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HPC Sample Job: Gromacs

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Overview

Gromacs can be run using four main classes of resources:

- small jobs using CPU cores in a single computer,
- small jobs using CPU cores and 1-2 GPUs in a single computer,
- large jobs using CPU cores in multiple computers connected over a network, and
- large jobs using CPU cores and 1-2 GPUs per computer in multiple computers connected over a network.

Input files for all the examples below are from the [HECBioSim](#) project's benchmark suite.

Refer to the [Slurm Quick Start User Guide](#) for more information on Slurm scripts.

Single-computer, non-GPU Gromacs Job

Working from the HECBioSim 20k atom model, create a Slurm job script named `gromacs_multicore.sh` to run the job:

gromacs_multicore.sh

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --cpus-per-task=28

INPUT=bench.tpr
OUTPUT=bench.log
module load gromacs
gmxdrun -nt ${SLURM_CPUS_PER_TASK} -s ${INPUT} -g ${OUTPUT}
```

Submit the job from the login node with the command `sbatch gromacs_multicore.sh`, and when the job completes, you should have several new files and `bench.log`, containing the Gromacs output.

Final directory listing for Gromacs multicore job

[Expand source](#)

Single-computer, GPU-enabled Gromacs Job

Working from the HECBioSim 20k atom model, edit the file `_bench.mdp` to adding a line ensuring that Gromacs uses the `verlet` cutoff scheme:

Section of Gromacs input file

```
cutoff-scheme = verlet
```

and changing the line:

Section of Gromacs input file

```
rcoulomb = 1.4
```

to:

Section of Gromacs input file

```
rcoulomb = 1.2
```

to match the `rvdw` setting.

Regenerate the Gromacs `.tpr` file from the HECBioSim topology file and your updated molecular dynamics parameters file:

```
gmxdump -f _bench.mdp -c bench.tpr -p 3NIR.top -o bench_gpu.tpr
```

Create a Slurm job script named `gromacs_gpu.sh` to run the job (the `--cpus-per-task` flag has been adjusted from 28 to 16 as one solution to how Gromacs will divide up the job):



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gromacs_gpu.sh

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --cpus-per-task=16
#SBATCH --gres=gpu:2

INPUT=bench_gpu.tpr
OUTPUT=bench_gpu.log
module load cuda80/toolkit gromacs
gmh mdrun -nt ${SLURM_CPUS_PER_TASK} -s ${INPUT} -g ${OUTPUT}
```

Submit the job from the login node with the command `sbathch gromacs_gpu.sh`, and when the job completes, you should have several new files and `bench_gpu.log`, containing the Gromacs output.

Final directory listing for Gromacs GPU job

[Expand source](#)

Multi-computer, non-GPU Gromacs Job

Working from the HECBioSim 20k atom model, create a Slurm job script named `gromacs_mpi.sh` to run the job:

gromacs_mpi.sh

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=2
#SBATCH --cpus-per-task=4

INPUT=bench_gpu.tpr
OUTPUT=bench_mpi.log
module load gromacs
mpirun `which mdrun_mpi` -ntomp ${SLURM_CPUS_PER_TASK} -s ${INPUT} -g ${OUTPUT}
```

Submit the job from the login node with the command `sbathch gromacs_mpi.sh`, and when the job completes, you should have several new files and `bench_mpi.log`, containing the Gromacs output.

Final directory listing for Gromacs MPI job

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Multi-computer, GPU-enabled Gromacs Job

Working from the HECBioSim 20k atom model, edit the file `_bench.mdp` to adding a line ensuring that Gromacs uses the `verlet` cutoff scheme:

Section of Gromacs input file

cutoff-scheme = verlet

and changing the line:

Section of Gromacs input file

rcoulomb = 1.4

to:

Section of Gromacs input file

rcoulomb = 1.2

to match the `rvdw` setting.

Regenerate the Gromacs `.tpr` file from the HECBioSim topology file and your updated molecular dynamics parameters file:

```
gmh grompp -f _bench.mdp -c bench.tpr -p 3NIR.top -o bench_mpi_gpu.tpr
```

Create a Slurm job script named `gromacs_mpi_gpu.sh` to run the job (the `--cpus-per-task` flag has been adjusted from 28 to 8 as one solution to how Gromacs will divide up the job):

gromacs_mpi_gpu.sh

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=2
#SBATCH --cpus-per-task=8
```



QUESTIONS? ASK AWESOME

```

#SBATCH --gres=gpu:2

INPUT=bench_gpu.tpr
OUTPUT=bench_mpi_gpu.log
module load cuda80/toolkit gromacs
mpirun `which mdrun_mpi` -ntomp ${SLURM_CPUS_PER_TASK} -s ${INPUT} -g ${OUTPUT}

```

Submit the job from the login node with the command `sbatch gromacs_mpi_gpu.sh`, and when the job completes, you should have several new files and `bench_mpi_gpu.log`, containing the Gromacs output.

Final directory listing for Gromacs MPI GPU job
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Improving Performance for Gromacs Jobs

Please read the Gromacs documentation section [Getting good performance from mdrun](#) for more information about benchmarking Gromacs and improving your job runtimes.

Though it's assumed that adding more processors to a given job will automatically increase performance, various model sizes will reach peak performance with different processor counts. Additionally, simply adding minimal GPU support to an input file might not improve performance without more extensive changes.

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