Analysis of parallel molecular dynamics for MPI, CUDA and CUDA-MPI implementation

Utkin A V
Khristianovich Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences, Institutskaya 4/1, Novosibirsk 630090, Russia
utkin@itam.nsc.ru

One of the most difficult issues in molecular dynamic modelling is a large computation time of the task even for relatively small systems of atoms. The main method of solving this problem is implementation of highly efficient parallel codes. In the framework of current study three implementations of parallel MD algorithms were compared. The first approach was based on design of highly parallel program for a computer cluster with distributed memory using Message Passing Interface (MPI). The second type of parallel algorithms was implemented on CUDA based General Purpose GPUs by NVIDIA. It should be noted, that modern high performance computing systems are a combination of MPI clusters equipped with GPGPUs, what turns them into so-called heterogeneous computing clusters. In this case MPI technology is used for internode communications, while all computations are carried out by GPUs. Thus, the third approach to the parallelization discussed in this study was based on design of a CUDA-MPI algorithm. The detailed studies and comparison of all three approaches (MPI, CUDA and CUDA-MPI) were performed in order to define optimal parameters and conditions of applicability of each algorithm.