Introduction to Lattice Simulations

Cellular Automata

What are Cellular Automata or CA?

A cellular automata is a discrete model used to study a range of phenomena. These models have applications in:

computability theory, mathematics, physics, complexity, biology etc

Cellular Automata

CAs generally consist of a grid of cells, each of which has a finite number of possible states.

This is what we mean when we say it is a discrete model.

The simplest CA cells have two possible states “on” or “off.

Cellular Automata

These cells represent the ‘state’ of the simulation.

Each cell is updated based on the rules of the CA and the states of the neighbouring cells.

This is the ‘dynamics’ of the simulation.

Cellular Automata

A Cellular Automata is usually run over many generations to see how the system behaves.

Wolfram’s Cellular Automata

One famous Cellular Automata is Wolfram’s CA. This is a one dimensional cellular automata which the value of each cell depends on its state and the state of its two neighbours. These rules can be encoded easily into an integer.

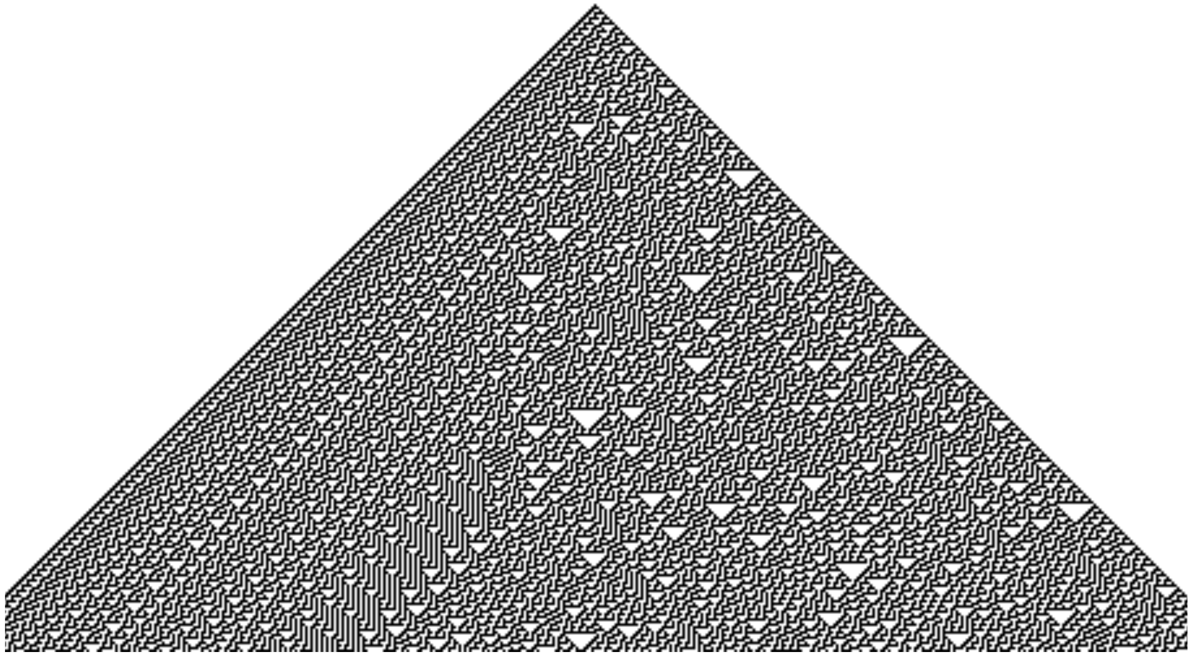
Wolfram's Cellular Automata

Rules for this automata can be easily built from the following representation:

111	**110**	**101**	**100**	**011**	**010**	**001**	**000**
0	0	0	1	1	1	1	0

This rule set can be represented by the integer 30.

Wolfram's Cellular Automata



111	110	101	100	011	010	001	000
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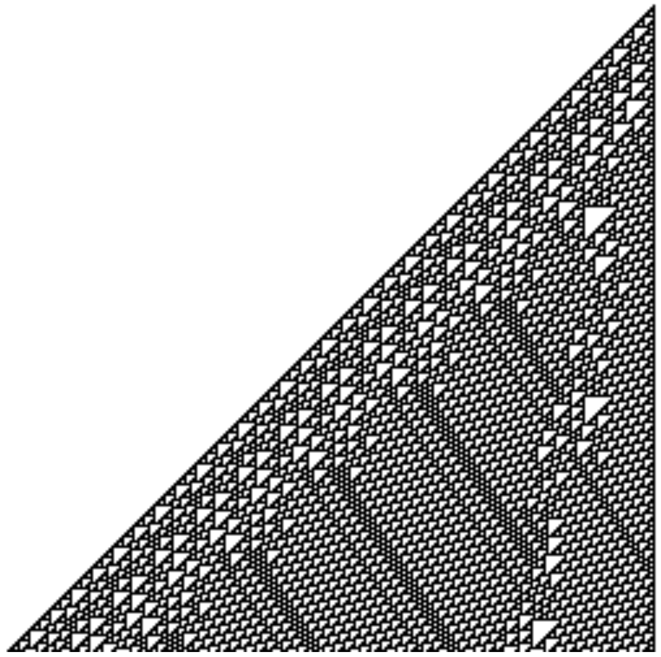
Wolfram's Cellular Automata



111	110	101	100	011	010	001	000
0	1	1	0	1	1	1	0

Conway’s Game Of Life

Conway’s game of life is an automata designed to simulate life. Each cell in this automata can be either ‘alive’ or ‘dead’.

Conway's Game Of Life

1. Any live cell with fewer than two live neighbours dies, as if caused by under-population.
2. Any live cell with two or three neighbours lives onto the next generation.
3. Any live cell with more than three live neighbours dies, as if by overcrowding.
4. Any dead cell with exactly three live neighbours becomes a live cell, as if by reproduction.

Conway’s Game Of Life

A simple two-dimensional CA like this can exhibit quite remarkable behaviour.

This simple game shows patterns and complex ‘organisms’ emerging from extremely simple rules.

Ising Model

The Ising model is model of ferromagnetism named after the physicist Ernst Ising.

Each cell in this model represents a magnetic dipole or atomic ‘spins’ in one of two states ‘up’ or ‘down’.

Ising Model

Each of these atomic spins interacts with its neighbours and either remains the same or flips.

The rules or dynamics of the model are:

Ising Model

1. If the spin is different to two or more neighbours, change spin.
2. If the spin is different to zero or one neighbours, change with some probability.
3. Else remain the same.

Metropolis Algorithm

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Metropolis Algorithm

Randomly select a spin and compute the energy E(s).

Change the spin and calculate the new energy E(s’).

Calculate the change in energy

$\Delta E = E(s') - E(s)$

Metropolis Algorithm

Accept the change if:

$\Delta E <= 0$

or with probability

$\exp(-B*\Delta E)$

Ising Model

Given this update method all we need to define the Ising model is the energy function or Hamiltonian:

$$H(\sigma) = -\sum_{<i\ j>} J_{ij}\sigma_i\sigma_j - \sum_j h_j\sigma_j$$

Ising Model

This is no longer a simple cellular automata because the dynamics depends on some probability.

Changing this probability now controls how the model behaves.

Potts Model

The Potts model is very similar to the Ising model.

However, rather than simply allowing an atomic spin to be ‘up’ or ‘down’ it has Q states.

The Potts model with Q=2 is the Ising model.

Potts Model

The Potts model is also updated using the Metropolis algorithm, so all we need is the Hamiltonian. The Hamiltonian for the Potts model is simply:

$$H_p = -J_p \sum_{(i,j)} \delta(s_i, s_j)$$

Potts Model

This model also shows a phase transition depending on temperature.

This is quite an extensible model. Q can be increased to allow each spin to have more possible states. Increase Q enough and this model becomes the XY model.

XY Model

The XY model is the extension of the Potts model into continuous space. Rather than a discrete value for each cell, each spin is represented by an angle.

XY Model

This model also uses the Metropolis algorithm so all we need is the Hamiltonian:

$$H(\mathbf{s}) = -\sum_{i \neq j} J_{ij}\, \mathbf{s}_i \cdot \mathbf{s}_j - \sum_j \mathbf{h}_j \cdot \mathbf{s}_j$$

Heisenberg Model

The final extension of this model is the Classical Heisenberg Model where each spin is a three-dimensional vector.

Heisenberg Model

Once again this model can be described by a Hamiltonian:

$$\mathcal{H} = -\sum_{i,j} \mathcal{J}_{ij} \vec{s}_i \cdot \vec{s}_j$$

Lattice Simulations

These models should show an obvious progression from a simple discrete case of the Ising right through to the more physically realistic Heisenberg Model.

Programming Lattice Simulations

Studying these models often requires many simulations and measurements. This is an obvious case when it makes sense to use parallel programming.

Programming Lattice Simulations

Task parallelism – The easiest and most obvious way to split up these simulations is to use task parallelism.

If you have 1000 simulations to run and 10 machines available. Simply have each machine run 100 simulations and combine the statistics afterwards.

Programming Lattice Simulations

This is the best approach if you are using a cluster. Another attractive alternative is to use GPUs.

In this case the tasks can’t simply be split between the processors in a GPU because of memory issues.

Programming Lattice Simulations

Instead it is better to have each GPU work on one simulation at a time. This is known as data-parallelism.

However, for the type of simulation we have discussed there is a significant problem with this:

The Metropolis Algorithm

Programming Lattice Simulations

Think about the way that the Metropolis Algorithm works. Randomly pick a spin and update it based on the value of its neighbours.

If two threads happen to pick spins next to each other, they will update both spins at the same time and update both of them.

Programming Lattice Simulations

This may not seem like a big deal but it can have a subtle impact on the behaviour of the simulation. As even a subtle change affects the statistics of the model this is unacceptable.

Programming Lattice Simulations

The common solution to this problem is the checkerboard or red/black update method.

In this algorithm each cell is colored like a checkerboard.

When a model is update, first all the ‘black’ cells are updated and then all the ‘red’ cells are updated.

Programming Lattice Simulations

This way no two neighbouring cells are updated at the same time.

This is generally accepted to be a suitable solution to the problem.

Programming Lattice Simulations

However, it does have an impact on performance. Most memory prediction and caching assumes that sequential memory address will be accessed.

This is normally the case for most programs, iterate through a sequence accessing each one.

Programming Lattice Simulations

For GPUs this is an even bigger requirement for performance. Sequential threads accessing sequential memory addresses can read all the values in a single transaction, if this condition is not fulfilled the memory reads must be broken into multiple transactions.

Programming Lattice Simulations

One method of overcoming this problem is a method called crinkling. This method rearranges the checkerboard so that sequentially access values are stored sequentially.

Programming Lattice Simulations

A small change like this can have a large impact on the performance of a simulation.

Summary

Cellular Automata

Lattice Models

- Ising
- Potts
- XY
- Heisenberg

Metropolis Algorithm

Programming Lattice Simulations