Order of updates in Monte Carlo computations of quantum fields

(Supervised by M.J. Peardon)

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The order of updates, in Monte Carlo computations of quantum fields, has been found to have an impact on the accuracy of the correlation function; this impact is dependent on the temperature given to the system. The model analysed was the Ising Model. It was assessed in one, two and three dimensions. New states of the system were produced using the Markov Chain Monte Carlo method and the Metropolis algorithm. The states were divided into bins and averaged over them to reduce the dependence between consecutive states in the chain. The mean correlation function and its standard deviation over the chain were computed. The order of updates was defined, inter alia, by the Hilbert and Lebesgue space-filling curves.

I. INTRODUCTION AND THEORY

In order to effectively carry out numerical analysis of thermodynamic systems as well as quantum fields, it is required to construct a very large, representative sample of systems often called a statistical ensemble. However, the creation of such an ensemble is usually costly and time-consuming. Hence in this report, we propose that the order of updates in simulations of quantum fields affects the efficiency of the computations and examine whether our proposition is true.

The model considered in this analysis is a mathematical model of a ferromagnetic material, the Ising model, named after the physicist Ernst Ising. It consists of points representing magnetic dipoles usually arranged in a lattice. Each site represents a magnetic dipole and can hold a value of ± 1 that imitates the 'spin'. Sites with the same value of the spin are said to be 'parallel' and have lower energy than those that have opposite values i.e. are 'anti-parallel'. Hereunder we consider only the nearest-neighbour interaction, that is, the energy of a system is decided by alignment (or misalignment) of all sites with sites right next to them. The aim of numerical methods that we will use is to approximate the canonical ensemble - a statistical ensemble consisting of all possible states, where the number of particles is fixed and the temperature is specified.

A. Monte Carlo and the Metropolis Algorithm

The technique used to analyse the system is a Markov Chain Monte Carlo (MCMC) method with the Metropolis algorithm which was first proposed in [1].

The Monte Carlo (MC) methods are a broad range of numerical methods that employ repeated random sampling and are most commonly used for numerical integration, optimisation problems, and problems with a probabilistic interpretation. Applying the 'pure' MC method by randomly assigning spins to all sites would give each state an equal probability of occurring, however, this is not the case for real systems. States with lower energies at finite temperatures are more likely to occur than those with higher energies. Hence, it is necessary to consider the energy and temperature when creating a new state. This is done by generating a sequence of states (Markov chain) to average over whose distribution approximates the canonical distribution. The states are generated using the Metropolis algorithm.

The first step is to initialise the lattice by randomly assigning a spin of ± 1 to each site. Then, we choose a dipole and consider 'flipping'/updating it (changing the sign of its spin). If the new energy is lower than the old energy then we accept the change, and if the energy is higher then the probability of accepting this change is weighted by the Boltzmann-like term,

$$p \propto e^{-\beta \Delta U}, \tag{1}$$

where $\beta = \frac{1}{k_b T}$ with k_B being the Boltzmann constant and T the temperature, and ΔU is the change in energy. After completing the process for all points we obtain a new state.

B. Analysis of the Ising Model

The Ising model can be described by the Hamiltonian

$$H(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_i h_i \sigma_i, \tag{2}$$

where σ_i represents the site i and h_i represents an external magnetic field acting on this site. In our case there is no external magnetic field, ergo we can write

$$H(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j. \tag{3}$$

The summation is over all the nearest-neighbour pairs and the term J_{ij} represents the interaction between them.

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To further simplify we can consider ferromagnetic interactions only, $J_{ij} > 0$, and that the interaction is the same between all the sites, i.e. $J_{ij} = J$. (For simplicity we take $J = 1$.) Then the change in energy for a prospective flip of spin σ_i is

$$(\Delta U)_{\sigma_i \to \tilde{\sigma}_i} = 2\sigma_i \sum \sigma_j. \tag{4}$$

It is also noteworthy that periodic boundary conditions were applied.

To analyse the correlation between the sites we define a function

$$F_{i,i+d} = \sum_i \langle \sigma_i \sigma_{i+d} \rangle, \tag{5}$$

where d is the separation between the sites.

For low β we expect weak correlation with the nearest-neighbours ($0 < F_{i,i+1} \ll 1$) and no correlation with other sites ($F_{i,i+d} \approx 0$ for $d \geq 2$). This is because at high-temperature values (low β values), the thermal fluctuations are significant enough and the system is in disorder. For high β we expect a significant correlation between all sites since at low temperatures thermal fluctuations will be too weak to reverse the tendency of dipoles to align with each other and lead to systems with lower energy.

II. METHODOLOGY

The project was divided into two main parts. The first part was to program the Ising model in the C language. The second part was to define a number of paths, use them to generate a Markov chain, and compare them.

To create the Markov chain a large number MCS = 10000 of states was generated. The states were divided into bins of size BINS_SIZE = 100, and the correlation was calculated for each state in a bin and then averaged over all members of the bin. This was done to reduce the correlation between consecutive states in the Markov chain. Then the correlation from all bins was averaged and the standard deviation was found. We expected that the correlation for all paths will be (almost) identical, hence the need for standard deviation which will allow us to determine which path is the most accurate.

A. 1-Dimension

The 1-dimensional Ising model was used as a stepping-stone to the more complicated and more interesting 2&3-dimensional models. In this version, there is no phase transition and a limited number of possible update paths. The ones used were: random (random number generator was used to decide the order of updates), order (left-to-right), every 2nd, and every 3rd.

B. 2&3-Dimensions and Space-Filling Curves

For 2&3-dimensional models following paths were used: random, order (row-by-row), Hilbert curve, and Lebesgue curve. Also for 2-dimensional model, a fractal curve made by the authors denominated G-curve was used. The recursive algorithm used to produce the space-filling curves was modelled on work done by G. Breinholt [2].

The Hilbert and Lebesgue curves are common examples of a class of continuous curves called the space-filling curves. In practice, they can also be thought of as fractals, as each apparent shape or pattern can be split up into further seemingly unitary shapes as the size of the space increases. The main characteristic of a space-filling curve is that in its limit the range of the curve is the entire unit square (or more generally n-dimensional unit hypercube) [3]. Due to the nature of these curves, the size of the lattice will be restricted to certain values as the Hilbert and Lebesgue curves require the lattices to be of side length 2^n. The Fig. 1 to Fig. 5 show the first 3 generations of the 2&3-dimensional Hilbert and Lebesgue curves and 2-dimensional G-curve.

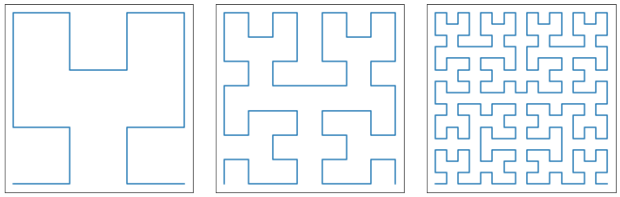

FIG. 1: The first three generations of the 2-dimensional Hilbert curve.

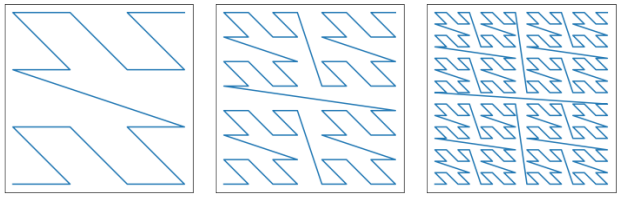

FIG. 2: The first three generations of the 2-dimensional Lebesgue curve.

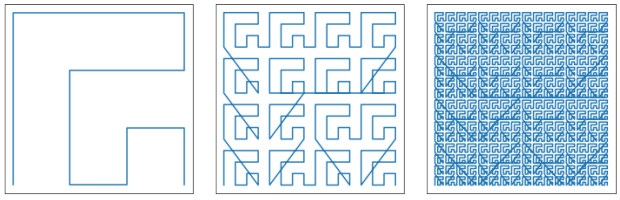

FIG. 3: The first three generations of the 2-dimensional G-curve.

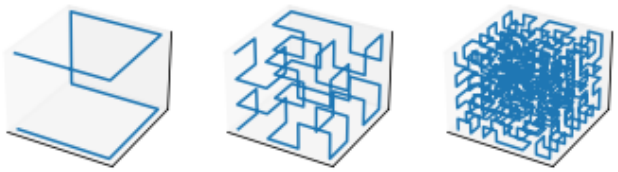

FIG. 4: The first three generations of the 3-dimensional Hilbert curve.

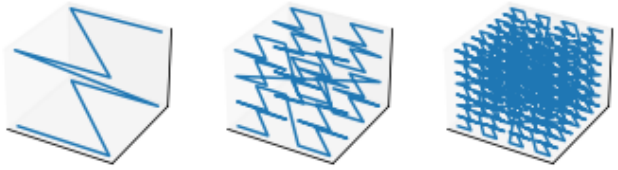

FIG. 5: The first three generations of the 3-dimensional Lebesgue curve.

III. RESULTS AND CONCLUSIONS

The models were run for $\beta = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$. Full list of graphs can be found in the Appendix.

In general, it was found that the order of updates does affect the efficiency of computations, and the choice of the most efficient update path depends on the specifications of the model.

Our expectations about the correlation function were accurate. The correlation at low values of β (and high values of temperature) between sites that are not nearest-neighbours is low or zero depending on the model and exact value of β. At higher values, the correlation is non-zero and tends to 1 as β increases. The discrepancy between path orders is also visible at this level of β, however, it is important to take the large error bars into account, and hence it is difficult to make unambiguous conclusions.

The behaviour of the correlation for the update path 'order' for 1-dimensional model is noteworthy. The behaviour for the nearest-neighbour is different from the other path orders, namely, it is zero for all values of temperature. This is most likely because this update path tends to get 'stuck' in a cycle of states. Hence, it is recommended to avoid this update path.

When it comes to the standard deviation, the behaviour is more complex. At higher β, once again, the error bars are very significant, and do not allow us to make clear conclusions.

[1] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *Equation of state calculations by fast computing machines*, Tech. Rep. (1953).

[2] G. Breinholt and C. Schierz, Algorithm 781, ACM Transactions on Mathematical Software **24**, 184 (1998).

[3] H. Sagan, *Space-Filling Curves* (Springer New York, 1994).

[4] D. V. Schroeder and H. Gould, An introduction to thermal physics, Physics Today **53**, 44 (2000).

IV. APPENDIX

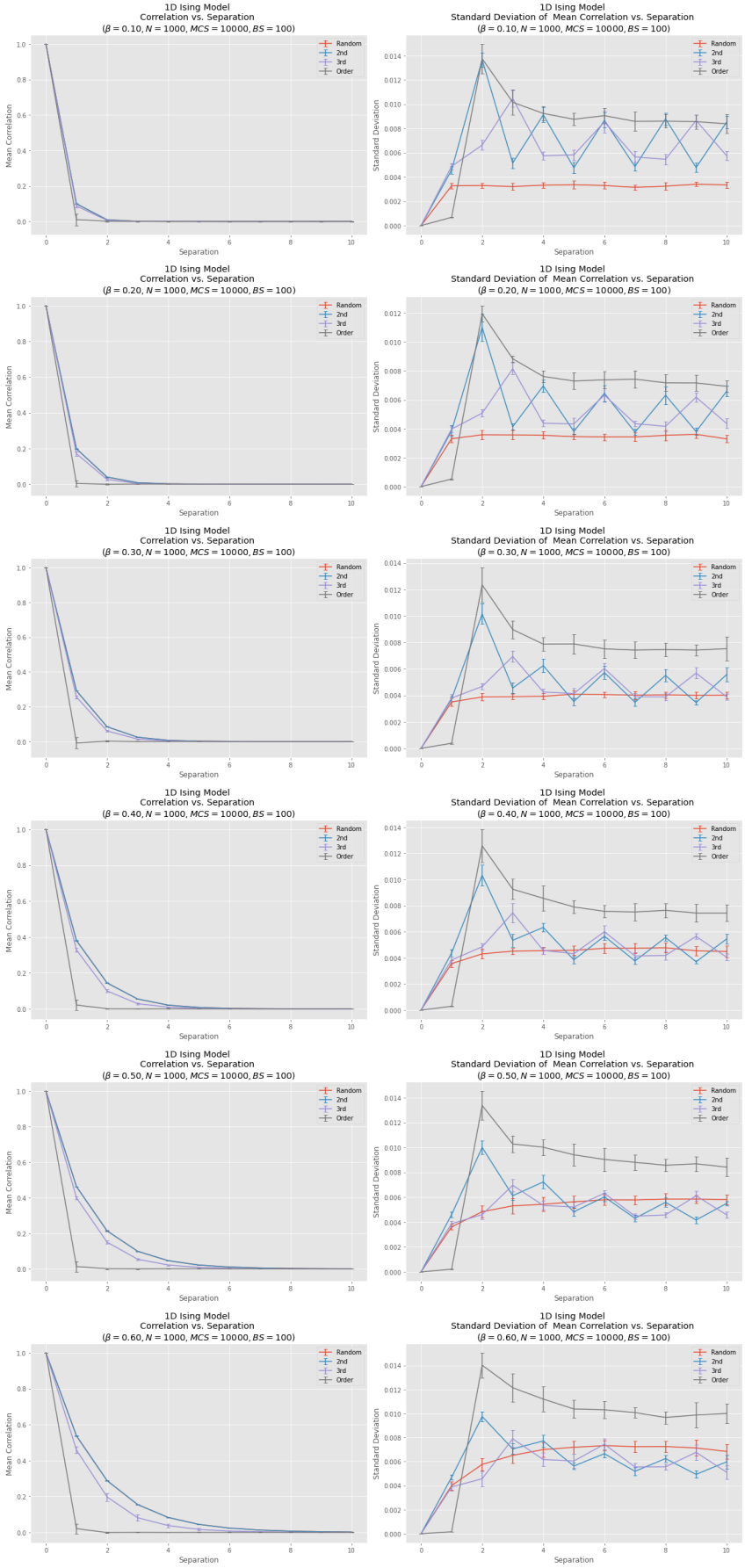

FIG. 6: The mean correlation and the standard deviation of mean correlation for the 1-dimensional Ising model.

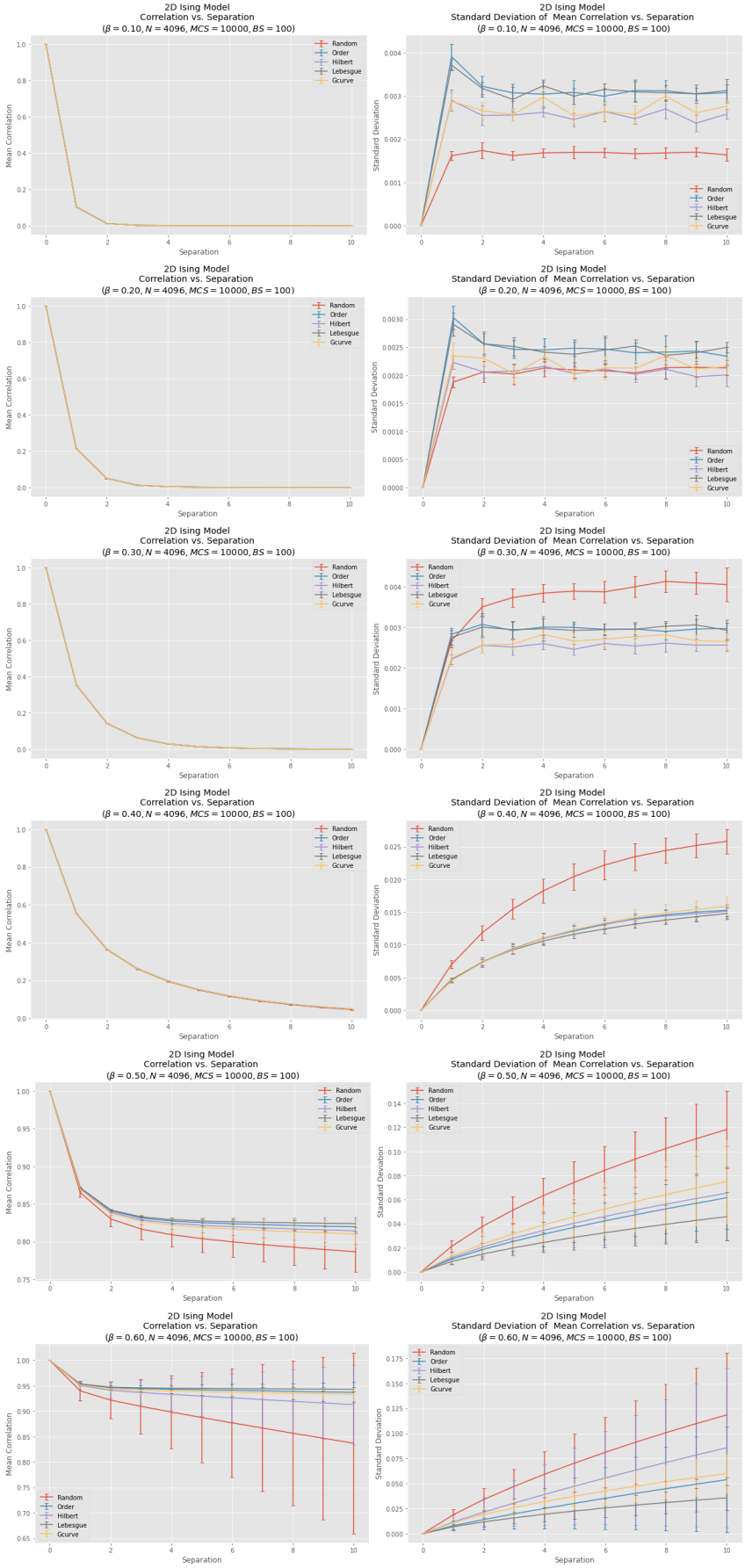

FIG. 7: The mean correlation and the standard deviation of mean correlation for the 2-dimensional Ising model.

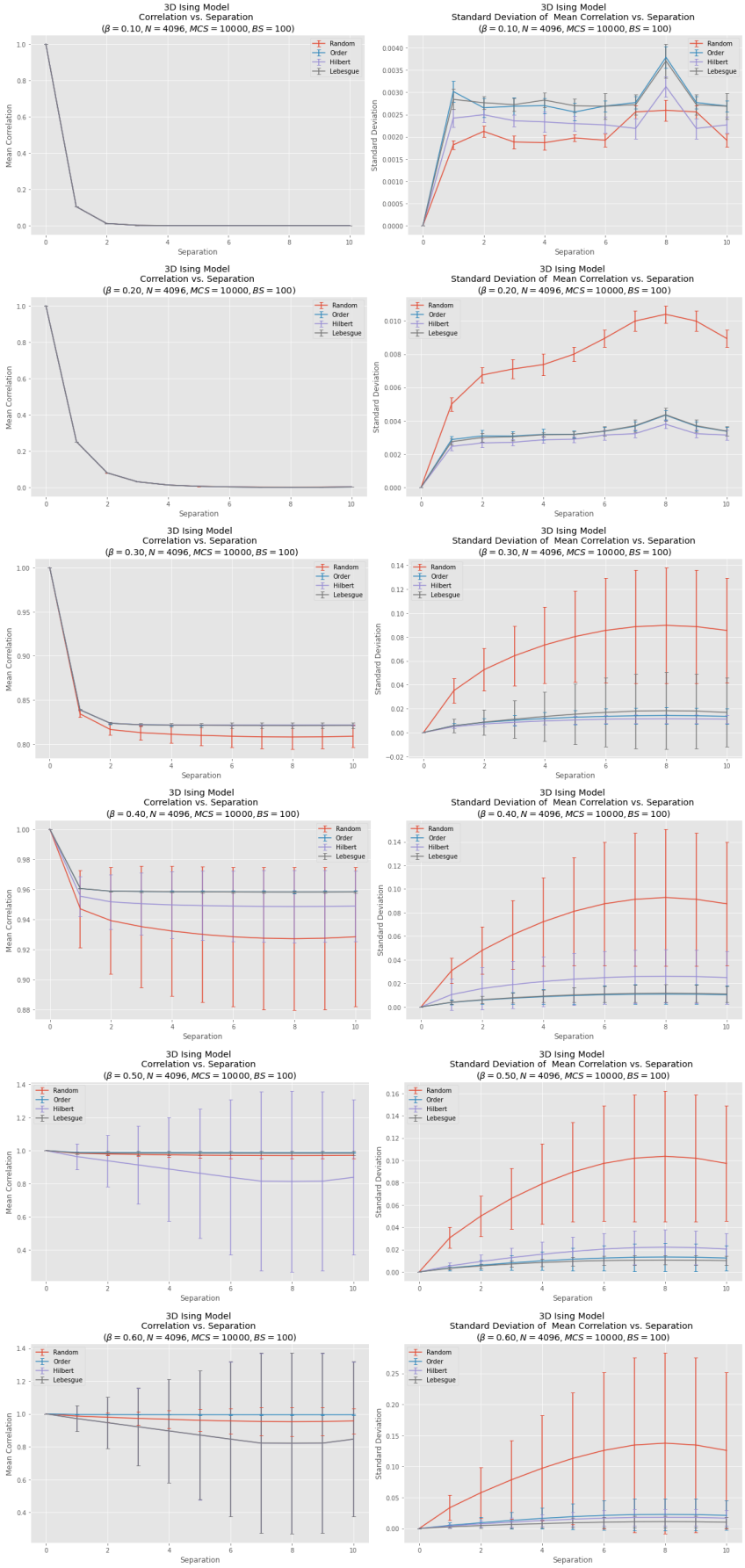

FIG. 8: The mean correlation and the standard deviation of mean correlation for the 3-dimensional Ising model.