Graphics processing unit portability of atomistic modeling codes

Nikolskiy V P[1,2,@] **and Stegailov V V**[1,2]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vnikolskiy@hse.ru

LAMMPS [1], GROMACS [2] and OpenMM [3] provide support for CUDA and OpenCL technologies. The new ROCm HIP technology delivers maximum performance on AMD graphics processing units (GPUs). In our recent work [4], a backend for ROCm HIP was added to LAMMPS. In this study, platform-dependent errors in the source code of the LAMMPS package were found and fixed. There was found a huge increase in memory consumption using the Tersoff potential with OpenCL, which severely limits the available size of systems. To solve this, a cross-platform implementation of the radix sorting algorithm for the GPU was created, which allowed us to transfer the calculation of the neighbors lists to the GPU. This reduced the memory consumption of the Tersoff model by 6 times. To provide the ability to compile the OpenCL backend on modern AMD accelerators, corrections were made in this work to improve compliance with the OpenCL 2.0 standard. Porting of the VASP [5] package to the ROCm HIP framework for using AMD hardware is discussed. The main part of the code is written in Fortran, the part related to CUDA is written in C and uses the old versions of cublas and cufft libraries. The talk describes a method of adapting such code for AMD infrastructure.

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[2] Abraham M J *et al* 2015 *SoftwareX* **1–2** 19–25
[3] Eastman P *et al* 2017 *PLOS Computational Biology* **13** 1–17
[4] Kuznetsov E *et al* 2020 Performance and portability of state-of-art molecular dynamics software on modern gpus *Parallel Processing and Applied Mathematics* (Cham) pp 324–334
[5] Hafner J 2008 *J. Comput. Chem.* **29** 2044–2078