Cellular Automata Algorithms for Lattice Models

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We explore a cellular automaton-based method for simulating the Ising model. We calculate nearest-neighbor correlations, magnetization, and internal energy, and find good agreement with experimental results. We also estimate the critical exponent $\beta = 0.1069(25)$, not consistent with the exact value. Next, we generalize the algorithm for the q-state Potts model and find magnetization responses consistent with the exact critical temperature for $q = 3, 4, 5$. We estimate $\beta = 0.0658(64)$ and $\beta = 0.0650(21)$ for $q = 3$ and $q = 4$, respectively; neither agrees with the exact result. We believe the discrepancies in β come from finite-size effects near T_c that have not been properly accounted for.

I. INTRODUCTION

For our purposes, we can define a cellular automaton (CA) as consisting of the following two pieces of data: (1) A lattice of *cells*, each of which holds some internal state s_i which can take on values within a set S. And (2) an *update rule*, which takes in the state of a cell and its neighbors, and returns a new state for the center cell.

The CA is seeded at $t = 0$ with an initial state. The update rule is then applied in parallel to each cell at once to advance the CA to the next time point $t = 1$, then again to $t = 2$, and so on.

Cellular automata are capable of extremely deep and rich behavior; in fact the best-known example, Conway's Game of Life, can emulate a universal Turing machine and is therefore capable of arbitrary computation. We are interested in a less ambitious question, inspired by a surface-level similarity between a CA's lattice of states and the Ising model: can a CA algorithm be used to simulate a lattice system at finite temperature?

There are many reasons to believe this may be difficult. One main reason is that a lattice system is defined in terms of an ensemble and a probability distribution, whereas a CA is fundamentally dynamical, defined in terms of trajectories and (deterministic or stochastic) time evolution. In fact, it can be shown that no cellular automaton, even one where the update rule is probabilistic, can successfully emulate a Boltzmann distribution at equilibrium so long as the update rule is applied to every cell simultaneously [1, 2].

Despite this, it turns out that it is possible to simulate the Ising model quite successfully using a reasonably simple CA. This is interesting from a philosophical and practical point of view. On one hand, it provides an example of deterministic – even non-ergodic – dynamics that is nevertheless useful for simulating a thermodynamic system. On the other hand, the CA model lends itself naturally to massively parallel computation, and does not require floating-point numbers or any source of high-quality randomness apart from seeding initial configurations, so in principle there are computational advantages too.

In this work, we explore a simple CA algorithm for simulating the Ising model. In Section II, we present the model and compare its prediction of the nearest-neighbor spin correlation against the known exact results for an Ising model in 2D, following Ref. [1]. We also use the Ising CA to find internal energy and magnetization estimates as well as an estimate of the critical exponent β. In Section III, we present an extension of the Ising CA model to the Potts model. There, we compute the order parameter as a function of temperature and check for consistency with the known transition temperature; we also compute β for $q = 3, 4$.

II. THE ISING MODEL

As a reminder, the Ising model has a spin $\sigma_i = \pm 1$ on each point of a lattice, and its Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{1}$$

We will scale energy such that $J = 1$ for computational simplicity, and work on a 2D square lattice with periodic boundary conditions.

II.1. The algorithm

We begin with a simple, fully deterministic algorithm proposed by Creutz [1]. The specifications are as follows:

Cell state. Each cell i contains three state variables: (b_i, e_i, p_i). Here b_i is a single bit tracking the Ising spin through the relationship $\sigma_i = 2b_i - 1$. Next, e_i is a nonnegative integer representing an energy reservoir attached to each site; its purpose will become clear later. Finally, p_i is a parity bit; its only purpose is to encode a checkerboard-style updating pattern. It is initialized so that red squares have $p_i = 0$ and black squares have $p_i = 1$.

Update rule. If $p_i = 0$, then set $p_i = 1$ but do nothing else. If $p_i = 1$, then calculate the change in Ising

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energy $E_i = -\sum_{j\in\langle ij\rangle}\sigma_i\sigma_j$ that results from flipping b_i. If this change in energy can be absorbed by increasing or decreasing p_i such that $E_i + 4e_i$ remains conserved, then flip the spin and change p_i accordingly. If the change in energy cannot be absorbed into e_i (i.e. if e_i would have to become negative) then do nothing. Also set $p_i = 0$.

II.2. Discussion of the algorithm

We can clearly see that the algorithm implements an energy-conserving dynamics; in particular the update step will conserve H, defined by $H = \sum_i \left(\frac{E_i}{2} + 4e_i\right)$. In essence, the quantity $4e_i$ serves as a "reservoir energy" attached to each site. The energy can be transferred into or out of the spin part of the CA system by flipping the corresponding spin σ_i; by flipping two adjacent spins energy can be effectively transferred between two adjacent reservoirs. Thus, the system can be thought of heuristically as an Ising system coupled to a secondary set of energy reservoirs.

A quick aside: the purpose of the parity bit is simply to circumvent the fact mentioned in the introduction that no CA whose update rule hits all sites at once can emulate the Ising model.

It is natural to ask whether the dynamics generated by Creutz' CA is ergodic. Creutz himself recognizes while proposing the model that it is not. For instance, the dynamics are symmetric with respect to translations in either the x or y direction by two lattice sites, as well as under the usual global spin flip symmetry. Consequently, the initial state will restrict the properties of all states that can be in its future trajectory [1]. However, we do note that the model is extremely sensitive to its initial conditions [1]. So in practice, for finite-volume systems, we can dodge this issue by simply seeding several randomly chosen initial configurations within the desired energy range and then averaging over the results.

Another question is how to get thermodynamics from the CA dynamics. These dynamics are microcanonical in nature – a total energy is specified and subsequently conserved – whereas we seek results in which the system is in equilibrium at some temperature. In fact, a temperature can be extracted from the CA dynamics as well, allowing comparison with the usual canonical ensemble results. After many time steps, the reservoir energies will thermalize, and the resulting probability distribution is given by

$$P(e_i) \propto \exp(-4\beta e_i) \tag{2}$$

Therefore we can calculate a temperature by solving

$$\langle e_i\rangle = \frac{\sum_{n=0}^{\infty} n e^{-4\beta n}}{\sum_{n=0}^{\infty} e^{-4\beta n}} \tag{3}$$

Within this equation the average can be over either time or space [1]. By carefully choosing the initial conditions, we can control the total energy available to the reservoirs, which affects $\langle e_i\rangle$ and thus β after thermalization. In this way we have a controlled, albeit imprecise, way of varying the temperature of the system.

II.3. Simulation results

We present some selected thermodynamic quantities calculated using the CA algorithm, compared against their exact values. For these results we initialize the CA state as follows: all spin bits are originally set to 0 so that the system's spin energy is minimized. Each site that will be updated on the first time step has its reservoir energy set to 2 with a probability p; this controls the starting energy and therefore the temperature. All other reservoir energies are set to 0. For each value of p, we perform 20 runs of 20000 steps each, throwing away the first 2000 steps.

The first quantity we calculate, replicating the result of Ref. [1], is the nearest-neighbor correlation function $\langle\sigma_{0,0}\sigma_{0,1}\rangle$; the thermal average here is calculated as an average over the CA time evolution. All exact results in this section can be found in Ref. [3].

The nearest-neighbor correlation is plotted in Fig. 1. We find good agreement within errorbars except near the critical temperature $\beta_c = \frac{1}{2}(1+\sqrt{2})$.

We also observe that the error bars are larger for $\beta > \beta_c$, suggesting that the CA algorithm's performance is worse in the ordered phase. There is an intuitive explanation for this, namely that equilibration of reservoirs requires energy to move between them, which can only happen in conjunction with spin flips. But when the temperature (or energy) is too low, spin flips are rare and energy transfer is poor [4]. This is analogous to the usual freezing out of degrees of freedom at low temperatures, except that in this case it is fatal to the performance of the CA algorithm. In fact, at β not too much higher than the range we explore, this freezing-out occurs and in order to maintain good performance it is necessary to design an update rule containing an energy-transfer mechanism that freezes out at lower temperature, or incorporates randomness so that in some sense it carries its own source of thermal energy [4].

The second quantity is the internal energy per site, u, as a function of temperature. This is the part of the energy that comes from the Ising spins only, and not from the reservoir energies. Both the Ising CA data and the exact energy are plotted in Fig. 2. Once again we find good agreement within errorbars.

The third quantity is the magnetization, which is again straightforward to calculate directly. Our results are plotted in Fig. 3, and once again we see good agreement except near the critical point.

Lastly, we seek to estimate the critical exponent β; we recall it is defined by

$$m \sim \left(-\frac{T - T_c}{T_c}\right)^{\beta} \tag{4}$$

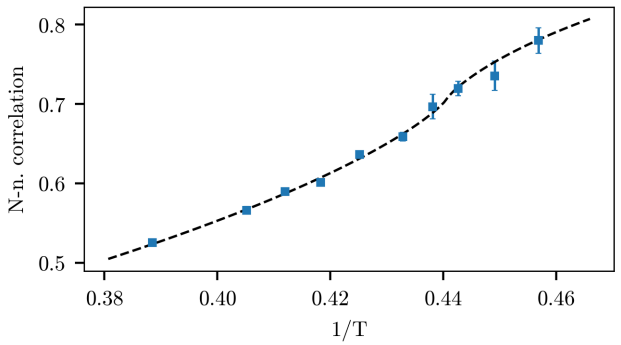

FIG. 1. Nearest-neighbor spin-spin correlation estimated using the Ising CA, compared with exact results. Several errorbars are covered by the plot markers.

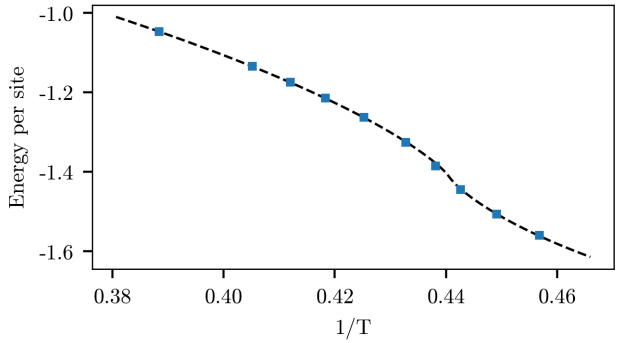

FIG. 2. Energy per lattice site estimated using the Ising CA, compared with exact results. Errorbars are covered by the plot markers.

as $T \to T_c$ from below. To accomplish this, we run a more fine-grained set of simulations near the critical temperature, with a 256×256 lattice. The data points from this run are plotted in Fig. 4.

To calculate β, we simply take these data points, convert the x-axis from β to $\frac{T-T_c}{T_d c}$, and perform an orthogonal distance regression (similar to least-squares, but it allows accounting for the error in measuring T). The resulting estimate is $\beta = 0.1069(25)$. The exact value is $\beta = \frac{1}{8}$, so our estimate is not accurate (deviates by around 7σ). Since we have access to the exact result, we can see that the main cause is the finite-size error near T_c, which is underaccounted for in our purely statistical error estimates. Given that our crude estimate is already close to the true exponent, there is good reason to believe that a more sophisticated finite-size scaling analysis would produce a value that agrees with the exact result.

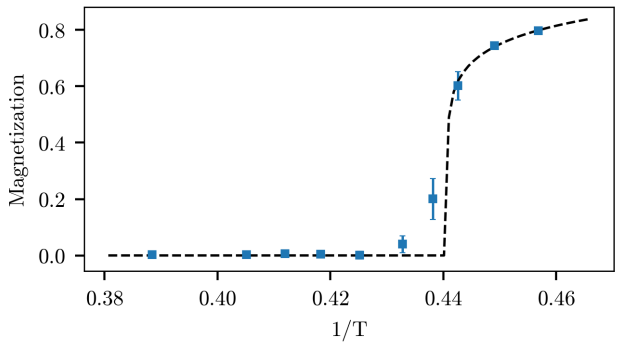

FIG. 3. Magnetization estimated using the Ising CA, compared with exact results. Some errorbars are covered by the plot markers.

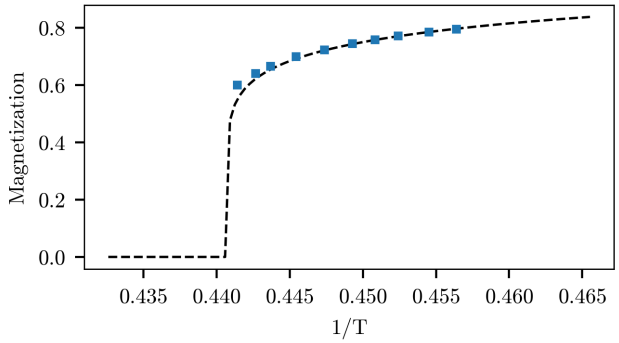

FIG. 4. Magnetization data points, obtained from a 256×256 lattice, used for estimating β. Errorbars are covered by the plot markers.

III. EXTENSION: THE POTTS MODEL

The Potts model is a natural extension of the Ising model. The q-state Potts model has each spin taking values $\sigma_i \in \{0, 1, \ldots, q-1\}$, and then the Hamiltonian is given by

$$H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j} \tag{5}$$

There are a few ways to define an order parameter here; for simplicity we will use a complex order parameter

$$m = \frac{1}{N} \sum_i e^{\frac{2\pi i}{q} \sigma_i} \tag{6}$$

A simple modification of the Ising CA allows it to simulate the Potts model.

Cell state. Each cell i contains three state variables: (σ_i, e_i, p_i). Here σ_i is an integer in the range $\{0, 1, \ldots, q-1\}$ directly tracking the Potts spin. The roles of e_i and p_i are the same as before.

Update rule. The same parity logic applies. For active cells, calculate the change in Potts energy $E_i =$

$-\sum_{j\in\langle ij\rangle}\delta_{\sigma_i,\sigma_j}$ that results from setting the value of σ_i to a random integer chosen uniformly from the range 0 to $q-1$, inclusive. Then apply the same energy-conservation update rule as before, except that the conserved quantity is E_i+e_i instead of E_i+4e_i. [This means the probability weight in Eq. (2) becomes $e^{-\beta n}$ rather than $e^{-4\beta n}$.]

We note that the spin update rule is now probabilistic. We originally tried to design a deterministic update rule, but simple ideas (e.g. incrementing each active spin modulo q) turned out to be unsuitable. In particular, deterministic attempts underestimated the critical temperature for $3 \le q \le 6$, the range that we tested. Additionally, in the ordered phase, the variation between runs was on the order of the magnetization itself. This suggests that the deterministic dynamics are freezing out, and the resulting trajectories do an extremely poor job of traversing the phase space. It is easy to see, for instance, how the increment-all-spins rule traverses the space of configurations very slowly and leads to long-lasting correlations between spins of the same checkerboard parity that are low-probability in a thermal distribution.

Given how well the Ising CA works, however, we expect that a deterministic rule could be formulated that avoids these issues and allows proper thermalization in a wide range of temperatures. For instance, one might begin from the energy-exchange mechanism proposed in Ref. [4]. However, within the scope of this work, we chose to sacrifice determinism in the name of expediency.

Fig. 5 provides plots of magnetization for Potts model with $q = 3, 4, 5$, together with the exact transition temperatures, $T_c = \log(1+\sqrt{q})$ [5]. We can see that the Potts CA successfully predicts a phase transition and in each of the three cases produces data consistent with the exact transition temperature.

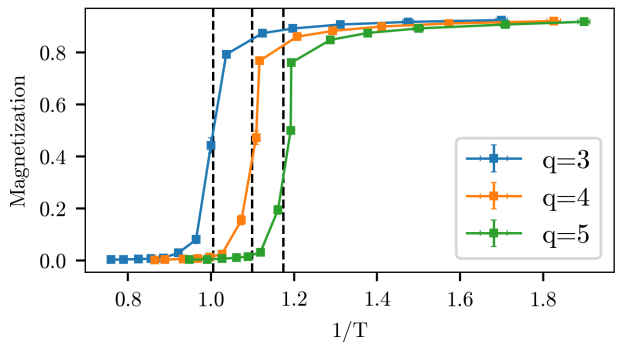

FIG. 5. CA-calculated magnetization data for the Potts model with $q = 3, 4, 5$. The dashed lines denote the exact critical inverse temperatures for $q = 3, 4, 5$ going from left to right. Errorbars are covered by plot markers.

For $q > 4$, the Potts model undergoes a first-order transition. But for $q \le 4$ it undergoes a second-order phase transition, and therefore β is well-defined [5]. So we estimate β for $q = 3, 4$, using the same method as before, on 200×200 lattices. The data points used are depicted in Fig. 6.

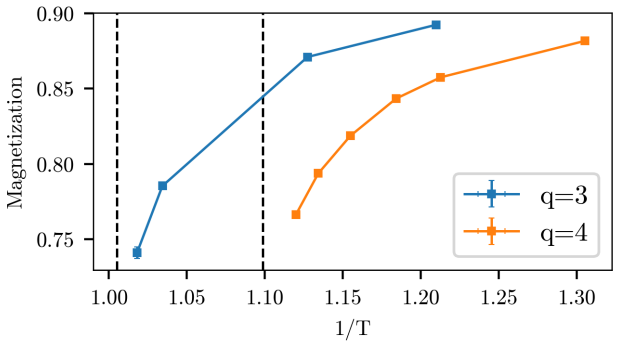

FIG. 6. Data from the ordered phase of the Potts CA on 200×200 lattices for $q = 3, 4$. The dashed lines denote the exact critical inverse temperatures for $q = 3, 4$ going from left to right. Errorbars are covered by plot markers.

After carrying out the calculation, we find $\beta = 0.0658(64)$ for $q = 3$ and $\beta = 0.0650(21)$ for $q = 4$. Neither of these agree well with the exact values, $\beta = \frac{1}{9}$ for $q = 3$ and $\beta = \frac{1}{12}$ for $q = 4$ [5]. It seems likely that the same finite-size effects that we saw in the Ising model are at play here.

IV. CONCLUSION

We have implemented and run a cellular automaton algorithm for simulating the Ising model. Its predictions for thermodynamic responses agree well with the exact results. We attempted a very simple estimate of β and obtained an answer near the exact answer, though not in true agreement with it. By comparison to the exact magnetization, we were able to see that the discrepancy arose from finite-size effects near T_c that were not accounted for in the error analysis. We have also attempted to generalize the cellular automaton to simulate the Potts model. It produces a plausible-looking magnetization response that drops to zero near the exact transition temperature; the estimated value of β is however in quite poor agreement with the exact value. Our speculation is that the error comes from the same source as in the Ising model, namely unaccounted-for finite-size effects.

We conclude with some ideas for further work. First, can critical exponents be accurately extracted with a better finite-size scaling? Second, is there a deterministic update rule for the Potts model? Finally, in principle, the Ising CA could be generalized to any system in which spins take on a discrete set of values. It would be quite interesting to implement a q-state clock model in a CA, and and try to generalize to the large-q limit and approximate continuous-spin systems such as the XY model. The dynamical nature of the CA model could then allow interesting explorations of vortex dynamics and the BKT transition.

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