Simulation of the critical behavior of a complex spin systems by the parallel Wang-Landau method

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The computer simulation of a complex spin systems is actual area of theoretical physics research and it requires a lot of supercomputer resources (as much as there is). Last time we have wide range of algorithms to explore the critical behavior of a complex spin systems. One of them is the Wang-Landau method [1] that have few advantages relative to other Monte Carlo methods like Metropolis and cluster algorithms. There are no critical slowing down effect and wide range of applications e.g. exploring of polymer chains, protein folding, phase transitions in spin glasses. The Wang-Landau algorithm based on random walking at the energy space of spin system, and, when the energy space is large enough (especially for three-dimensional Heisenberg system), it can be observed the divergence of the algorithm and the modeling time tends to infinity, because histogram of energy levels visits will never be flat. To break those constraints the energy space can be divided on the subinterval by few replicas [2]. This approach will allow to beat divergence.

In this work we investigate the critical behavior of the three dimensional Heisenberg spin system model by serial and parallel Wang-Landau algorithm developed with use of OpenMP technology and we observe how resulting density of energy states, thermodynamical quantities and estimation time changed with the use of parallel method. Important question is about how effective this method relative to classical algorithms [3] e.g. Metropolis on three-dimensional Heisenberg model and can we use Wang-Landau method to explore properties of thin-film structures?

Most of the supercomputer systems have a lot of the computational cores and threads. Modern supercomputers often have hybrid architecture and scientists use GPUs to reduce the simulation time [4]. Therefore, we need to develop parallel methods of existing Monte Carlo algorithms to explore large and complex spin system, thin-films and multilayer structures.

This research was supported by the grants 17-02-00279, 18-53-00003 of Russian Foundation of Basic Research and by the grant MD-6868.2018.2 of Russian Federation President. The simulations were supported in through computational resources provided by the Shared Facility Center “Data Center of FEB RAS” (Khabarovsk).

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