# Optimization of the Hybrid Monte-Carlo Algorithm for the Edwards-Anderson Model

Dmitrii Yu. Kapitan[a,b], Alexey E. Rybin[a,b], Petr D. Andriushchenko[c], Aleksandr G. Makarov[a,b], Yuriy. A. Shevchenko[a,b], Konstantin S. Soldatov[a,b] , Vitalii Yu. Kapitan[a,b] and Konstantin V. Nefedev[a,b]

[a] *Department of Computer Systems, School of Natural Sciences, Far Eastern Federal University, Vladivostok, 690922, 10 Ajax Bay, Russian Federation*
[b] *Institute of Applied Mathematics, Far Eastern Branch, Russian Academy of Science, Vladivostok, 690041, 7 Radio St., Russian Federation*
[c] *ITMO University, Kronverksky Pr. 49, bldg. A, St. Petersburg, 197101, Russian Federation*

**Abstract**

This article describes the principle of using Hybrid Monte-Carlo method in spin glasses using the Edwards-Anderson model as an example. We consider efficient algorithm for searching ground states of frustrated systems. We discuss two optimizations for this algorithm in order to find the most efficient. We implement and test algorithm on a two-dimensional square lattice of Edwards-Anderson model. The advantages of using the Hybrid Monte-Carlo method in spin glasses are revealed.

**Keywords 1**

Hybrid Monte-Carlo algorithm, Spin Glass, Ground State, Edwards-Anderson model

## 1. Introduction

Frustrated magnetic interactions are one of the most fiercely debated topics in condensed matter physics [1, 2]. Interest in spin systems where frustrations, as a result of a special lattice topology or competition exchange interactions, suppresses the Neel antiferromagnetic order is greatly stimulated by the search for new magnetic ground states and unique excitations which can arise instead. A magnetic system with disorder in bonds often exhibits a short-ranged order, indicating that the system cannot form a true thermodynamic ground state and thus becomes frustrated. This state of matter, so-called spin glass, with a multitude of a ground state degeneracy has drawn colossal interest over the past decades.

Spin glasses are disordered magnetics which characterised by two main characteristics that strongly distinguish these systems from others: in such systems there is a strong competition between ferromagnetic and antiferromagnetic interactions, i.e., 'frustrations', and disorder - the freezing (or solidification) of atoms at different locations during alloy formation. These factors provide key features of such structures. In such systems with competing interactions, unlike conventional magnetics, no long-range magnetic order arises with decreasing temperature. But neither does a slow, gradual freezing of spins occur. Spin glasses have long relaxation times and a rough energy landscape, so both analytical description and numerical modelling of such systems is challenging. The processes occurring in such systems cannot be described in terms of classical phase transition theory.

This paper proposes optimized versions of the hybrid algorithm for finding the ground state values of the Edwards-Anderson model.

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EMAIL: kapitan.diu@students.dvfu.ru (Dmitrii Yu. Kapitana)
ORCID: 0000-0001-9815-1891 (Dmitrii Yu. Kapitana)

## 2. Edwards-Anderson model

In 1975 S. Edwards and P. Anderson suggested changing the distribution function of the exchange interaction in the Ising model to a more complex one, such as the one where the exchange integral $J_{ij}$ is a random function and the average value of $J_{ij}$ is zero[3].

The interaction $J_{ij}$ between a spin pair $(ij)$ changes as one goes from one pair to another. The Hamiltonian is then expressed as:

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j \; - \; h \sum_i s_i, \tag{1}$$

where $S_i$, $S_j$ are spins of the system, $\langle i,j \rangle$ denotes summarizing over the lattice with size N, h - external magnetic field. The interaction can be ferromagnetic or antiferromagnetic: in the first case, the interaction arranges spins along one direction; in the second case, the state with antiparallel direction of spins becomes the most advantageous for the system. The exchange interaction can occur directly between a pair of magnetic particles (direct exchange interaction), as well as in the presence of the intermediary particle (indirect exchange interaction). Therefore, the magnitude of the exchange interaction may strongly depend on the lattice geometry (mutual arrangement of atoms) and the distance between spins [4].

## 3. Hybrid Monte-Carlo

Monte Carlo methods, such as the Metropolis or Wang-Landau algorithms, are not only actively used to study various physical systems [5,6,7,8,9] but also continue to actively develop and improve due to current Monte Carlo methods have some weaknesses. Single-spin sampling methods suffer from critical deceleration and applying of multicanonical methods has difficulties in calculating the thermodynamics of relatively large systems. The use of single-spin Monte-Carlo methods (e.g. the Metropolis algorithm) to calculate the ground state of systems with coarse energy landscapes is problematic [10]. To overcome the large energy barriers separating the quasi- degenerated configurations of the frustrated Ising magnetic, which prevent one from finding their energy-preferred low-energy states, applying of quasi-Markov processes in the thermodynamics of multi-spin clusters is required.

To solve the problem of thermodynamics of frustrated vector models of complex systems with many interacting bodies, searching for ground state configurations, we propose new optimizations for the Hybrid multi-spin method, described in [11].

### 3.1. HMC with Monte-Carlo inside kernel

First, authors tried to divide the lattice into sub-lattices with modulation inside such kernels. The algorithm is worked as follows:

- Spin lattice with periodic boundary conditions is created
- For each spin from the lattice the neighbours are defined
- The initial energy calculation is performed
- Spin lattice is divided on several sublattices, as shown in Figure 1
- Inside those small areas Monte Carlo simulation is started
- The configuration with the lowest energy in kernel is taken
- Kernels are moved in lattice
- After the termination of n cycles, the algorithm is stopped

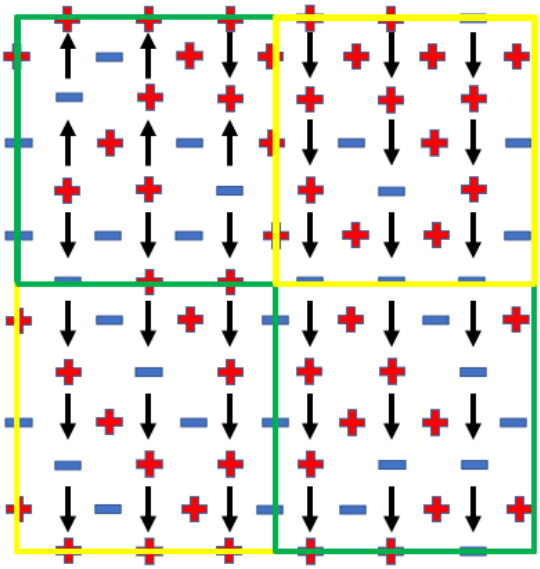

**Figure 1**: Dividing of lattice into sublattices

This algorithm has shown a good efficiency, however accuracy of this method in searching Ground State is still inappropriate. This is the reason for another suggestion.

## 3.2. HMC with exact solution inside kernel

Next assumption was to choose spins as midpoint of kernel with the highest energy. The work of this algorithm is presented below: An example of numbered list is as following.

1. Spin lattice with periodic boundary conditions is created
2. For each spin from the lattice the neighbours are defined
3. The initial energy calculation is performed
4. Spins are randomly chosen from the list of spins with max energy as shown in Figure 2
5. The energy and magnetization of all possible configurations of kernels and the boundary block of spins are computed by brute force algorithm

Step 5 is repeated until thermodynamic equilibrium is reached in the system. The criterion for stopping the algorithm can be a given number of iterations or reaching a given temperature value.

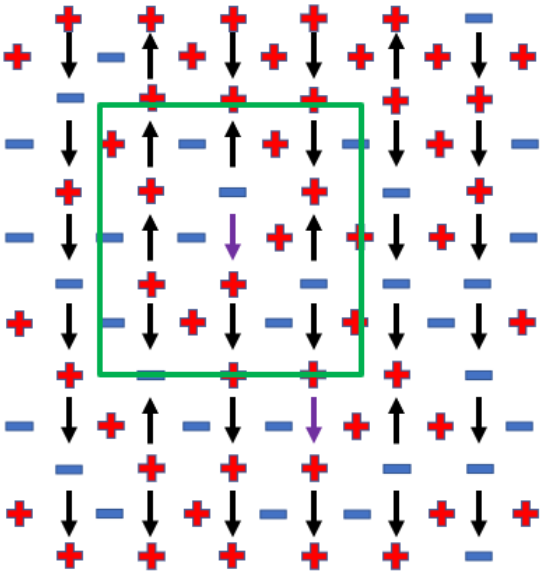

**Figure 2**: Example of choosing a spin with max energy

## 4. Results

To compare the two algorithms, a program was created on the C++. The algorithms were tested on a square lattice of the two-dimensional Edwards-Anderson model, where bonds have had bimodal distribution, i.e. amount of ferromagnetic and antiferromagnetic bonds was equal. To calculate the ground state of different systems, the number of spins was set as N = 6x6, 10x10, 20x20, 30x30. Calculations were carried out for a supercomputer cluster. To compare the results, the data were obtained using the algorithm of exact solution, and the parallel tempering algorithm. The results are showed good potential of Hybrid Monte-Carlo with exact solution in kernel in searching ground states of frustrated models, see Table 1. Hybrid Monte-Carlo with MC in kernel, despite its efficiency, had not shown an appropriate result. This can probably be explained by problems with defining direction of spins on the border between sublattices. After choosing the algorithm, authors started to investigate the behaviour of staggered magnetization as a function of different values of the external magnetic field on the example of Edwards-Anderson model with size N = 6x6. The results were compared to algorithm of exact solution, please, check Table 1 3. Also, authors decided to study the values of the ground state spin excess. The results were compared to algorithm of exact solution, as well, see Table 1 4.

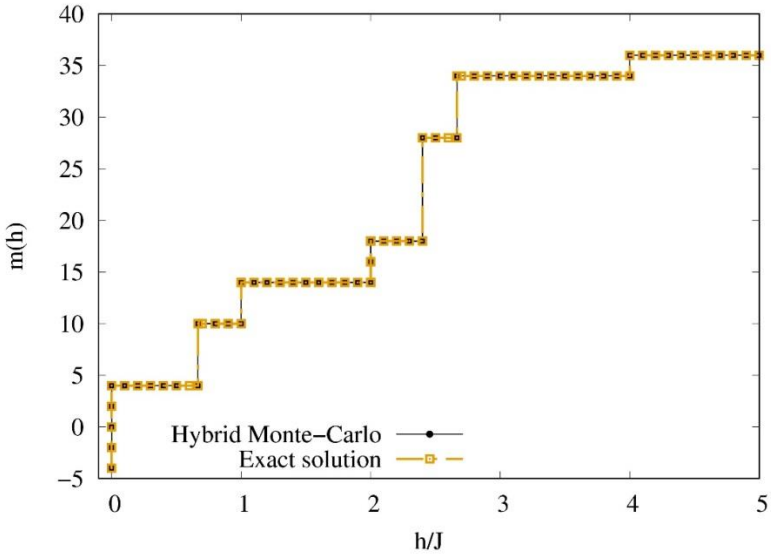


**Figure 3**: Staggered magnetization retrieved from optimized HMC and exact solution for the system with N=6x6

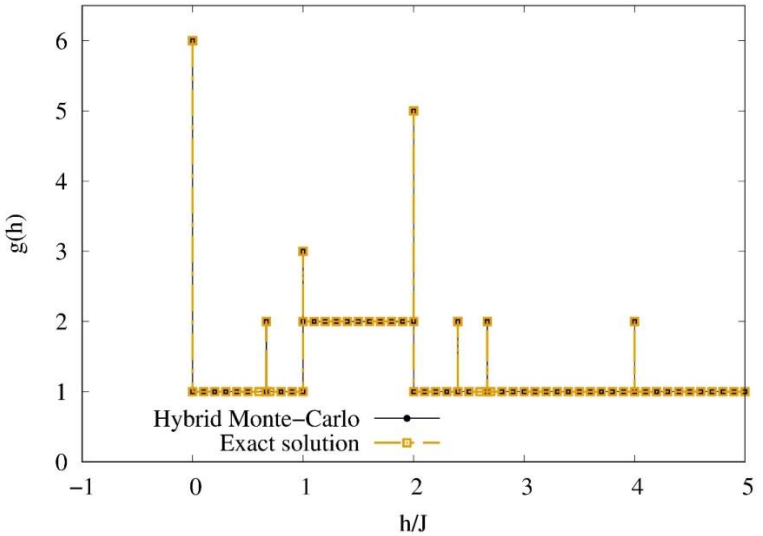


**Figure 4:** Values of the ground state spin excess retrieved from optimized HMC and exact solution for the system with N=6x6

**Table 1**
Comparison of GS values reached by each method

| N | Exact Solution | Parallel Tempering | HMC with MC step in kernel | HMC with exact solution step in kernel |
|---|---|---|---|---|
| 6x6 | -1.50 | -1.27 | -1.33 | -1.50 |
| 10x10 | -1.40 | -1.24 | -1.32 | -1.40 |
| 20x20 | - | -0.98 | -1.06 | -1.34 |
| 30x30 | - | -0.76 | -0.79 | -1.34 |

## 5. Conclusion

In this paper, algorithms were considered for finding ground states in the Edward-Anderson model. Authors looked at Hybrid Monte-Carlo algorithms with different approaches during modulation of kernels: exact solution and Monte-Carlo. A program was also written to compare two algorithms within the framework of the conditions we are interested in. After that, using the best approach key characteristics were calculated. On the basis of the obtained results, it can be concluded that when choosing an algorithm for searching ground states, one should use a Hybrid Monte-Carlo algorithm with exact solution inside kernel.

In the future, the approach can be extended to the case of a complex sign-variable exchange long-range interaction. Also, it is interesting to investigate the ground state of three-dimensional Edwards-Anderson spin glass.

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