THE EFFECTIVENESS OF MONTE CARLO ALGORITHMS USED TO CALCULATE THE KINETICS OF CHEMICAL REACTIONS

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Microscopic stochastic models are most common model describing the dynamic of systems with probabilistic nature of interactions, such as chemical reactions. Evolution of the system calculated by Monte Carlo methods in accordance with the basic process has defined by kinetic scheme. In contrast to mathematical models based on differential equations, microscopic models don't require conditions for application of the mean-field and allow us to study macroscopic behavior of the system, based on micro level.

The main challenge of using it is huge dimension of the lattice model, and therefore the request of computing resources for the Monte Carlo method. It's more important to find efficient algorithms for extend the application of the microscopic stochastic models.

In this work[1] we considered six frequently used Monte Carlo algorithms. The algorithms have been tested in calculation of complex wave dynamics of two heterogeneous catalytic reactions: the reaction $NO+CO/Pt\{100\}$ and Lotka-Volterra reaction. We estimated complexity and performance of each method.

Studies have shown that the computation time can vary by 2-3 order of magnitude, and the most popular Monte Carlo methods are not optimal. The most effective method was the lesser-known multi-level method based on the tree-structure [1]. Oscillatory dynamics of systems on lattices up to 4 million cells was investigated with this algorithm. The mechanism of nucleation of macroscopic fluctuations in micro level was clarified [2].

References.

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