Cellular Automata and Discrete Physics[1]

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Contents

Chapter 14

Cellular Automata and Discrete Physics

This paper provides an introduction to cellular automata (CA). The concept of CA is reviewed with emphasis on its properties which make it attractive for physical modeling. This leads to a brief discussion of cellular automata machines (CAMs) which can perform real-time simulations. Applications of CA and CAMs are discussed including some recent results in simulating wave propagation.

14.1 Introduction

An *automaton* is a simple computer which has a finite number of internal states (*discrete values*). Through a specific function, or "rule", the internal state of the automaton depends on one or more inputs. In the simplest case, the "output" of the automaton consists of an integer representing the internal state. For the present discussion, we will call such a simple automaton a "cell".

A *cellular automaton* consists of a regular lattice (array) of identical cells (*discrete space*). As an imaginary clock ticks (*discrete time*), every cell is simultaneously updated according to a rule which receives as input the state of the cell, as well as the states of some of its closest neighbors. (See Figure 14.1.)

Lately, there is much interest in using cellular automata to model physical systems. Part of the reason for this is that cellular automata provide representations of physical systems which are different from traditional ones. This new perspective often provides additional insights into the behavior of

Fig. 1

Figure 14.1: A two-dimensional, rectangular array of cells. The dashed line identifies the set of cells which define the “MOORE” neighborhood for the center cell. This neighborhood is also called a “3 x 3” neighborhood.

the system under study. CA can also provide a more “direct” representation which explicitly embodies many of the physical properties of space, such as locality of interactions, finite speed of information propagation (finite speed of light) and relativity. Many practitioners also point out that the CA’s “restriction” to a finite amount of information per cell (i.e. information per unit volume) is also a reasonable assumption for space [1].

As abstract ideas, these properties may not be very exciting. It is very exciting, however, that CA models have been used to simulate physical processes, such as diffusion, diffusion-reactions, wave propagation, fluid flow, growth mechanisms, phase transitions on spin lattices, the evolution of non-equilibrium and thermodynamic systems, and other phenomena. Effective modeling of these processes creates the possibility of using CA simulations for complex engineering design, such as the blades of a high temperature turbine, a complex chemical reactor bed, or exotic lithographic processes for electronic device fabrication [2]. Some advocates claim that cellular automata models offer the promise of performing such simulations much faster and more accurately than conventional models.

Today, most CA practitioners use supercomputers such as Crays or Connection Machines because of their high speed. The intrinsic regularity of cellular automata, however, permits the construction of high-speed, low-cost hardware coprocessors called “cellular automata machines”. CAMs have excellent cost/performance characteristics for CA simulations. Examples of such hardware are RAP-1, LGM-1, CAM-6, and its newer cousin CAM-PC, and others [3, 4, 5, 6].

Cellular automata machines can also be used for animated, real-time visualizations of the process under study. Traditionally, many researchers observe their simulations with a short sequence of still images. It is much easier, however, to comprehend the temporal evolution of a simulation by using high-speed computation and display, which is provided by appropriately equipped supercomputers or a low-cost CAM. CA machines also allow the user to interactively experiment with different rules and boundary conditions.

Much larger and more expensive CA machines are already being designed and built [7, 8]. While cellular automata models are intellectually stimulating and even entertaining, it is the potential engineering applications that provide the primary justification for constructing large machines [9].

Before using CA models to simulate physical systems that have not yet been built, it is necessary to compare several critical CA simulations with laboratory experiments to gauge how well they approximate the systems under study. One of the most successful CA flow simulations to date was reported recently by the Lattice Gas group at Los Alamos. A flow simulation was performed using the digitized geometry of a thin slab of rock. The measured and simulated 2D flow permeability were found to agree within 5%, which is remarkable for **any** model. The Los Alamos group has challenged practitioners of more conventional methods to obtain equal or better results [10]. Work is in progress at Los Alamos to extend the simulation technique to three dimensions.

It is important to realize that cellular automata models, in general, and for physical systems, in particular, are really still in their infancy. It is possible, but not likely, that the empirical results described above are fortuitous. The work must be repeated several times elsewhere before it is accepted as solid scientific evidence. In addition, most large corporations already use conventional methods for process and structural engineering design simulations, however no one is yet using CA models for this purpose. Furthermore, the tools for using CA methods are rather primitive, whereas engineering tools that incorporate traditional methods have been evolving for decades. The many barriers to overcome before CA models effectively compete with traditional methods in applications are providing worthy challenges to the present generation of scientists.

The above discussion was intended to show the reason for interest in cellular automata and cellular automata machines by physicists, materials scientists and chemists, among others. In the remainder of the paper, we describe in more detail how CA and CAMs can be used.

14.1.1 A Well-Known Example: *Life*

To understand CA for physical simulations, it is helpful to have a concrete example in mind, which illustrates the relationship between the underlying lattice and the rule. The example we have chosen is John Conway's "Life", because of its simplicity and the fact that it is widely known.

Life is an example of a "two-state" cellular automaton on a two-dimensional rectangular lattice. Each cell becomes active or inactive ("alive" or "dead", or takes values 1 or 0) based upon its current state and the number of active cells nearby. More specifically, each cell counts how many of its eight neighbors are alive. The new value of the cell depends on its current value and on the sum of active neighbors as follows:

- 0 or 1 neighbors alive: die from isolation
- 2 neighbors alive: stay as you currently are
- 3 neighbors alive: become alive, or stay alive (trisexual mating?)
- 4 or more neighbors alive: die from overpopulation

Because it is two-dimensional, we can think of the state of this CA as a binary image. Perhaps suprisingly, this simple rule can lead to very complex evolving patterns when the sequence of states are observed on a computer or CAM display. Since the rule is fixed, the behavior depends entirely on the initial pattern of living and dead cells in the array. Starting with a random initial configuration, the system usually appears "active" for some time and then eventually stabilizes into either a static or periodic pattern.

A great deal of effort went into studying all aspects of the Life rule, particularly during the 1970's. See [11, 12, 13] for more in-depth discussions about Life.

The emergence of complex behavior from massive quantities of very simple components, as in Life, encouraged thinking about the possibility of modeling complex physical systems with more general cellular automata.

14.1.2 Cellular Automata

A cellular automaton as defined in the introduction is an abstract, mathematical object. There are precise, formal ways to define a cellular automaton, but for the present purpose, it is convenient to think of an array of "cells" with the following properties:

- discrete space: N-dimensional array of cells
- discrete states: finite # of bits at every cell
- discrete time: clock ticks away, everyone updates on each tick
- synchronous updating
- homogeneous rule: update rule is the same everywhere
- deterministic rule

- spatially local rule: only look at nearby cells

- temporally local rule: only current state (and maybe previous state) affects new state

Occasionally, a few of these properties are relaxed for particular simulations. For example, one might use a pseudo-non-deterministic update rule or a rule with continuous values. Such extensions to the basic notion of cellular automata are important but will not be discussed in this paper.

At first, cellular automata may seem very restricted because every parameter is discretized, and one might wonder how it is possible to have much variety. In fact, tremendous variation is possible, as the following argument suggests. Consider an n-state cell, which is updated according to the states of k neighbors (possibly including itself). There are n^k possible state combinations that a cell's neighborhood may assume. For each possible combination, the cell may take on any of the n states. Thus, there are a total of n^{n^k} rules. For the 3 x 3 neighborhood used in Life ($n = 2$, $k = 9$), this number is 2^{2^9}, or approximately 10^{154}. Running out of rules to try doesn't seem to be an immediate concern. On the other hand, randomly trying different rules isn't very constructive. Some way is needed to generate rules which do something interesting or useful.

The first comprehensive study to classify cellular automata was conducted by Stephen Wolfram [14]. In particular, Wolfram examined one-dimensional, two-state CA with a "radius" of one, meaning the value of the current cell plus both of its immediate neighbors determine the new value for the cell (1-D, n=2, k=3). (With a radius of two, the new value would also depend on the next-nearest neighbors, and so on.) Since this class of CA has only $2^{2^3} = 256$ rules, Wolfram classified the typical behavior of all of them, starting with various initial configurations. He showed that there are several distinct types of cellular automata which all have physical analogs. He also illustrated comprehensive approaches to analyzing the algebraic and statistical mechanical properties of cellular automata (mostly based on studies of 1-D systems).

Others have attempted to classify higher-dimensional automata. One of the more interesting approaches uses Chris Langton's *lambda* parameter, a simple analogy of temperature, to describe the space of CA rules. Current results indicate that there is some kind of "phase transition" in the region of the rule space between rules which settle down to periodic behavior, and rules which exhibit chaotic behavior. At the transition between the two, the system will follow extremely long transients, which may be a sign of computational capacity [15, 16, 17].

Such studies provided more specific evidence for the belief that cellular automata could model various types of complex physical systems.

14.1.3 The Information Mechanics Group

While Wolfram and others emphasized the ensemble properties of cellular automata, several individuals focused on the "microscopic" properties. In particular, the Information Mechanics Group at MIT contributed a series of papers which discussed the characteristics that CA have in common with physical space-time:

- spatially local rule — there is no action at a distance
- there is a finite speed of information propagation –"speed of light"
- homogeneous rule — the laws of physics are the same, no matter where you are
- deterministic rule — rules are generally forward-deterministic; by making them backward-deterministic as well, it is possible to create microscopically reversible rules

Toffoli and Margolus of the Information Mechanics Group made the bold claim that these factors could allow construction of much more efficient computers for physical simulations. They then designed and built a series of small cellular automata machines (CAM-1 through CAM-6) to demonstrate their points!

The Information Mechanics Group has studied a wide variety of applications of CA with their various machines. Many of these applications are described in their book [18], which is currently the only introductory book on the subject of physical modeling with cellular automata. Although it heavily uses CAM-6 notation to describe the rules, it is still a valuable introduction to the subject in general.

The Information Mechanics Group is now developing a much larger machine, called CAM-8 [7].

14.2 Physical Modeling

14.2.1 CA Quasiparticles

Up to now, most CA applications to physics generally use collections of CA "quasiparticles" for simulation of both statistical ensembles and "continuum" fields.

The simplest example of a CA simulation for a statistical ensemble is a spin lattice, where each site has a spin variable that can take on values "up" or "down". A variety of multistate spin lattices and Potts models have been studied with CA. Several references can be found in [19].

For simulating "continuum" fields, it is convenient to think of each quasiparticle as representing an imaginary particle whose collective properties are similar to those of the field. Feynman had a very nice way of expressing this:

> We have noticed in nature that the behavior of a fluid depends very little on the nature of the individual particles in that fluid. For example, the flow of sand is very similar to the flow of water or the flow of a pile of ball bearings. We have therefore taken advantage of this fact to invent a type of imaginary particle that is especially simple for us to simulate. This particle is a perfect ball bearing that can move at a single speed in one of six directions. The flow of these particles on a large enough scale is very similar to the flow of natural fluids. [20]

The model described by Feynman is known as a *lattice gas*. Note that **any** integrable vector field, such as an electrostatic field, or a classical gravity field, can be described in terms of the flow of imaginary particles.

A cellular automaton provides a direct way to implement such a set of simple particles. Figure 14.1 shows a cellular automaton which can be used to implement fluid-like particles that can move in one of four directions, instead of six. In fact, by playing tricks with the rules, a square-lattice automaton can also be used to implement the lattice gas described by Feynman.

By using a particle representation of a "continuous" field, the techniques of statistical physics are applicable, just as particles are used in quantum field representations of electromagnetic fields. For fluid simulations, however, CA quasiparticles are much simpler than the photons that make up an electromagnetic field, which provides an enormous computational simplification. An introduction to the statistical properties of 1D CA is [21].

14.2.2 Physical Properties from CA Simulations

In simulation of statistical ensembles, properties over the whole system are important, such as the number of particles in a particular state, or conservation of a particular type of particle.

A necessary component of a model is that it has certain properties which can be measured and studied, such as mass, velocity, momentum, etc. There are both intrinsic and extrinsic properties of a cellular automaton system.

The latter are very straightforward. Consider mass as an example. In a 2-state CA, the total mass of the system can simply be defined as the number of cells which are in state 1. (Vacuum is then defined as state 0.) In a system with more than 2 values per cell, it may be desirable to determine the mass from particular states. For example, cells with an even value might count toward the total mass, while odd cells might not. In this case, odd values would have another interpretation, such as a quantum of energy.

A next step might be the definition of momentum. Suppose the current rule is one in which particles (non-zero values) propagate in various directions. The momentum of a cell could simply be its mass multiplied by its direction of motion (a unit vector). These vector quantities could be summed over the entire array, thus giving a value for the total momentum of the system. By summing only over particular regions or clusters of active cells, it would be possible to measure the momentum of a particular region or structure in space.

Intrinsic properties such as pressure may also be defined. To use the propagating particle example again, suppose that the model also has fixed walls which deflect the particles. The force at any given instant might be defined as the total number of particles currently adjacent to the wall — either about to collide or just after colliding. The pressure would then be defined as the average number of such particles per unit area.

This leads to an interesting observation about the measurement of certain properties of a cellular automaton: namely, that an *averaging* technique is often very useful. This technique is used regularly in studies of lattice gas models, which will be described shortly. In some cases, it is only meaningful to speak in terms of local averages. For example, to measure the density of a particular area in a particle model, it wouldn't be very useful to speak of the density of a single cell, which is either zero or one. Instead, such quantities are measured in a local area, for example an $N \times N$ block of cells (where finding the optimum value for N is a problem in itself). Similar techniques are used in kinetic theory, where it is desirable to use a volume that is large enough to contain many particles, but small enough to treat as infinitesimal compared to the size of the system. It is partly for this reason that simulations with enormous numbers of cells are desirable.

14.2.3 Diffusion

A class of CA applications to ensembles is the study of the behavior of a large number of diffusing particles. This is important for simulation of fluid flow, electron scattering in solids, or chemical reactions. In this case, the CA quasiparticle might be thought of as representing an individual molecule of the ensemble, even though this is not achievable in practice. Although the model described below is very simple, it demonstrates a few of the techniques and limitations that often arise in particle-based CA models.

Note that in traditional models of particle systems, a list of structures is maintained, with each structure describing the attribute of a particle, such as position, velocity, etc. In a cellular automaton model, a very different approach is used. Instead of simulating many particles which move around in space, we simulate many regions of space through which particles move. Literally, a particle or a "bit of matter" moves through space by passing a value from one cell to the next. In this sense, each cell is "a piece of space".

Consider a lattice in which particles move horizontally and vertically, as in Fig. 14.1. All particles move at the same speed. Each cell will be able to hold up to four particles at once. No two particles, however, may be in the same location moving in the same direction (like the Fermi exclusion restriction). Thus, a "full" cell would have one particle moving in each of the four orthogonal directions. We must also be sure that under the update rule, it will not be possible for more than 4 particles to converge upon one cell.

One way to mathematically describe this implementation is to use an array of 4-vectors, where each 4-vector represents a cell. The components of the vector can take on values 0 or 1.

Thus, for example, a state like $(0,1,0,0)_{ij}$ might represent the presence of a particle moving "South" in $cell_{ij}$, while for the same cell, $(1,0,0,0)_{ij}$ might represent a particle moving "North". The existence of particles moving "East" and "West" can be represented using the other vector components. Note that state $(0,0,0,0)_{kl}$ represents the absence of any particles, or a vacuum, at $cell_{kl}$. With the help of this notation, it should be easy to see how this simple lattice gas can be implemented with a 16-state rectangular CA.

For behavior that resembles diffusion to occur, particles must interact with each other in some way, or else the particles would move independently and the model would not be very interesting. Some sort of *collision rule* is needed to describe what happens when particles meet. If we require that momentum is conserved in all collisions, there is only one possible collision which can alter the paths of particles. Namely, when two particles hit head-on, they can both be deflected by $90°$; the net momentum before and after is zero.[1] With any other combination of particles, deflecting any of them would require a change in total momentum.

Next, a method of applying or organizing the rule is needed. The

[1] Note that it is irrelevant whether particles are deflected clockwise or counterclockwise, since all particles are identical.

Fig. 2

Figure 14.2: The complete HPP update cycle, shown in two parts. First, the collision transformation is applied, and then the propagation rule.

Fig. 3

Figure 14.3: a. Two types of particles in the array | b. The particles have begun to mix

propagation-collision cycle is a very common and simple technique to accomplish this. Two different rules are applied on alternating time-steps. First, a rule is used in which every particle moves one cell in whichever direction it is going; then, the collision-rule is applied. This changes the direction of motion of some of the particles. By alternating between the two, we get motion and interaction. In fact, these two steps can be combined into a single rule, but it is often useful to think of the two phases separately, which also makes code-development easier. Figure 14.2 illustrates a complete update-cycle.

This model is called the HPP lattice gas, from the initials of those who first extensively studied its properties [22, 23]. Besides its pedagogical utility, the HPP model is of historical importance because it introduced the concept of the propagation-collision update cycle which is a key step in implementing lattice-gases.

Let's now run an experiment using this rule. We will start with a pattern of uniform density, but color a portion of the particles black, and the rest gray[2] (see figure 14.3-a). After about 50 time-steps, the two types of particles are somewhat mixed, as shown in figure 14.3-b. The number of time steps required to thoroughly mix the particles depends on the size of the system and on how the black particles are distributed. This behavior is very similar to the mixing of two gases with identical dynamics.

Extensions to the basic HPP model address some of it's deficiencies.

[2] In order to trace individual particles through collisions, we can simply assume all head-on collisions rotate particles clockwise, or counter-clockwise, or flip a coin in each case.

One important extension was discovered by Frish, Hasslacher and Pomeau (the FHP model) [24]. They found that by allowing six velocities on a hexagonal lattice, that the resulting lattice gas accurately approximated the behavior of the Navier-Stokes Equation. This derived from the improved set of symmetry properties of rules on this lattice. Later additions of a small number of additional speeds, including particles "at rest" were shown to futher improve the behavior for many types of fluid simulations [26, 27]. The search for minimal extensions to the basic rule continues to be an active area of research.

14.2.4 Sound waves

The HPP model has been modified to model many things besides molecular gas diffusion. One such application is the motion of sound waves.

In section 14.2.3, we discussed systems at equilibrium (the two colors of particles obeyed the same rules, and so the system was always at dynamical equilibrium). Now, we investigate the results of disturbing the equilibrium in one region of the array.

Consider an experiment where we place a solid block of particles in an otherwise empty array, and apply the HPP rule. For a brief time, there will be an interaction between the particles. Shortly thereafter, however, we will see four groups of particles rush out in the four directions of propagation, never to interact again (assuming an infinite lattice). Obviously, the behavior of a dense cluster of particles in a vacuum is very anisotropic.

Now consider a similar experiment, where we again have a solid block of particles, but instead of being placed into an empty array, we place the cluster of particles into an array that has particles randomly distributed at a density of 40%. The presence of these "background" or "noise" particles will cause the mean free path in the system to be very small relative to the size of the array. If we now apply the HPP rule to the new configuration, we get a *circular* compressional wave propagating outward from the disturbance, as shown in figure 14.4. The behavior is isotropic — by observing the density variation of the wave, it is nearly impossible to determine the orientation of the lattice. Toffoli and Margolus observe that "the overall effect is much like that of a bucket of water dumped into a pond" [18]. Note that, as in a wave on the surface of water, the particles in the array do not travel with the wave; the wave is simply a propagating density variation whose velocity is faster than the random-walk motion of the particles, but slower than the velocity of the individual particles in the system. The random background therefore serves as a medium in which the sound waves may travel.

Other properties of fluids have been studied with lattice gas models as well. In fact, lattice gas methods of hydrodynamics is currently one

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Fig. 4

Figure 14.4: A circular wave emerges from the dynamics of particles on a square lattice.

of the most actively studied applications of cellular automata, around the world. As mentioned in the introduction, a group at Los Alamos has been very successful with flow simulations through porous media. Many other experimental results and mathematical analyses of CA hydrodynamics have appeared [24, 9, 25, 26].

Other approaches to acoustic wave propagation are described in [28, 29].

14.2.5 Optics

The same HPP model, with minor modifications, has also been used to perform simple experiments with optics, such as reflection and refraction. In fact, in this section the wave phenomena is more similar to sonics than optics since a background gas or "ether" is used, but the description is easier to follow in the language of optics. A different CA approach to optics with a demonstration of interference in a "double-slit experiment", is described in [30].

Reflection is fairly simple to accomplish by introducing a new type of quasiparticle which doesn't move, but with which the normal particles interact. Either specular collisions or a reversal of momentum ("no-slip") can be used. These "wall" particles are considered to have infinite mass. Thus they don't move during collisions. Reflective surfaces of arbitrary shape (such as a parabolic mirror) made of these special particles can be drawn in the array.

Note that these extra particles can be mathematically described by extending the vector representation discussed previously. Thus, a 5-vector can be used to describe the lattice gas particles and the immobile barrier ($2^5 = 32$ states/cell).

Implementing refraction might seem like a more difficult task, but actually only requires another very simple modification. A way to give different regions different *indices of refraction* is needed. This means that the "speed of light" should be different in these different regions (i.e. slower in a lens than in a vacuum). This can be accomplished by marking certain sites of the array with a flag. These sites will have the special property that they will only be updated *half as often as normal cells.* While at first this may seem like a very nonstandard extension, it is possible to implement this as part of the local rule, by sufficiently increasing the number of states per cell. By updating the cells in the lens region half as often, the index of refraction, which is defined as $n_2 = c/v_2$, should have a value of 2, while the vacuum's index of refraction n_1 will simply be 1. Note that other update-frequency ratios can be used, giving other relative indices of refraction.

With the addition of these "slow cells", it is possible to draw lenses of any shape, such as circular or planar lenses. By sending planar "light" waves through these lenses, their properties can be observed and measured. It is possible to construct a planar "light" wave by activating an entire row or column with particles ("photons"). Several adjacent columns can be activated in this way for a stronger signal. As usual, the random background noise will be present in the array.

The result of a planar wave passing from a vacuum into a lens that has an index of refraction of 2 is shown in Figure 14.5. The angles θ_i are the angles between the propagation vectors and the normal to the interface. When these angles are measured from the figure, the empirical index of refraction can be calculated from $n_1 sin(\theta_1) = n_2 sin(\theta_2)$. The experiment shown yields $n_2 = 1.99 \pm 0.07$, which is very close to the expected value. Note also that there is a faint *reflection* from the surface of the lens; this too matches the behavior in a physical system. While at first it seems that there is no reason for a reflection, there is a simple explanation. The HPP rule is reversible; when a wave passes from vacuum into lens, it slows down, thus compressing as it moves into the lens. However, the waves we have been using are so dense that in order to compress, they would have to exceed the maximum possible particle density. Since this cannot happen, and since in a reversible system no information can be lost, there is necessarily a reflection.

The empirical index of refraction corresponds to the predicted value over a wide range of angles whether the planar wave is moving from vacuum into lens or lens into vacuum. However, the measured values begin to deviate as the critical angle [3] is approached. Beyond the critical angle, no wave exits from the lens, which is the correct behavior.

A shortcoming in this model is the following. When a wave passes from lens into vacuum, there is no internal reflection from the surface. The above argument for the necessity of a reflection when moving from vacuum to lens does not apply here, because the wave *expands* upon exiting the lens, and will not exceed the maximum density. However, by adjusting the

[3] When the wave is moving inside the lens toward the vacuum, this is the angle at which the outgoing ray is refracted to 90° from the normal to the surface. Thus, the wave travels along the lens surface and the situation is referred to as *total internal reflection.*

Fig. 5

Figure 14.5: A planar wave, originally vertically oriented at the left edge of the array, is reflected and refracted as it moves toward the right. The white area represents a vacuum, the grey area a lens. To improve the clarity of the image, several copies of the system were run. Each copy began with an identical initial wave, but a different random distribution of the background noise. By correlating the different copies of the system, some of the background noise was filtered out in this image, and the clarity of the waves was improved.

boundary conditions between the two media, and making a small extension to the rule, this problem can be overcome as well. If we allow a *third* medium which has a higher index of refraction than either of the others, and then place an "infinitesimal" (single-cell) layer of this new medium at the interface between lens and vacuum, then our information-loss argument will again apply (since the wave has to compress to pass through the new layer). A lens which has had its surface treated in this way seems to produce results which are correct within the measured precision. Further analysis will determine how successful it really is under different conditions.

14.2.6 Chemical Reactions

In addition to the physical systems discussed in earlier sections, there is also interest in using cellular automata to model the evolution of chemical reactions [31, 32, 33, 34, 35, 19]. We will present one example in some detail below. This is a model of a surface-reaction which exhibits a kinetic phase transition. This system is of interest for its collective (statistical) properties rather its spatial behavior. Thus, this example illustrates the use of CA for simulation in an abstract parameter space.

$CO - O_2$ Surface Reactions

A system that has been studied a great deal is the oxidation of carbon monoxide. This system consists of the following components: (1) adsorption of the reactants on the surface, (2) reaction of the species, (3) desorption of the product. More specifically, O_2 and CO are adsorbed onto the surface, where the reaction $CO+O \rightarrow CO_2$ can take place, and the resulting CO_2 is desorbed. In our cellular automaton model, each cell in the two-dimensional array represents a site on the surface of the catalyst. It will be a 3-state CA, the states being (**A**) *empty*, (**B**) O, and (**C**) CO. The model will be probabilistic. The gas above the surface consists of a CO concentration X_A, and O_2 concentration $X_B = 1 - X_A$. We will ignore the effects of the surface reactions on the composition of the gas, and thus assume that the concentration X_A (and therefore X_B) is constant.

CA models of this surface-reaction system have been studied by Ziff *et al.* [31], Dickman [32], and by Droz and Chopard [33]. We will discuss the version described in [33]. A simplified version of their rule is as follows:

- if there are two adjacent empty sites, they will become state **B** (containing an O atom) with probability $1 - X_A$. Upon adsorption, O_2 dissociates into two O atoms residing on adjacent sites.
- An empty site (regardless of its neighbors) will assume state **C** (a CO molecule) with probability X_A.
- A site in state **B** will become empty if it has a neighbor in state **C**, and a cell in state **C** will become empty if a neighbor is in state **B**. This represents the reaction of CO with O on adjacent sites, and desorption of the product.

Analysis and experiments were done by Droz and Chopard using a CAM, to study the properties of this model. The results of experimentation indicate that two second-order phase transitions exist near two critical concentrations X_{A1} and X_{A2}. When the concentration of CO exceeds the critical value X_{A1}, the surface will become permanently "poisoned" with CO; a similar poisoning with O occurs when the concentration X_A of CO falls below the threshold X_{A2}. The behavior of the system near these two values exhibits second-order transitions between zero production-rate of CO_2 and non-zero rates. Further analysis indicates that the model corresponds well with mean-field theory analyses. The mean-field-like behavior emerges as a result of the "randomness" [4] of the gases above the surface. This prevents correlations on the surface which might emerge in a model which explicitly simulated the gas above the surface.

14.3 Hardware

A wide variety of machines have been built that can perform CA computations at high speeds. Some of the more widely known past and future

[4] The probability concentration X_A can be implemented either with external hardware or as a diffusing gas on a CAM.

machines are described below. A good bibliography of machines built by various research groups is included in [36].

- CAM-6 costs under $2000, plugs into an IBM PC or compatible, and updates a 256x256 array of 16-state cells, 60 times per second. For this type of application, CAM-6 is as fast as the Cray-1. The amazing performance/cost ratio makes it clear that special-purpose hardware is desirable for CA simulations. Unfortunately, this product was last produced in early 1989 and there are no current plans to restart production.

  A new product, however, called CAM-PC, is based on the CAM-6 specifications, but includes several enhancements that have been suggested by members of the CAM-6 User's Group and other CA researchers. It is being developed by a new company with help from the Information Mechanics Group to make CAM available to the research community at a reasonable cost [37].

- CAM-8 is currently being designed at MIT. A single module will have 64 times the storage capacity of CAM-6. More details of the architecture is described in [7].

- RAP2 is currently being designed and built for lattice gas simulations at the National Center for Scientific Research in France. This is described in [4].

- Another lattice gas machine, LGM-1, is under construction at Princeton [5].

- For a mere $10 million, you can get a fully-loaded Connection-Machine 2, with 65,536 processors or a fully-loaded Cray Y-MP which can cost up to three times as much. These machines run cellular automata simulations faster than any other currently available machines.

- A lattice gas machine has been proposed [8] which will run at approximately 10^8 times the speed of a Cray Y-MP, at about 2/3 the cost.

14.4 Current Sources of Literature

Major research institutions around the world support research in cellular automata. For example, the Los Alamos Alamos National Laboratory, IBM Research, the French National Center for Scientific Research and the

Trieste International School for Advanced Studies, in addition to science and engineering departments in major universities around the world.

CA research is published in diverse places. Several regular sources of current information are:

- Complex Systems — This journal is edited by S. Wolfram who has made many contributions to CA science. CA articles appear here regularly.
- Physica D — CA articles are frequently published in this journal. Physica 10-D contained the proceedings of the 1986 CA conference. The proceedings from the 1989 CA conference will be published in an upcoming volume of this journal.
- Scientific American — A.K. Dewdney's "Computer Recreations" column has featured CA many times (see [38] for three recent articles). Martin Gardner's "Mathematical Games" column, an ancestor of Dewdney's column, was where the game of Life was first introduced to the mass public.
- Algorithm – A.K. Dewdney has started this new computer magazine. It is expected to be a source of CA-related articles in the future.
- Various introductory articles have appeared in Byte and other personal computing magazines (e.g. [39, 40]).

14.5 An Outstanding Problem in CA Simulations

Many fields of research have difficult problems whose solution opens or closes many avenues of investigation and application. The field of cellular automata is still relatively young and there are many such problems. While most of the CA applications research focuses on gases and incompressible fluids, one of the outstanding problems in cellular automata research is the representation of solid elastic bodies. This requires that many "particles" move in a correlated way. A solution to this problem has been described for one-dimensional objects [41] and it has been implemented on a CAM [42]. A general rule which allows a representation of arbitrarily shaped two- and three-dimensional bodies is desired. This would enable complex simulations that combine objects having different length scales. For example, it may be desirable to simulate the deformation of an elastic tube in a fluid stream, or the buckling of a support under a high pressure gas. By treating both solid bodies and particles or fluids on the same footing, some very complex transformations within the simulation are possible, such as a volcanic explosion which scatters a large fractal structure into small solids that fly and spin through space.

The solid body problem is a correlation problem. A solution to this problem may also have an impact on the simulation of other systems with can be described in terms of correlations of massive numbers of particles, such as superfluids and the electronic structures in metals and semiconductors [43]. There are other representation problems that need to be addressed, but in the authors' view, a solution to the "solid body" problem would provide tremendous rewards.

14.6 Exercises

Note: Many of the following exercises are for cellular automata on a square lattice. In order to facilitate a discussion of the rules, the following nomenclature, which is identical to that of [18], is introduced. For 2-state automata, the value of the state of a cell is referred to as CENTER. The values of the states of the nearest neighboring cells are called NORTH, SOUTH, EAST and WEST. The values of the states of the second nearest neighboring cells are called NORTHEAST, SOUTHEAST, SOUTHWEST and NORTHWEST.

Most of the rules here make use of the "MOORE" neighborhood which uses the values CENTER, NORTH, SOUTH, EAST, WEST, NORTHEAST, SOUTHEAST, NORTHWEST and SOUTHWEST.

1. How would you extend the representation discussed in section 14.2.3 to describe the lattice gas on an hexagonal array?

2. Write a rule to simulate a self-diffusing gas on a hexagonal lattice. Assume that momentum is conserved. Is more than one rule possible?

3. Write a rule to simulate 3 diffusing gases on a square lattice. Assume that momentum is conserved and that all particles have the same mass. Is more than one rule possible?

4. Consider the following rule on a square lattice of 2-state automata: For a given cell, compute the sum of the values in its MOORE neighborhood. If this number is greater than 4, set the cell state to 1, otherwise set the cell state to 0. This is known as a voting rule. Given a random initial condition, what happens to the pattern over many time steps?

5. Describe what happens when 2 sound waves collide in the HPP model.
6. How would you extend the mathematical representation of the HPP model to handle both reflecting and refracting materials?
7. Consider the following rule on a square lattice of 2-state automata. For a given cell, examine NORTH and SOUTH. If SOUTH is 0, set the state of the cell to NORTH. If SOUTH is 1, don't change the state of the cell. What does this rule do to an initial condition consisting of a row of 6 consecutive cells in state 1 if all the other cells are in state 0?
8. Describe how to setup a cellular automata simulation of an equilibrium reaction between a diatomic molecule and its atomic constituents. Assume that the atomic species freely diffuse and that two atoms form a diatomic molecule whenever they are in adjacent cells. Also assume that there is a catalyst at a finite number of locations which decomposes the molecule into atoms. Also conserve the total number of atoms.
9. Compute the mean free path as a function of density for the self-diffusion model on both square and hexagonal lattices.
10. Write a rule on a square lattice that computes the instantaneous force on a movable wall.
11. Describe how to implement the correlated motion of three particles arranged in a row on a 2-D square lattice (hint: use a short period sequence of rules)
12. Describe how to implement the correlated motion of an elastic body of arbitrary shape on a 2-D lattice. How would you handle a collision between two such bodies?
13. In a 2-D system in which each cell has an integer value between 0 and 255 (8-bit cells), consider the following rule: add the values of the center cell and its eight neighbors, and divide by nine. In other words, each cell's new value will be the average value in its current neighborhood. This has been used to model *heat flow* (see [44], for example). Why do you think this model works? (a) What will happen if we start with random initial configurations, and let the system run for a very long period of time? Will the system ever become stable or periodic? If so, what is the physical analogy of the stable configuration? (b) When finding the average value of the local neighborhood, some method of truncation or rounding must be used. What effect

will different methods have on the dynamics of the system? (c) How can the system be generalized, i.e. what simple change could we make to introduce one or more parameters with physical meaning?

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