Cellular Automata Modeling of Physical Systems

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This book provides a self-contained introduction to cellular automata and lattice Boltzmann techniques.

Beginning with a chapter introducing the basic concepts of this developing field, a second chapter describes methods used in cellular automata modeling. Following chapters discuss the statistical mechanics of lattice gases, diffusion phenomena, reaction-diffusion processes and nonequilibrium phase transitions. A final chapter looks at other models and applications, such as wave propagation and multiparticle fluids. With a pedagogic approach, the volume focuses on the use of cellular automata in the framework of equilibrium and nonequilibrium statistical physics. It also emphasizes application-oriented problems such as fluid dynamics and pattern formation. The book contains many examples and problems. A glossary and a detailed list of references are also included.

This will be a valuable book for graduate students and researchers working in statistical physics, solid state physics, chemical physics and computer science.

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To Viviane
Cléa, Tristan and Daphné

and Dominique
Anne-Virginie and Philippe

Everything should be made as simple as possible but not simpler
A. Einstein

Preface

The cellular automata approach and the related modeling techniques are powerful methods to describe, understand and simulate the behavior of complex systems. The aim of this book is to provide a pedagogical and self-contained introduction to this field and also to introduce recent developments. Our main goal is to present the fundamental theoretical concepts necessary for a researcher to address advanced applications in physics and other scientific areas.

In particular, this book discusses the use of cellular automata in the framework of equilibrium and nonequilibrium statistical physics and in application-oriented problems. The basic ideas and concepts are illustrated on simple examples so as to highlight the method. A selected bibliography is provided in order to guide the reader through this expanding field.

Several relevant domains of application have been mentioned only through references to the bibliography, or are treated superficially. This is not because we feel these topics are less important but, rather, because a somewhat subjective selection was necessary according to the scope of the book. Nevertheless, we think that the topics we have covered are significant enough to give a fair idea of how the cellular automata technique may be applied to other systems.

This book is written for researchers and students working in statistical physics, solid state physics, chemical physics and computer science, and anyone interested in modeling complex systems. A glossary is included to give a definition of several technical terms that are frequently used throughout the text. At the end of the first six chapters, a selection of problems is given. These problems will help the reader to become familiar with the concepts introduced in the corresponding chapter, or will introduce him to new topics that have not been covered in the text. Some problems are rather easy, although they usually require some programming effort, but other problems are more involved and will demand significant time to complete.

Most of the cellular automata simulations and results presented in this book have been produced on the 8k Connection Machine CM-200 of the University of Geneva. Others have been computed on an IBM SP2 parallel computer, also installed at the University of Geneva. Although a parallel supercomputer is quite useful when considering large scale simulations, common workstations and even modern personal computers are well adapted to perform cellular automata computations, except for on-line display which is alway very desirable. Dedicated hardware is also available but, usually, less flexible than a general purpose machine.

Despite our effort, several errors and misprints are still likely to be present. Please report them to us* (as well as any comment or suggestion).

We would like to thank all the people who have made this book possible and, in particular Claude Godrèche who gave us the opportunity to write it. Special thanks go to Pascal Luthi and Alexandre Masselot who made several original and important simulations which are presented in this book. Other people have played a direct or indirect role in the preparation of the manuscript. Among them, we thank Rodolphe Chatagny, Stephen Cornell, Laurent Frachebourg, Alan McKane, Zoltan Racz and Pierre-Antoine Rey.

Finally we acknowledge the Swiss National Science Foundation who funded some of the research reported here and the Computer Science Department and the Theoretical Physics Department of the University of Geneva for making available the necessary environment and infrastructure for this enterprise.

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Contents

1
Introduction

1.1 Brief history

Cellular automata (often termed CA) are an idealization of a physical system in which space and time are discrete, and the physical quantities take only a finite set of values.

Although cellular automata have been reinvented several times (often under different names), the concept of a cellular automaton dates back from the late 1940s. During the following fifty years of existence, cellular automata have been developed and used in many different fields. A vast body of literature is related to these topics. Many conference proceedings [1–8]), special journal issues [9,10] and articles are available.

In this section, our purpose is not to present a detailed history of the developments of the cellular automata approach but, rather, to emphasize some of the important steps.

1.1.1 Self-reproducing systems

The reasons that have led to the elaboration of cellular automata are very ambitious and still very present. The pioneer is certainly John von Neumann who, at the end of the 1940s, was involved in the design of the first digital computers. Although von Neumann's name is definitely associated with the architecture of today's sequential computers, his concept of cellular automata constitutes also the first applicable model of massively parallel computation.

Von Neumann was thinking of imitating the behavior of a human brain in order to build a machine able to solve very complex problems. However, his motivation was more ambitious than just a performance increase of the computers of that time. He thought that a machine with such a complexity as the brain should also contain self-control and self-repair mechanisms. His idea was to get rid of the difference which exists between processors and the data, by considering them on the same footing. This led him to envisage a machine capable of building itself, out of some available material.

Rapidly, he considered the problem from a more formal viewpoint and tried to define the properties a system should have to be self-replicating. He was mostly interested to find a logical abstraction of the self-reproduction mechanism, without reference to the biological processes involved.

Following the suggestions of S. Ulam [11], von Neumann addressed this question in the framework of a fully discrete universe made up of cells. Each cell is characterized by an internal state, which typically consists of a finite number of information bits. Von Neumann suggested that this system of cells evolves, in discrete time steps, like simple automata which only know of a simple recipe to compute their new internal state. The rule determining the evolution of this system is the same for all cells and is a function of the states of the neighbor cells. Similarly to what happens in any biological system, the activity of the cells takes place simultaneously. However, the same clock drives the evolution of each cell and the updating of the internal state of each cell occurs synchronously. These fully discrete dynamical systems (cellular space) invented by von Neumann are now referred to as *cellular automata*.

The first self-replicating cellular automaton proposed by von Neumann was composed of a two-dimensional square lattice and the self-reproducing structure was made up of several thousand elementary cells. Each of these cells had up to 29 possible states [12]. The evolution rule required the state of each cell plus its four nearest neighbors, located north, south, west and east. Due to its complexity, the von Neumann rule has only been partially implemented on a computer [13].

However, von Neumann had succeeded in finding a discrete structure of cells bearing in themselves the recipe to generate new identical individuals. Although this result is hardly even a very primitive form of life, it is quite interesting because it is usually expected that a machine can only build an object of lesser complexity than itself. With self-replicating cellular automata, one obtains a "machine" able to create new machines of identical complexity and capabilities.

The von Neumann rule has the so-called property of universal computation. This means that there exists an initial configuration of the cellular automaton which leads to the solution of any computer algorithm. This sounds a surprising statement: how will such a discrete dynamics help us to solve any problem? It turns out that this property is of theoretical rather than practical interest. Indeed, the property of universal computing means that any computer circuit (logical gates) can be simulated by the rule of the automaton. All this shows that quite complex and unexpected behavior can emerge from a cellular automaton rule.

After the work of von Neumann, others have followed the same line of research and the problem is still of interest [14]. In particular, E.F. Codd [15] in 1968 and much later C.G. Langton [16] and Byl [17] proposed much simpler cellular automata rules capable of self-replicating and using only eight states. This simplification was made possible by giving up the property of computational universality, while still conserving the idea of having a spatially distributed sequence of instructions (a kind of cellular DNA) which is executed to create a new structure and then entirely copied in this new structure.

More generally, artificial life is currently a domain which is intensively studied. Its purpose is to better understand real life and the behavior of living species through computer models. Cellular automata have been an early attempt in this direction and can certainly be further exploited to progress in this field [18,19].

1.1.2 Simple dynamical systems

In a related framework, it is interesting to remember that it is precisely a simple ecological model that has brought the concept of cellular automata to the attention of wide audience. In 1970, the mathematician John Conway proposed his now famous *game of life* [20]. His motivation was to find a simple rule leading to complex behaviors. He imagined a two-dimensional square lattice, like a checkerboard, in which each cell can be either alive (state one) or dead (state zero). The updating rule of the game of life is as follows: a dead cell surrounded by exactly three living cells comes back to life. On the other hand, a living cell surrounded by less than two or more than three neighbors dies of isolation or overcrowdness. Here, the surrounding cells correspond to the neighborhood composed of the four nearest cells (north, south, east and west) plus the four second nearest neighbors, along the diagonals. Figure 1.1 shows three configurations of the game of life automaton, separated by 10 iterations.

It turned out that the game of life automaton has an unexpectedly rich behavior. Complex structures emerge out of a primitive "soup" and evolve so as to develop some skills. For instance, objects called *gliders* may form (see problems, section 1.4). Gliders correspond to a particular arrangement of adjacent cells that has the property to move across space, along straight trajectories. Many more such structures have been identified in the vast body of literature devoted to the game of life [21,22]. As for the von Neumann rule, the game of life is a cellular automata capable of computational universality.

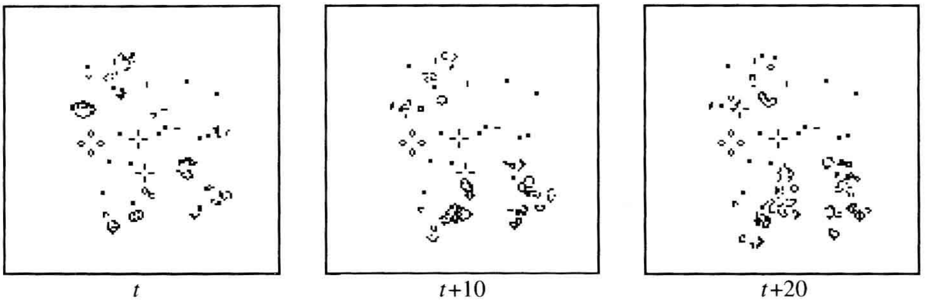

Fig. 1.1. The game of life automaton. Black dots represents living cells whereas dead cells are white. The figure shows the evolution of some random initial configurations.

In addition to these theoretical aspects, cellular automata were used in the 1950s for image processing [23]. It was recognized early on that much tedious picture analysis could be carried out automatically, according to a cellular automata computing model: the pixels of an image can be treated simultaneously, using simple local operations. Special-purpose machines based on cellular automata logic have been developed for noise reduction, counting and size estimation in images obtained from observations with a microscope.

At the beginning of the 1980s, S. Wolfram studied in detail a family of simple one-dimensional cellular automata rules (the now famous Wolfram rules [24,25]). He had noticed that a cellular automaton is a discrete dynamical system and, as such, exhibits many of the behaviors encountered in a continuous system, yet in a much simpler framework. A concept such as complexity could be investigated on mathematical models allowing an exact numerical computer calculation, because of their Boolean nature (no numerical errors nor truncation as in more traditional models). Wolfram's results have contributed to prove that cellular automata are important objects to consider for statistical mechanics studies and, at the present time, Wolfram's rule are still the topic of much research.

1.1.3 A synthetic universe

The property of many cellular automata rules being a universal computer made several authors think that the physical world itself could be a very large cellular automaton. Tommaso Toffoli [26] compares cellular automata to a synthetic model of the universe in which the physical laws are expressed in terms of simple local rules on a discrete space–time structure.