Molecular dynamics applications on modern heterogeneous systems

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Classical molecular dynamics applications show significant performance increase using graphics accelerators (GPUs), which provides the best price-performance ratio on modern general-purpose systems [1]. For a long time, the "default" GPU platform was Nvidia CUDA, but now there are strong competitors—new exascale systems are being built on AMD and Intel hardware, which indicates the importance of performance portability research. LAMMPS implements GPU acceleration using two modules, Kokkos [2] and GPU [3], which embody two different approaches to portability. Kokkos provides high-level abstractions for algorithms and minimizes data transfer between the GPU and the main memory, while the GPU-module implements portability at the preprocessing level and at each timestep it perform data exchange. Both modules allow one to compile the code to run on AMD and Nvidia hardware. AMD ROCm support was added to the GPU module in our previous work [4]. The report will provide a comparative overview of approaches to portable heterogeneous computing in MD applications and a comparison of performance using the benchmark model as an example. The study was implemented in the framework of the Basic Research Program at the HSE University in 2022.

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