

Order of updates in Monte Carlo computations of quantum fields

J.J. Vázquez, A. Prymek, O. Stoicescu supervised by M.J. Peardon

Trinity College Dublin

Objective

The main objective of this project is to discover if the order of updates in the simulation of a quantum field affects the computation. Hereunder is a full list of objectives:

- To program the Ising model in the C language.
- To produce new states of the system using the Markov Chain Monte Carlo Method (MCMC) and the Metropolis algorithm.
- To use the following space-filling curves: Hilbert curve, Lebesgue curve, and our own curve called G-curve to change the order of updates in the Metropolis algorithm.
- To compare the update paths by computing the correlation between sites and its standard deviation.

Process

- 1 Initialise the lattice by randomly assigning ± 1 to each site.
- Choose a site according to an order path and update the site (if $(\Delta U)_{\sigma_i \to \tilde{\sigma}_i} < 0$ then accept the flip, otherwise accept it with $p \propto e^{-\beta \Delta U}$).
- 3 The update paths compared:
- Random;
- Row-by-row (order);
- Hilbert curve;
- Lebesgue curve;
- G-curve.
- The correlation $F_{i,i+d} = \sum_i \langle \sigma_i \sigma_{i+d} \rangle$ for all sites σ_i was computed (for $0 \le d \le 10$).
- 5 The states in the Markov chain were divided into bins and averaged over them, to reduce the dependence between consecutive states in the chain.
- 6 The mean correlation over all bins and its s.d. were computed, and the results for update paths were compared.
- 7 The process was repeated for a number of different β values.

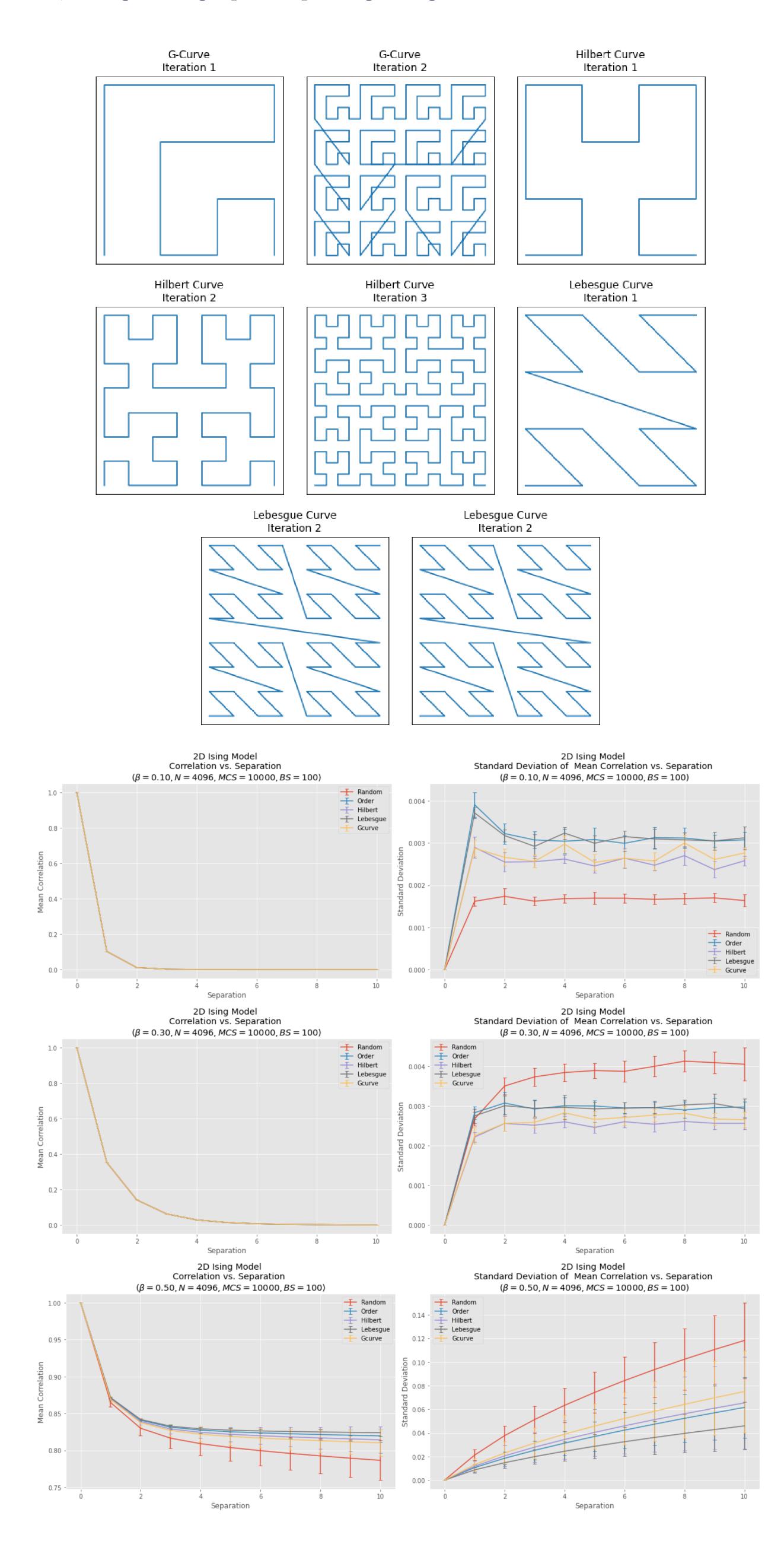
Findings

- The order of updates does affect the efficiency of computations. The choice of the most efficient update path depends on the specifications of the model.
- For low $\beta \sim 0.1$, the thermal fluctuations are significant and the system is in disorder resulting in zero correlation between states that are not the nearest-neighbours.
- For high $\beta \sim 0.5$, the thermal fluctuations are not strong enough, and the system tends to the lowest energy, i.e. to organised state; hence the correlation is close to 1.
- Large random fluctuations and high errors prevent us from being able to make clear conclusions on effectiveness of each specific update path.

Contact Information

• prymeka@tcd.ie - vazquezj@tcd.ie - stoiceso@tcd.ie

Hereunder you can observe a part of our data collected for the 2-dimensional model, along with graphs depicting the geometries used:



References

- [1] G. Breinholt and C. Schierz. Algorithm 781. ACM Transactions on Mathematical Software, 24(2): 184–189, jun 1998. doi: 10.1145/290200.290219. URL https://doi.org/10.1145%2F290200.290219.
- [2] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller. Equation of state calculations by fast computing machines. Technical report, mar 1953. URL https://doi.org/10.2172%2F4390578.
- [3] H. Sagan. Hilbert's space-filling curve. In *Universitext*, pages 9–30. Springer New York, 1994. doi: 10.1007/978-1-4612-0871-6_2. URL https://doi.org/10.1007%2F978-1-4612-0871-6_2.