Multiscale modeling 2

Panov Mikhail

26 декабря 2024 г.

Содержание

1 Part 1

I ran scripts from [this link](https://group.miletic.net/en/tutorials/gromacs/1-tip4pew-water/) and processed the output to get images of potential energy, temperature, pressure, and diffusion coefficient.

1.1 Graphs

Scales are not the same as in examples but shapes of the graphs look correct.
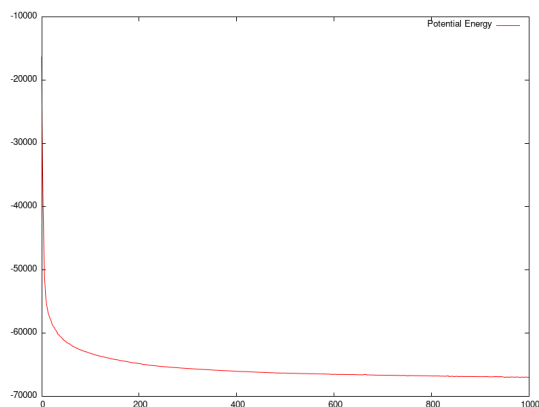

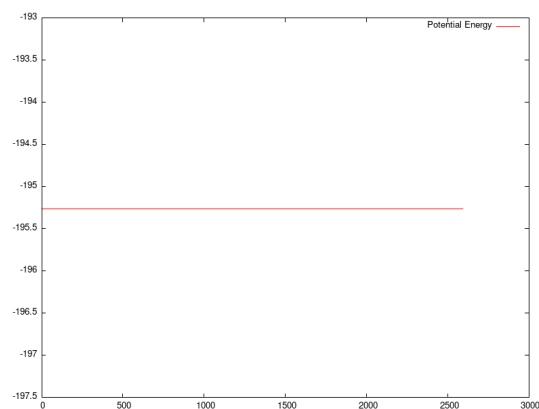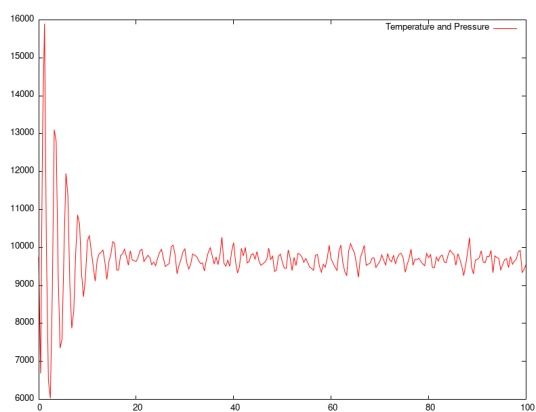
Рис. 1: Potential Energy 1

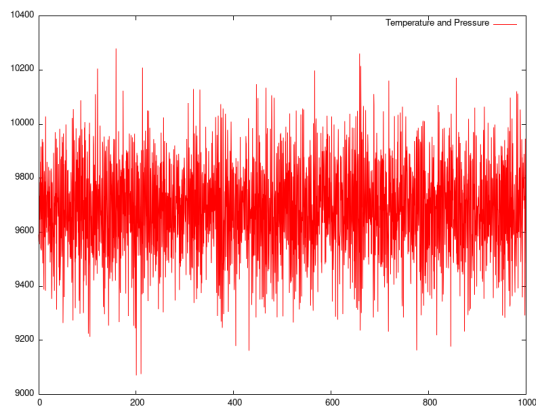Рис. 2: Potential Energy 2
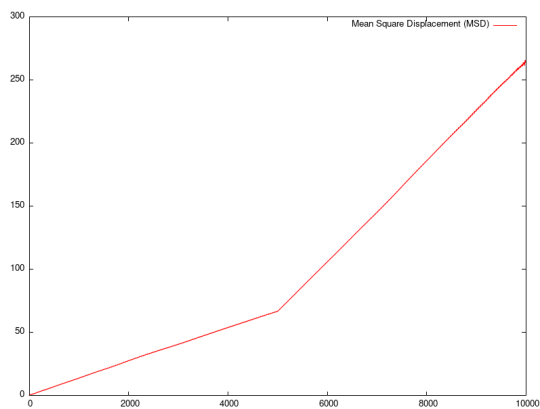
Рис. 3: Temperature

Рис. 4: Pressure

Рис. 5: Diffusion Coefficient

3

1.2   Output Files

Output SLURM files should be attached to the PDF. If any additional files, such as SBATCH, bash, or configuration files, are needed, they are available on the supercomputer and can be provided upon request.

2   Part 2

Results are mostly strange. One core performances are better than any multicore probes by far. All jobs showed very bad scale with number of cores. Single core results are not showed on the graphs below because they would be so high that all other scores would be indistinguishable.
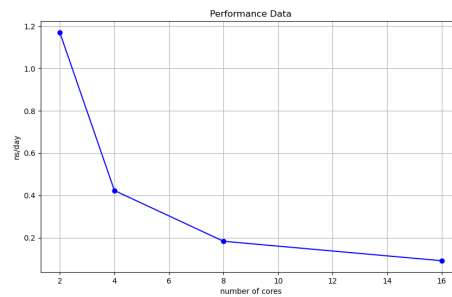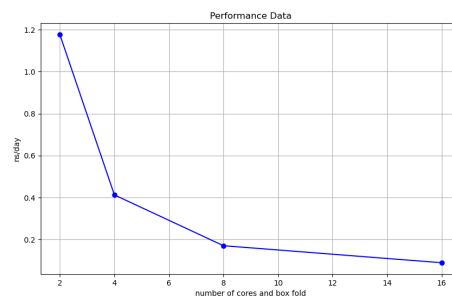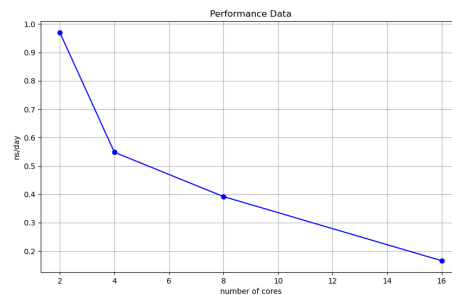

Рис. 6: Strong scaling

Рис. 7: Weak scaling

Рис. 8: Fixed 18832 particles GPU