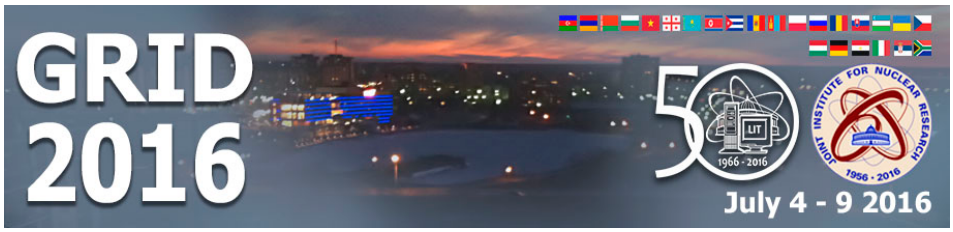

Contribution ID: **140** Type: **Sectional reports**

Comparison of CPU and GPU performance for the charge-transfer simulation in the 1D molecular chains

Thursday 7 July 2016 17:00 (15 minutes)

The process of charge transfer in biopolymers is modeled by specific ODE system. To estimate the thermodynamic properties of the model, we use direct simulation - calculation of the set of trajectories and averaging over ensemble. Such calculations require a lot of computer time. We compared the three program realization, using MPI, openMP, and GPU technology.

At present, attention of researchers attracts possible application of biological macromolecules in nanobioelectronics, especially DNA, for example, in the development of electronic biochips and use as molecular wires. Therefore, the study of thermodynamic characteristics and conducting properties of biopolymers is of interest [1,2].
The model of charge transfer along the chain of sites is described by the self-consistent system of ODE. To simulate thermostat, we add friction term and random value with special properties in the right-hand side (Langevin equation). In computationally, the resource-intensive part of the problem is the calculation of a large number of samples (the dynamics of the charge distribution from the different initial data and with different values of the random force), since the accuracy of the mean is proportional to the square root of the simulation amount. Such task imply the natural parallelization "one sample - one core" using MPI technology.
The problem of attaining the thermodynamic equilibrium can require huge integration time [3]. To reduce the computation time, we have studied the possibility of paralleling using openMP, and program realization based on GPUs with NVIDIA CUDA technology.
Although explicit iterative method use for numerical integration of the ODE system, but the equations includes explicitly only the nearest neighbors. So we can "divide" the chain into several fragments, which are integrated in one step independently on different cores with openMP. To realize the GPU program version, we assemble a single array of several implementations with dividers - Resettable sites. Number of samples depends on the amount of sites in the chain. Due to hardware multithreading operations, calculations are carried out in parallel simultaneously on all components of the vector.
The results of tests and comparison of the performance of these three program realizations are discussed.
The work was done with partial support from the Russian Foundation for Basic Research, projects No. 16-07-00305, 14-07-00894, 15-07-06426, and Russian Science Foundation, project 16-11-10163.

[1] Nanobioelectronics - for Electronics, Biology, and Medicine. Eds. Offenhousser A., Rinaldi R. New York: Springer, 337 p., 2009.
[2] Lakhno V.D.: DNA nanobioelectronics. International Journal of Quantum Chemistry, 108 (11): 1970-1981, 2008.
[3] Lakhno V.D., Fialko N.S. On the dynamics of a polaron in a classical chain with finite temperature. JETP, 120: P.125-131, 2015.

Authors: SOBOLEV, E (Institute of Mathematical Problems of Biology RAS - the Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences.); LIKHACHEV, I (Institute of Mathematical Problems of Biology RAS - the Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences.); Dr FIALKO, Nadezhda (Institute of Mathematical Problems of Biology RAS –the Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences)

Presenter: Dr FIALKO, Nadezhda (Institute of Mathematical Problems of Biology RAS –the Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences)

Session Classification: 4. Scientific, Industry and Business Applications in Distributed Computing System

Track Classification: 4. Scientific, industry and business applications in distributed computing systems