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Parallelization in the modeling of dynamics of a polaron in a constant electric field along molecular chain in Langevin thermostat

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Charge transfer processes in biopolymers such as DNA are actively investigated using mathematical and computer modeling. A large number of works are devoted to studies of polaron mechanism of charge transfer. We have modeled the dynamics of Holstain polaron in a chain with small random perturbations and under the influence of a constant electric field.

In the semi-classical Holstein model the region of existence of polarons in the thermodynamic equilibrium state depends not only on the temperature but also on the chain length. Therefore when we compute the dynamics from the initial polaron data, the mean displacement of the charge mass center differs for different-length chains at the same temperature. For a large radius polaron, it is shown numerically that the "mean polaron displacement"(which takes account only of the polaron peak and its position) behaves similarly for different-length chains during the time when the polaron persists. A similar slope of the polaron displacement enables one to find the polaron mean velocity and, by analogy with the charge mobility, assess the "polaron mobility".

For a temperature prescribed, we compute a set of realizations (dynamics of the system from different initial data and with different pseudo-random time-series) and then calculate trajectories averaged over realizations. This formulation allows for trivial parallelization (using MPI) "one realization –one node"with an efficiency of almost 100%.

To reduce the calculation time, parallelization was performed on a node containing multi-core processors when calculating a realization using shared memory and openMP. The dynamic equations for the n-th site of the chain explicitly include only its closest neighbors. Therefore, the chain is divided into short parts that are integrated at the step independently on different cores of the node, while only for the boundary sites the data calculated by other processes are required. All processes must go to the next iteration synchronously; the synchronization operation also takes time. The longer the chain, the smaller the ratio of exchanged data to calculated data, and the greater the gain from parallelization.

Test studies of the gain t1/tp were made (t1 denotes the execution time of the sequential variant, tp denotes the execution time of the task parallelized using openMP on p threads). Maximum t1/tp ~ 0.9 p allows to significantly reduce the machine time of a realization.

The calculations were performed on the supercomputers k-60 and k-100 installed in the Supercomputer Centre of Collective Usage of KIAM RAS

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