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Hybrid Monte Carlo algorithm for studying the Edwards-Anderson model

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Abstract: The complexity of the study of spin glasses is related to their frustrations, due to which classical Monte Carlo algorithms experience serious difficulties when trying to calculate such systems. The main object of research in this paper is two-dimensional Edwards-Anderson model on a square lattice. In the paper, we propose an optimized Hybrid Monte Carlo method for calculating the values of thermodynamic averages and ground state energies of the frustrated spin glass model. The validity of the results is confirmed by comparison with numerical simulation with the parallel tempering Monte Carlo method, complete enumeration algorithm and robust machine learning approach-RBM neural network. The proposed algorithm has a number of advantages: possible high parallelization of the algorithm to speed up simulation, calculation accuracy and low resource consumption, which allows to calculate lattices of relatively large size. This algorithm can be applied to calculations of lattices with different geometry and sizes.

Keywords: Edwards-Anderson model, Monte Carlo algorithm, ground state, frustration

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Гибридный алгоритм Монте-Карло для изучения модели Эдвардса-Андерсона

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Аннотация. Сложность исследования спиновых стекол связана с фрустрациями, из-за которых классические алгоритмы Монте-Карло испытывают серьезные трудности

при попытке расчета таких систем. Основным объектом исследования в данной работе является двумерная модель Эдвардса-Андерсона на квадратной решетке. В работе предложен оптимизированный гибридный метод Монте-Карло для расчета значений термодинамических средних и энергий основного состояния модели фрустрированного спинового стекла. Достоверность результатов подтверждается сравнением с численным моделированием с помощью параллельного отжига методом Монте-Карло, алгоритмом полного перебора и надежным алгоритмом машинного обучения - нейронной сети RBM. Предложенный алгоритм обладает рядом преимуществ: возможность параллелизации алгоритма для ускорения моделирования, точность расчетов и низкое потребление ресурсов, что позволяет рассчитывать решетки относительно большого размера. Данный алгоритм может быть применен для расчета решеток с различной геометрией и размерами.

Ключевые слова: модель Эдвардса-Андерсона, алгоритм Монте-Карло, основное состояние, фрустрации

Финансирование: Исследование гибридного алгоритма и разработка алгоритма численного расчета в целом проводились при финансовой поддержке гранта Президента Российской Федерации для государственной поддержки ведущих научных школ Российской Федерации (НШ-2559.2022.1.2). Разработка компьютерной программы и кодирование эффективного параллельного кода проводились в рамках государственного задания Министерства науки и высшего образования Российской Федерации (№ 0657-2020-0005).

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Introduction

Nowadays, frustrated spin systems, such as spin glasses and ices, are actively studied in modern condensed matter physics [1–3]. In such models, frustrations arise due to the special lattice topology or the competition of exchange interactions, which leads to the search for new magnetic ground states and unique effects that can arise.

Spin glasses are disordered magnetics, which are characterized by two unique properties that greatly distinguish these systems from others: in such systems there is strong competition between ferromagnetic and antiferromagnetic interactions, i.e., frustrations, and disorder, which is freezing (or solidifying) of atoms in different locations during alloy formation. Many processes occurring in spin glasses cannot be described within the framework of the classical theory of phase transitions and require some new non-standard approaches.

The process of reaching the ground states and studying the thermodynamic properties even in the simplest model, the Ising model, is associated with serious difficulties in theoretical analysis and numerical calculations. This problem is much more complicated than it seems at first sight. Creating an efficient algorithm for finding the ground states is one of the main challenges in the theory of frustrated magnetism.

The classical Monte Carlo algorithm and its many optimizations have their drawbacks. Single-spin sampling methods near critical points drastically lose in efficiency, the so-called ‘critical slowdown’ occurs. In addition, at very low temperatures, only a small fraction of spins makes a flip. The motion of the system in phase space is very slow, so the system requires generation of a very large number of states to move to an equilibrium state. In turn, the use of multicanonical methods has difficulties in calculating the thermodynamics of systems with a relatively large number of spins.

To solve the problem of searching for thermodynamics of frustrated models of many interacting bodies, as well as to search for ground state configurations, a new hybrid multispin method is applied, which is a logical continuation of the Metropolis algorithm.

Edwards-Anderson model

The main object of research in this paper is two-dimensional Edwards-Anderson model on a square lattice (see Fig. 1). Edwards and Anderson proposed in [4] to change the distribution function of the exchange interaction to a more complex one, where the exchange integral J_{ij} is a random function and the average value of J_{ij} is equal to zero. In such systems, half of the spins has ferromagnetic interaction with its nearest neighbors, and the other part is antiferromagnetic one.

The interaction J_{ij} between the spin pair (ij) changes during the transition from one pair to another. The Hamiltonian is then expressed as:

$$H = -\sum_{i,j} J_{i,j} S_i S_j - h\sum_i S_i, \tag{1}$$

S_i, S_j are the spins in lattice, $\langle i,j\rangle$ denotes summation over pairs of interacting spins in a system with the size N, h is the external magnetic field. Edwards and Anderson suggested in [4] that each J_{ij} distributed independently according to the probability distribution $P(J_{ij})$. In this work, we have used the bimodal distribution, i.e., the amount of positive and negative bond values is equal.

The average energy of the spin glass model at temperature T is calculated by Eq. (2) and the average magnetization by Eq. (3).

$$E(T) = \frac{1}{N}\langle H\rangle_T, \tag{2}$$

$$M(T) = \frac{1}{N}\left\langle \sum_i S_i \right\rangle_T. \tag{3}$$

Based on these two main characteristics, we can calculate the various thermodynamic properties, such as magnetic susceptibility (4) and specific heat (5)

$$\chi(T) = \frac{1}{N}\frac{\left\langle |M|^2 \right\rangle - \left\langle |M| \right\rangle^2}{k_B T}, \tag{4}$$

$$C(T) = \frac{1}{N}\frac{\left\langle E^2 \right\rangle - \left\langle E \right\rangle^2}{k_B T^2}. \tag{5}$$

In this study, we investigated models on the square lattice with different number of spins, such as $N = 6\times6$, 10×10, 20×20, 30×30.

Parallel Hybrid Monte-Carlo Algorithm:

Initially, the hybrid algorithm was proposed for field theory studies on a lattice with fermionic degrees of freedom [5]. Subsequently, this algorithm was transferred and adapted for various problems [6, 7]. More recently, we proposed an approach for studying the temperature behavior of the frustration parameter in a geometrically frustrated hexagonal lattice [8]. It is based on combining the canonical and multicanonical sampling of the Gibbs distribution.

However, after comparing the results of the algorithm with the complete enumeration method, it turned out that as the size of the systems increased, the algorithm did not arrive at the ground state. For this reason, the algorithm was optimized and reduced to the form presented below.

- → random *spins* and bonds initialization
- → **for** all *threads* do
  - → choosing random *spin* in the system
    if *cluster* borders are not crossing **then**
    - → copy cluster spin array to private memory
    - → **for** $2*N_c$ steps **do**
      - → **for** every *spin* in the *cluster* **do**
        - → current spin value = ((counter >> $2*Nc$ −1) & 1)
        - → **if** new energy<previous energy **then**
          - → save current configuration as minimal configuration
  - →collect *spin* values in main system array
- → ground state and thermodynamics calculation.

Results and Discussion

To demonstrate the work of the algorithm, we compare its accuracy with different methods [9–11], such as complete enumeration algorithm, ML approach using RBM, see Table 1. Algorithms were tested on a square lattice of the two-dimensional Edwards-Anderson model, with number of spins $N = 6\times6$, 10×10, 20×20, 30×30. As can be seen from the table, proposed hybrid Monte Carlo algorithm demonstrates the same accuracy as the complete enumeration algorithm, but, unlike the latter, it is much less resource-intensive, which allows us to calculate larger systems.

Table 1

Comparison of results obtained by different computational approaches

System size	E_{min}		
	CE	HM	RBM
6 x 6	–1.30	–1.30	–1.30
10 x 10	–	–1.40	–1.40
20 x 20	–	–1.38	–1.38
30 x 30	–	–1.34	–1.34

In contrast to the other algorithms presented in Table 1, the hybrid Monte Carlo algorithm can be used to study other important properties of the system, such as the dependence of the staggered magnetization and the system degeneracy multiplicity on the external magnetic field. It also allows the calculation of basic thermodynamic quantities such as heat capacity and magnetic susceptibility. A comparative graph of the dependence of heat capacity on temperature is shown in Fig. 1. We checked the accuracy of the proposed algorithm by comparing it with the parallel tempering (PT) method, which has proved [12–14] to be excellent for such problems.

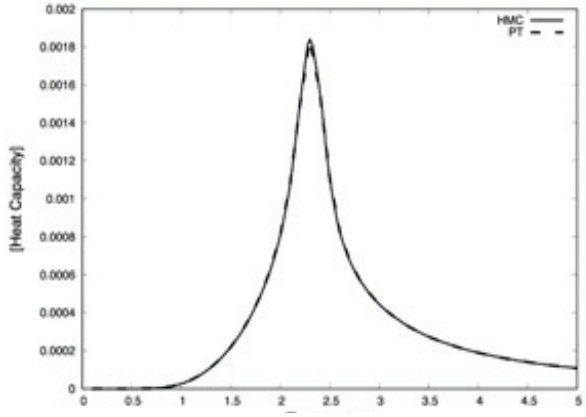

Fig. 1. Dependence of heat capacity on temperature according to Edwards-Anderson with $N = 20\times20$, obtained by Hybrid Monte Carlo (HMC) and Parallel Tempering (PT) algorithms

Based on the values obtained, we can conclude that the optimized hybrid Monte Carlo algorithm is well adapted to searching for the main states of complex lattices, as well as to the calculation of the main thermodynamic characteristics.

Conclusion

In this work, we proposed and implemented an optimization of a hybrid Monte Carlo algorithm. Using this method, various important characteristics on spin glass lattices with different numbers of spins were obtained, such as: energy of ground states, dependence of heat capacity and susceptibility on temperature. The validity of the obtained results was validated using well-proven algorithms. Due to its accuracy and versatility, this algorithm can be used to study systems with a large number of spins and different lattice geometries.

REFERENCES

1. **Belokon V., Kapitan V., Dyachenko O.,** The combination of the random interaction fields' method and the Bethe-Peierls method for studying two-sublattice magnets, Journal of Magnetism and Magnetic Materials. 401 (1) (2016) 651–655.

2. **Kapitan V. Y., Nefedev K. V.,** Labyrinth Domain Structure in the Models with Long-range Interaction, Journal of Nano-& Electronic Physics. 6 (3) (2014) 03005-1-03005-4.

3. **Nefedev K. V., Kapitan V. Y.,** Concentration phase transition and hysteresis phenomena in Co-nanofilms. Computer data processing and simulation, Advanced Materials Research. 718 (1) (2013) 69–73.

4. **Edwards S., Anderson P.,** Theory of spin glasses, Journal of Physics F: Metal Physics. 5 (5) (1975) 965–974.

5. **Duane S., Kennedy A., Pendleton B., Roweth D.,** Hybrid Monte Carlo, Phys. Lett. B. 195 (2) (1987) 216–222.

6. **Efendiev Y., Zachariah M.,** Hybrid Monte Carlo Method for Simulation of Two-Component Aerosol Coagulation and Phase Segregation, Journal of Colloid and Interface Science. 249 (1) (2002) 30–43.

7. **Nagai Y., Okumura M., Kobayashi K.,** Self-learning hybrid Monte-Carlo: A first-principles approach, Phys. Rev. B. 102 (4) (2020) 041124.

8. **Makarov A., Makarova K., Shevchenko Y., Andriushchenko P., Kapitan V., et al.,** On the numerical calculation of frustrations in the ising model, JETP Letters. 110 (10) (2019) 702–706.

9. **Andriushchenko P., Kapitan D., Kapitan V.,** A New Look at the Spin Glass Problem from a Deep Learning Perspective, Entropy. 24 (5) (2022) 697.

10. **Korol A., Kapitan V., Perzhu A., Padalko M.,** Kapitan D., et al., Calculation of the Ground States of Spin Glasses Using a Restricted Boltzmann Machine, JETP Letters. 115 (8) (2022) 466–470.

11. **Padalko M. A., Shevchenko Y. A., Kapitan V. Y., Nefedev K. V.,** Parallel Computing of Edwards-Anderson Model, Algorithms. 15 (1) (2022) 13.

12. **Hartmann A. K.,** Ground-state clusters of two-, three-, and four-dimensional $\pm j$ ising spin glasses, Phys. Rev. E. 63 (1) (2000) 016106.

13. **Bittner E., Nußbaumer A., Janke W.,** Make life simple: Unleash the full power of the parallel tempering algorithm, Physical review letters. 101 (13) (2008) 130603.

14. **Newman M. E., Barkema G. T.,** Monte Carlo methods in statistical physics, Clarendon Press, 1999.

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