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PARALLEL EVOLUTIONARY ALGORITHM IN HIGH-DIMENSIONAL OPTIMIZATION PROBLEM

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An implementation of a combined evolutionary algorithm for searching of an extremum of functions with many parameters is proposed. The algorithm is designed to optimize parameters of the molecular-dynamics reactive force field potential ReaxFF. It can be efficient for a variety of extremum searching problems with arbitrary complex objective function. The algorithm itself is a hybrid of two evolutionary methods: Genetic Algorithm which uses the principle of a natural selection in the population of individuals, and the Particle Swarm Optimization, which imitates the self-organization of the particle swarm. Individuals in a population as well as swarm particles can be considered as trial solution vectors. Combination of these two methods provides one with a possibility to work with objective functions with an unknown complex structure which often has a composition of specific peculiarities insurmountable by simple algorithms.

Genetic Algorithm parameterizations regarding choosing its main strategies for computations with different objective functions has been analyzed. Results for the classical test functions convergence speed testing are presented. Effectiveness of the algorithm working on the platform of the computational system with shared memory and on the platform of the distributed system has been compared. Good scalability of implemented algorithm is demonstrated for the distributed computational systems.

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