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Although their scope and methodologies overlap somewhat, one can distinguish the following main concepts and tools: self-organization, nonlinear dynamics, synergetics, turbulence, dynamical systems, catastrophes, instabilities, stochastic processes, chaos, graphs and networks, cellular automata, adaptive systems, genetic algorithms and computational intelligence.

The two major book publication platforms of the Springer Complexity program are the monograph series "Understanding Complex Systems" focusing on the various applications of complexity, and the "Springer Series in Synergetics", which is devoted to the quantitative theoretical and methodological foundations. In addition to the books in these two core series, the program also incorporates individual titles ranging from textbooks to major reference works.

Understanding Complex Systems

Founding Editor: J.A. Scott Kelso

Future scientific and technological developments in many fields will necessarily depend upon coming to grips with complex systems. Such systems are complex in both their composition – typically many different kinds of components interacting simultaneously and nonlinearly with each other and their environments on multiple levels – and in the rich diversity of behavior of which they are capable.

The Springer Series in Understanding Complex Systems series (UCS) promotes new strategies and paradigms for understanding and realizing applications of complex systems research in a wide variety of fields and endeavors. UCS is explicitly transdisciplinary. It has three main goals: First, to elaborate the concepts, methods and tools of complex systems at all levels of description and in all scientific fields, especially newly emerging areas within the life, social, behavioral, economic, neuro- and cognitive sciences (and derivatives thereof); second, to encourage novel applications of these ideas in various fields of engineering and computation such as robotics, nano-technology and informatics; third, to provide a single forum within which commonalities and differences in the workings of complex systems may be discerned, hence leading to deeper insight and understanding.

UCS will publish monographs, lecture notes and selected edited contributions aimed at communicating new findings to a large multidisciplinary audience.

Alfons G. Hoekstra · Jiří Kroc · Peter M.A. Sloot
Editors

Simulating Complex Systems by Cellular Automata

Springer

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Simulation based understanding of complex systems with cellular automata.

Foreword

What are Cellular Automata good for?
What you always wanted to ask about them
but where afraid of the answer.

Cellular automata (CA) are a paradigm of *fine-grained*, *uniform*, *parallel* computation. This mode of computing is supposedly one that is most naturally and efficiently supported by physics, since physics itself is at bottom a uniform parallel computing medium (thence the appeal of "cellular automata machines" and all that). Obviously, then, if you have a complex system (such as an urban traffic network or a simultaneous system of chemical reactions) and manage to represent it as a cellular automaton, then you can "run" it on CA hardware – which you'll be using effectively as a "numerical integrator," see what happens, and hopefully develop a better understanding of your systems structure and function. Just like with experimental mathematics, there is nothing wrong with this prescription – as long as it is taken only in *trace amounts*. But if you think that, just because you've managed to dress your system in the garb of a CA, then running it and watching its evolution will make you *understand* it – well, you are in for a big disappointment, and so will your readers.

Even though their distinguishing characteristic – that they lend themselves to efficient and *exact* numerical integration – plays a major role in our story (unlike partial differential equations, CA are not chronically beset by issues of approximation, convergence, and stability – and one does not have to be an expert in calculus and functional analysis to use one), nonetheless CA are primarily a *conceptual* tool. In this sense, they play a role, for understanding and taming a complex system, similar to that played by *mathematical physics* in making us understand physics itself.

As 50 years of development consistently testify, the best contribution that a CA approach can give to the understanding of a complex system is at the stage of *developing the model* – not running an industrial version of it. *A successful CA model is the seed of its own demise!* The reason is simple. A CA model is a plausible *microscopic* dynamics (no mysteries to it, no infinitesimals, no indeterminism) that yields in a well-understood way the emergence of a desired *mesoscopic* behavior. In principle, an astronomically large implementation of that model will also give us the full-fledged *macroscopics*. Suppose we have a CA that "predicts" the formation of water droplets or ice needles by means of a simple combinatorics of tokens. If we had the resources, by scaling the model billions of billions of times we could model fog, clouds, etc., all the way up to global weather. But once we have derived, from the CA, the bulk properties of a water droplet, we can feed these numerical parameters to a higher-level model (a finite-element model or a differential equation), in which all that counts is just droplets per cubic meter, temperature, and so forth, and *much more practically and efficiently* model a whole cloud. At a higher aggregation level, we can model regional – and ultimatelly global – weather. That is, once we have learned from a CA how a water droplet emerges and behaves, there is no point in re-running the entire process from scratch for every single droplet of a rainstorm – even though in principle we might! A better allocation of our computational budget is (a) to use CA to learn whether, under what conditions, and at what level there emerge recognizable *mesoscopic laws* out of simple microscopic mechanisms; and then (b) use these mesoscopic laws as a basis for higher-level analytical models ("equations") or numerical models ("simulations").

The present collection gives several examples of this *maieutic* role of CA.

In addition to that, recent developments in the theory of CA and their "lattice gas" variants suggest that these structures may play an even more blatantly conceptual modeling role, analogous to that of analytical mechanics. That is, after the arithmetization of physics (Galileo), the mechanization of physics (Newton, Faraday, Maxwell), and the geometrization of physics (Poincaré, Einstein), we may envisage the *informatization* of physics not only at the statistical level (Boltzmann, Gibbs) but also at the fundamental level.

According to *Hamiltons* "least action" *principle*, among all conceivable trajectories of a physical systems the effective ones are those whose *action* is stationary with respect to infinitesimal variations of the trajectory. According to *Noethers theorem*, in the dynamical systems typically dealt with by physics "to every continuous one-parameter group of symmetries there correspond a conserved quantity." (E.g., the existence of a conserved a quantity called *energy* comes from the fact that a systems laws do not change with *time*.) However, in spite of their sweeping generality, these principles are predicated only for physical systems that are continous, differentiable, invertible, and symplectic. Does that mean that nothing at all of these principles is left if one turns to systems that, like CA, share many properties with physics but are *discrete*?

To salvage some aspects of those principles for CA, one has to transliterate concepts, as far as possible, from the continouous to the discrete; to know how to do that, one first has to ask "What is the essential, most likely combinatorial, and inescapably tautological nature of those principles?", "What kind of *accounting* is it that they are doing?", or, "What is it that they are really trying to tell us?" (think of Boltzmann and his intuition that entropy has to do with *number* of states). More importantly for the advancement of science, we can reverse the roles of means and goal in the above endeavor. That is, let us work at fitting (as much as posible of) those principles into a CA context, hoping that that will reveal to all of us (CA aficionados and physicists alike) what those somewhat mystical and teleological principles "really mean." By using a CA as a *discrete* "kitchen experiment" of analytic mechanics, we bring "magical" aspects of theoretical physics down to earth. After the fair's magic show, the man in the street – any one of us, really – will then go home and tell his children (and, what's more important, to himself), "Oh, there was nothing to it! Here is how it must work – let me show you. . . ."

In conclusion, the discipline of modeling with cellular automata is an excellent way to identify, without being distracted by irrelevant technicalities, those element of a system that are *truly essential* – namely, those that are both necessary and sufficient to yield a *certain kind* of behavior. "Keep things simple!", or, in Donald Knuth's words, "Premature optimization is the root of all evil."

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Preface

Deeply rooted in fundamental research in Mathematics and Computer Science, Cellular Automata are recognized as an intuitive modeling paradigm for Complex Systems. Very basic Cellular Automata, with extremely simple micro dynamics such as the Game of Life, show an almost endless display of complex emergent behavior. By modeling natural or man-made Complex Systems with Cellular Automata we usually dissect the system to it's most fundamental and minimal properties and interactions, such that the simulated dynamics *mimics* the emergent behavior of the real Complex System, leading to a true *understanding* of the fundamental properties of the system under study.

For instance, Cellular Automata models of vehicle traffic are a beautiful example. A few simple rules relating to acceleration, deceleration, and maximum speed of vehicles in a one-dimensional Cellular Automata are sufficient to display all different types of motions that cars on a freeway can have (free flow, stop-and-go, jamming), as well as showing backward traveling density waves in stop-and-go traffic and reproducing the fundamental diagram of car throughput on a freeway as a function of car density.

Vice-versa, Cellular Automata can also be designed to *produce* a desired emergent behavior, using theoretical methodologies or using e.g. evolutionary techniques to find Cellular Automata rules that produce specified characteristics.

Cellular Automata can also actually *reproduce* the dynamics of Complex Systems *qualitatively*. For instance, Lattice Gas Cellular Automata are a class of Cellular Automata that reproduce many of the intricate dynamics in fluids. Likewise, other fundamental physical systems, such as Reaction–Diffusion or Advection–Diffusion can be qualitatively modeled. These Cellular Automata models can actually be used to *predict* the behavior of Complex Systems under many different circumstances. Nowadays there are many applications of Cellular Automata models in Computational Physics or – Chemistry, but also in for instance Systems Biology (e.g. models for diffusion limited gene regulatory networks).

Over the last decade or so, there has been a tremendous progress in studying Complex Systems with Cellular Automata. They are not only being used within their originating disciplines (say Physics, Computer Science, Mathematics), but are also applied in quite different disciplines such as epidemiology, immunology, sociology, and finance. Cellular Automata are quite successful in for instance modeling immune response after HIV infection, both the short term effects, as well as the long term effect that finally lead to the development of AIDS. Cellular Automata are also used to study the dynamics of crowds, for instance in situations where a crowd must escape from a confined space through a small door.

In this context of fast and impressive progress in the field the idea to compose this book emerged. Moreover, another experience convinced us that we should embark on this project that in the end resulted in this book. When teaching Complex Systems Simulations to Master students in the Amsterdam Master program on Computational Science, we always experience the great appeal that Cellular Automata have on the students, and we are always impressed by the deep understanding that our students – but we as well – obtain of a large range of complex systems they try to model and understand using Cellular Automata. These students come from many disciplines, as broad as the application areas of Cellular Automata mentioned earlier.

For us it became evident that an edited book focusing on all aspects of modeling Complex Systems with Cellular Automata was needed, as a welcome overview of the field for its practitioners, as well as a good starting point for detailed study on the graduate and post-graduate level. While Jiří Kroc was a visiting scientist in Amsterdam, in the period September 2007 to September 2008, the idea materialized and the "book project" went into high gear.

The book contains three parts, two major parts on theory and applications, and a smaller part on software. The theory part contains fundamental chapters on how to design and/or apply Cellular Automata for many different areas. This should give the readers a representative overview and strong background on many aspects related to modeling with Cellular Automata. In the applications part a number of representative examples of really using Cellular Automata in a large range of disciplines is presented. By providing a large set of examples, this part should give readers a good idea of the real strength of this kind of modeling and challenge them to apply Cellular Automata in their own field of study. Finally, we included a smaller section on software, to highlight the important work that has been done to create high quality problem solving environments that allow to quickly and relatively easily implement a Cellular Automata model and run simulations, both on the desktop and if needed, on High Performance Computing infrastructures.

We are very proud and happy that many prominent scientists agreed to join this project and prepared a chapter for this book. We are also very pleased to see it materialize in a way as we originally envisioned. We hope that this book will be a source of inspiration to the readers. We certainly challenge students on the graduate and post-graduate level to study this book in detail, learn from it, grasp the fundamental ideas behind modeling Complex Systems with Cellular Automata, and apply it to solve their own problems. For scientists working in many different fields we believe that this book will provide a representative state-of-the-art overview of this field. It not only shows what we *can* do, it also shows current gaps in our knowledge, open issues and suggestions for further study.

We wish all readers a fruitful time reading this book, and wish they experience the same excitement as we did – and still do – when using Cellular Automata for modeling complex systems.

Amsterdam, The Netherlands
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