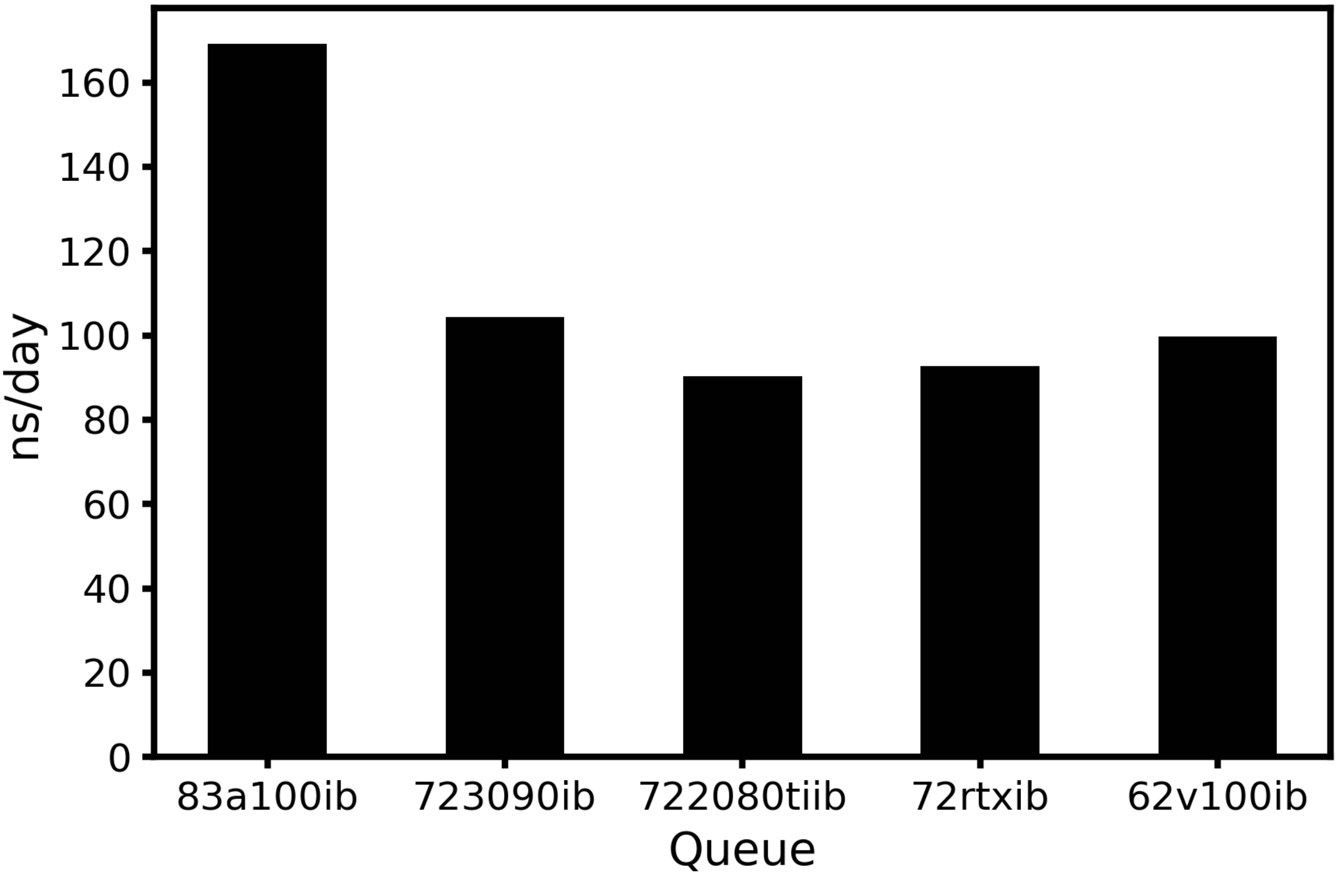
```
ATOM  102808(464 residues, 9nt DNA, 31709 SOL, 94 NA, 94 CL)
nsteps      = 25000000     ;50 ns
```

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



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

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□□□ 2019□□□□□□□□□□□□□□□□□□ GPU□□□□□□ 2021

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

????

```
#BSUB -q GPU_QUEUE
#BSUB -gpu "num=1"
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>□#
□□□□□□□□GPU□□
```

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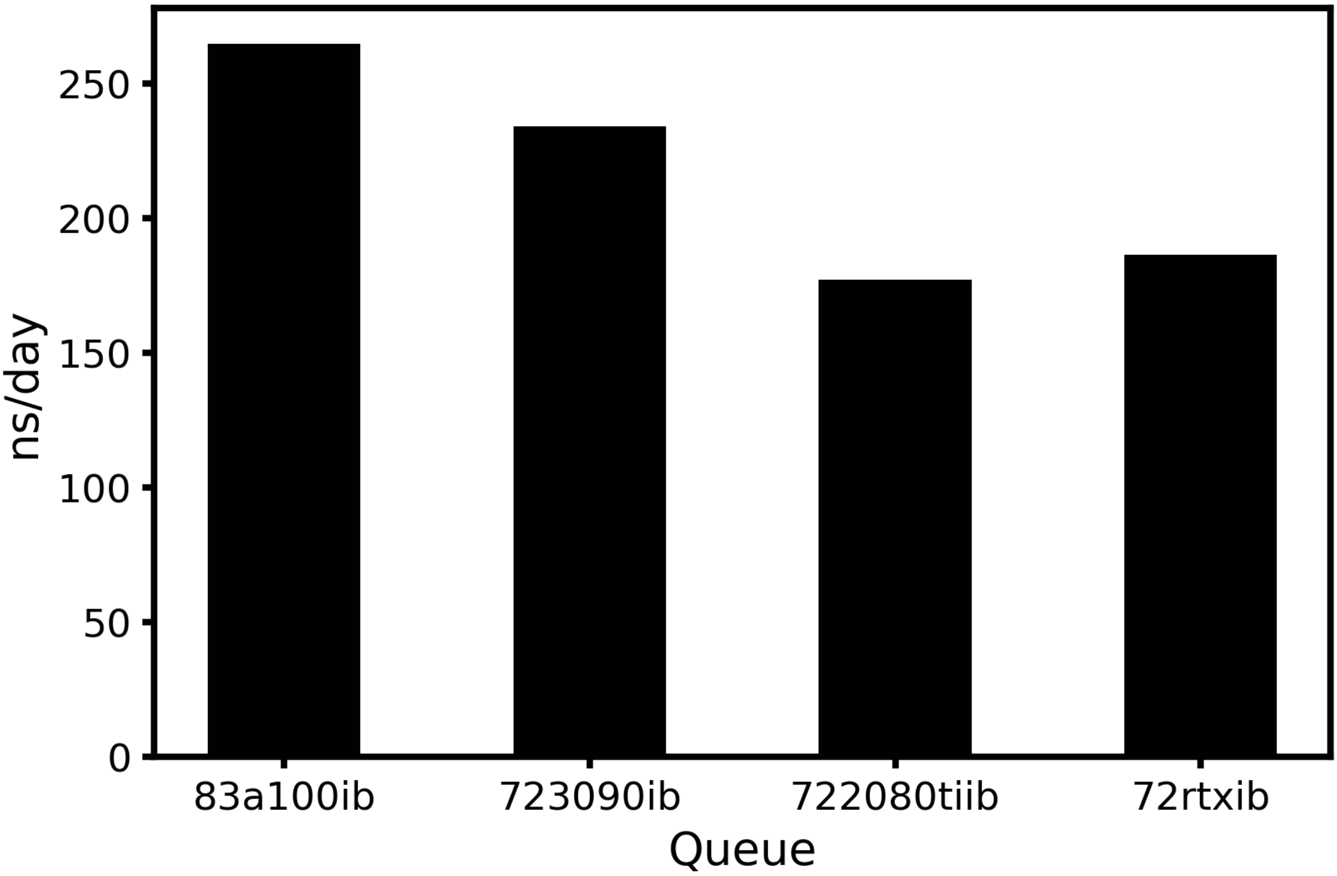
```
ATOM  102808(464 residues, 9nt DNA, 31709 SOL, 94 NA, 94 CL)
nsteps      = 25000000     ;50 ns
```

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



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1. □□ GPU□□□□□□□□□ GPU+CPU□□□□□□□□□□□□□□□ CPU □□□□□□□□□□ GPU□□□□□□□□□□

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□□ GPU□□□□□ CPU□□

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

Revision #24
Created 2021-11-16 15:18:31 CST by Yao Ge
Updated 2024-12-31 09:53:47 CST by Yao Ge