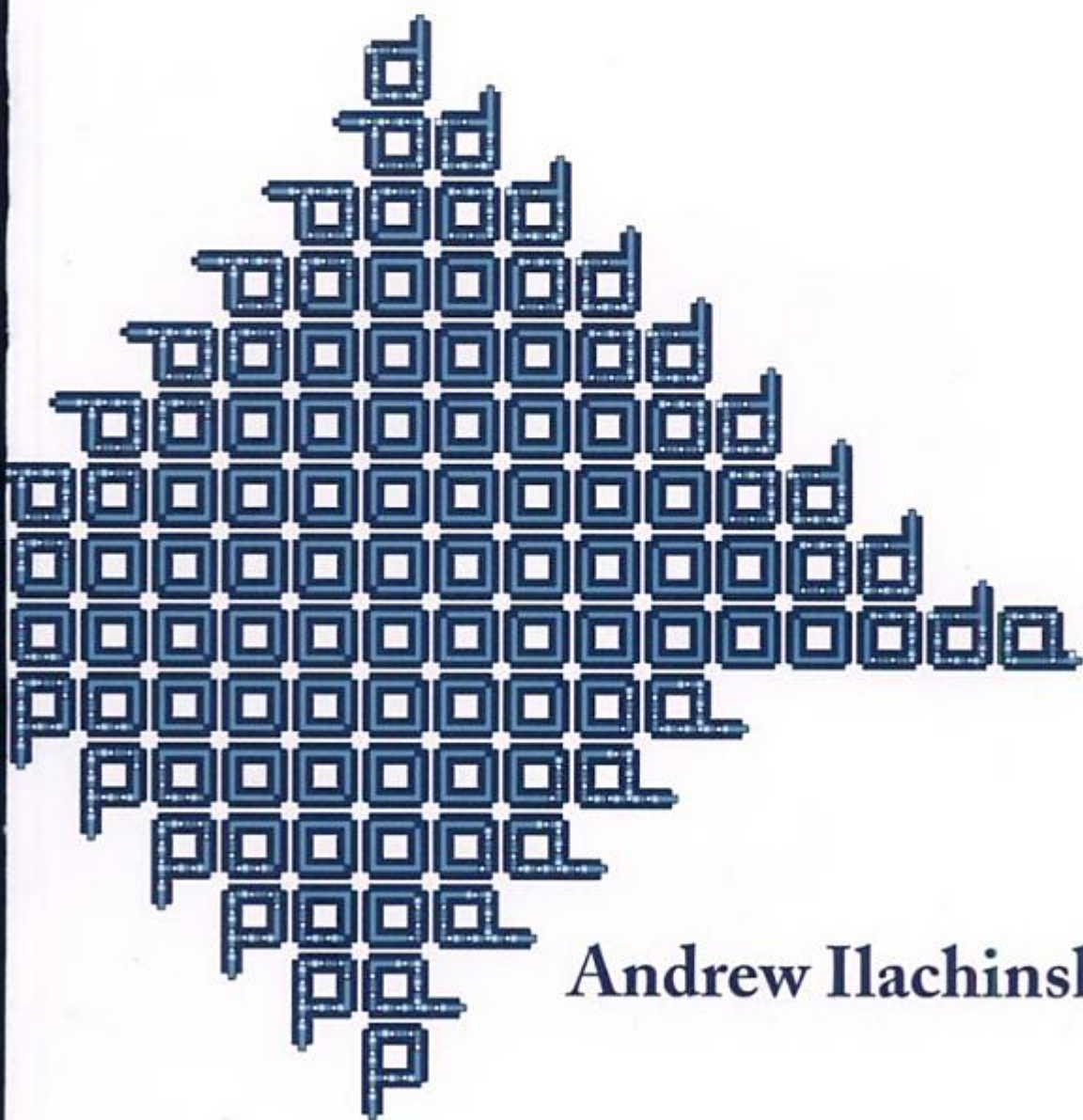


Cellular Automata

A Discrete Universe



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No writing project that takes as long to complete as this one takes place in a vacuum. Such projects are, at best, slow, cumulative processes that—in the end—owe at least twice as much debt to a large cadre of faithful friends and colleagues as they do to the author, whose only significant task (aside from inevitably introducing errors entirely his own) is to humbly commit to paper his own interpretation of the collective wisdom of his companions. Unfortunately, no list of acknowledgments can possibly be complete, for the tapestry of kind suggestions and criticisms has grown far too large over the years to lend itself to individual acknowledgment. Nonetheless, I certainly want to take this opportunity to sincerely thank everyone who has at one time or another, either knowingly or unknowingly, helped nurture this project; from conception, to long gestation, to even longer evolution, to final birth.

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*Whose morning coffee chats about physics, engineering and cosmology kept my sanity in check.

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My sincere, humble apologies to all those that belong on this short list, but cannot find their name so listed. Know that your absence from these acknowledgments conveys no other conscious message other than the obvious evidence it provides of the author's fallible memory.

My deepest thanks, of course, goes to my family: to my mom and dad, *Sam & Katy Ilachinski*, who are two of the most loving and humblest creatures ever to grace this world; to my wife *Irene*, who has so infinitely enriched my life that I feel as though I've been blessed with a glimpse of heaven; and to my son *Noah*, who (at the tender age of two) has already taught me that love has no bounds and that mother nature is infinitely wiser than we know. Without my family's unconditional love, support and patience this book truly could not have been completed,

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Third, *Rich Bronowitz*, who has been the most important teacher, and mentor, in my professional career. I owe Rich an unpayable debt for unreservedly believing in, and allowing me to explore – virtually unencumbered by otherwise ubiquitous bureaucratic obstacles – my vision of introducing cellular automata into the arsenal of mathematical tools used by the operations research community and of applying agent-based modeling techniques to help understand the fundamental processes of conflict. A heartfelt thanks for all you've done, Rich. Know that you have played a far more important, and active, role in my development as an analyst, and as a person, than you allow yourself credit for.

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Preface

In memory of my teacher, friend and mentor, Max Dresden

The book that you—kind reader—are holding in your hand represents a labor of love, in the purest sense, for most of the five-and-a-half years that it took to write; and the additional five years that, because of various setbacks and self-imposed periods of inactivity, it took me to struggle through in order to have it finally see the light of day. In the time that the book has matured from a vague but interesting idea—first brought up by the author’s thesis advisor while waiting for dessert to arrive during a casual luncheon—to its final unintentionally massive form, I have myself evolved dramatically from an idealistic, 28-year-old, sadly underpaid graduate physics student to a husband, father and senior defense analyst working for a naval think-tank,[†] currently developing one of the first cellular-automata-based *artificial-life* simulations of combat. I would like to briefly share a few personal notes about how this book came to be.

I received my Ph.D. in theoretical physics from the *Institute of Theoretical Physics* (ITP) at the State University of Stony Brook in 1988. My thesis research, entitled “Computer Explorations of Discrete Complex Systems,” was conducted under Professor Max Dresden, who was at the time nearing the end of his professional career; a career that began when Max was studying for his own Ph.D. under Uhlenbeck (of spin fame). I was, in fact, Max’s last Ph.D. student, and it was Max who one day suggested to me during one of our frequent lunches that he and I ought to write a book on cellular automata together.

At the time, Max had just had his well-received biography of the Dutch physicist

[†]The *Center for Naval Analyses* (CNA) is a not-for-profit federally funded research & development center.

Kramers[†] published, and was, I suspect, anxious to start a new writing project. The year was 1987: four years after Wolfram's groundbreaking review article on cellular automata that appeared in *Reviews of Modern Physics* [wolf83a], and three years after the founding of the *Santa Fe Institute*, now arguably one of the world's leading centers for complex systems research.

My own interest in cellular automata manifested itself during my first year as a physics graduate student, while I was exploring the conceptual foundations of physics by looking into novel approaches to unifying quantum field theory and relativity. What was then, and remains today, an essentially open problem (string theory notwithstanding), is the unification of quantum mechanics—whose laws operate on the microscopic level—with general relativity—which describes phenomena on the very macroscopic level.

An idea that I had been tinkering with, in early 1983, involved re-writing some microscopic equations of motion on a discrete dynamic lattice representation of space-time. I wanted to see if one could construct a toy universe in which the fundamental distinction between *figure* (i.e. particles) and *ground* (i.e. space-time) is blurred (or disappears completely). Though I did not know it at the time (this was many months prior to Wolfram's review article, and whatever else I may have read on cellular automata certainly was not memorable enough in my own mind to start its own cognitive meme), the formalism I was struggling with to create and understand was precisely that of cellular automata!

The day that Wolfram's article appeared at ITP's library is forever etched in my mind as one of those proverbial milestone events in one's life. I knew instantly that cellular automata embodied a profound new approach to looking at physics and the world; and that cellular automata were a subject about which I had to do a lot of thinking. I will forever be indebted to Max for allowing me to pursue musings that seemed—certainly to those making up the intellectual inner-circle of ITP at the time—comical, at best and childishly *unphysics-like*, at worst. So...

It was with great pleasure that—three years later, and at the tail-end of completing my dissertation—I accepted Max's kind offer to jointly write a book on CA. "One or two years," I thought, "is all it will take." I was wrong.

Following my successful thesis defense in early 1988, I moved down to Washington, D.C. to start what has become a more than decade-long professional occupation as research analyst for the US Navy. My new job was, (and still is!) profoundly time consuming. My official duties soon took me to several (many-week-long) naval exercises at sea, included an intensive several-month-long reconstruction effort of *Operation Desert Storm* (which itself included virtually around-the-clock work days), and culminated in a multi-year stint as CNA's field representative at the naval air station located on Whidbey Island in Washington state (during which time many of my duties introduced me to the unhappy sport of prolonged sleep deprivation).

[†]Max Dresden, *Kramers: Between Tradition and Revolution*, Springer-Verlag, 1987.

Needless to say, the time (and energy) that remained for making any progress on this book after the long work days that characterized this period of my life, kept taking increasingly bigger hits.

Adding to these difficulties of writing a book, Max's own schedule had also undergone significant changes, and he was soon to back off from making a deeper commitment. Soon after I received my Ph.D., Max retired to Professor Emeritus status at Stanford University in California. He became engrossed in editing journals, working on several new physics projects with a fresh set of post Docs, and lecturing throughout the country on extended trips.[§] His schedule thus, unfortunately, left precious little time for writing. Though we had contract offers from two distinguished and reputable publishing houses (we accepted the one from Springer-Verlag), the co-authored project that began in earnest in 1989, was first converted to single authorship (namely, mine), and not long afterward, began languishing from a terminal case of *much, much too much to do in too short a time!*

The premature end of the project seemed to finally come when I learned in 1995 that Max had been diagnosed with an inoperable form of cancer. At the time, I had completed roughly 80% of the book, and the reality of actually completing the Herculean task no longer seemed so farfetched. However, without Max—without his encouragement and always happy outlook—I found that, for psychological reasons, it was difficult for me to continue. The book thus remained in its semi-complete form for several years following Max's sad announcement. Max died a few years later in 1997. As all of us who were graced by this gentle soul know well, Max was a profoundly gifted and inspiring teacher. He will be intensely missed.

What finally saw the book through to its conclusion? I confess to not having a solid answer. However, I am fairly certain that, had it not been for a serendipitous intervention of Jungian synchronicity, the book would never have been completed. In my professional capacity as a research analyst for the US Navy (working for a think tank that also does work for the Marine Corps), I had the distinct privilege and honor of getting to know a truly visionary military thinker: *Lt.Gen (Ret) Paul van Riper*.

General van Riper, during the time when he was Commanding General at the Marine Corps Concept Development Command at Quantico, VA. (1994-1996), approached CNA with an idea for a study that asked, *What do all of these new ideas I've been hearing about – nonlinearity, complexity, complex adaptive systems – have to do with combat?* Since many at CNA knew of my deep interest in the subject, I was soon asked to direct a project addressing this question; a project that has since spawned a follow-on multi-year effort sponsored by the *Office of Naval Research* to develop an artificial-life model of combat.[¶] To say that Lt.Gen van Riper's appear-

[§]Max was particularly fond of giving (always well received) talks at frequently held Chautauqua conferences for schoolteachers.

[¶]Those parts of this research that involve cellular automata are described in chapter 11 of this book. For additional details, including all approved-for-public-release documentation, see

ance on the scene was “welcome” would be a gross understatement. His vision has led me down many interesting new intellectual paths I would likely otherwise have never encountered.

Thus, slowly, at first, then more strongly, my CNA complexity project eventually re-ignited the passion I had inexplicably lost for my *other* complexity project: this book! Thus, to both Max and Gen van Riper, I owe an absolutely enormous, sincerely heartfelt, thanks. To Max for originally igniting and encouraging what was to become a life-long passion; to Paul van Riper for reminding me, more recently, and just as forcefully, of the passion that life’s circumstances had somehow, inadvertently and – as it turns out – only temporarily, dislodged. Thank you both!

I conclude this preface with an observation. Despite the very long gestation period for this book (nearly ten years, from original concept to publication), no other graduate-level book on cellular automata, comparable to the length and scope of this one, has appeared in the interim. Most likely, this is a direct reflection of the very broad scope, along with the relative immaturity, of the field. In any case, I am humble enough to know that my own effort will likely prove to be neither definitive nor complete. This book is intended solely to provide the interested reader with a self-contained reference summarizing some of the groundbreaking work that has been done by a great many researchers.

My greatest pleasure will come from learning that, for those of you who are not immediately put off by the daunting sight of a behemoth of a book sitting on your favorite bookseller’s shelf, this book has inspired a few of you to muse about cellular automata on your own. I am convinced that CA, in one form or another, will eventually be found lurking at the very heart of how our universe really works.

Andy Ilachinski
Springfield, Virginia
March, 2001

Foreword

Cellular automata (CA) are among the simplest mathematical representations of complex systems; where, for the moment, we may take “complex system” to mean any dynamical system that consists of more than a few—typically nonlinearly—interacting parts. As such, CA are extremely useful idealizations of the dynamical behavior of many real systems, including physical fluids, neural networks, molecular dynamical systems, natural ecologies, military command and control networks, and the economy, among many others. Because of their underlying simplicity, CA are also powerful conceptual engines with which to study general pattern formation. They have already provided critical insights into the self-organization of chemical reaction-diffusion systems, crystal growth, pattern formation on seashells, and phase-transition-like phenomena in vehicular traffic flow, to name but a few examples. On a more practical side, CA may provide the basis for extremely powerful encryption algorithms, a subject about which there has recently been much heated debate. There is even some serious speculation that CA may provide the backbone of a radically new discrete fundamental physics (an idea that we will focus our attention on in Chapter 12).

While the history of CA can be traced back to early *Systems’ Theory* and rigorous mathematical analyses conducted primarily by Russian researchers in the 1930s and 40s, their more recent incarnation as simple models of complexity in nature can arguably be traced to a single landmark review paper published by Wolfram in the *Reviews of Modern Physics* in 1983 [wolf83a].

Indeed, the sudden, almost explosive, emergence of CA as a major scientific and intellectual discipline is one of the most important developments in the decade from 1975–1985. It is always difficult and, in fact, a bit arbitrary to pinpoint particular dates as the definitive starting point of a new development, but it is striking how after a slow beginning, much influenced by the scientific demands of World War II, ideas leading to CA and computers entered the literature at an increasing rate. Around 1970, about 300 to 400 mathematically oriented papers dealing with automata were published; at the same time, the number of physics papers was at most a tenth of that. Some ten years later (~ 1980), evidence of a

shift in interest was already appearing: the numbers of mathematics and physics oriented papers was now roughly comparable, 50 to 100 each. In the succeeding five years the physics, or physically motivated, papers increased dramatically (400 to 500), while the number of mathematics papers slowly declined. The number of physics papers continues to increase even today. It is clear that CA can be anticipated to play an increasingly significant, if not major, role in future physics, and these developments should be analyzed and evaluated.

In spite of the large number of papers published on CA, their direct impact on the *mainstream* of physics was (and, depending on what researcher you ask today, still is), rather minor. Although many research studies make use of the computer experience and expertise which has been (and continues to be) developed in connection with CA, this influence remains primarily technical and computational rather than conceptual or philosophical. The contributions of CA have so far consisted of somewhat disjoint investigations which are largely isolated from modern physics—although they are arguably an integral component of an emerging new interdisciplinary research genre, that includes physics, called *complexity theory* (about which we will have more to say later). Complexity theory—as defined by, say, research being done at the *Santa Fe Institute* in New Mexico—is very much an immature, even infant science. This fact, along with it being a fundamentally interdisciplinary field, precludes us from branding it as mainstream *physics*. However, as this book hopes to show, CA are being increasingly recognized as important both for natural ability to simulate the dynamics of real physical systems and for providing powerful conceptual models with which to build (possibly radically new) physical theories.

Whenever a new field emerges, many different individuals contribute to its development. This is of course also true for CA, yet three persons stand out as originating and shaping the field: Alan Turing (1936), John von Neumann (1948) and Stephen Wolfram (1983). In addition, Stanislaw Ulam (1950) and John Conway (1969) each made specific, original contributions of long-lasting fundamental significance. It is interesting that four of these founders were mathematicians, while the sole physicist worked in particle physics and cosmology (rather than many-body theory or macroscopic physics, where current CA techniques find their primary use).

The scientific, mathematical orientation of these founding fathers had a major impact on the early development of CA. It is most remarkable that von Neumann, arguably the dominant figure, came to CA via the unlikely path of an interest in formal logic and the foundations of mathematics. In the 1920s, many of the usual procedures in classical mathematics were severely criticized by Brouwer and Weyl, who argued that the methodology and philosophy of set theory were fundamentally unsound. The intuitionist dogma was that all mathematical results should be constructive: proofs and derivations should be obtained via finite algorithms. Hilbert suggested a systematic program to counter this intuitionist criticism.

John von Neumann, under Hilbert's influence, actually produced a paper in which he showed that a subsystem of classical analysis could be obtained in a fini-

tistic manner. He further showed, by finitistic means, that this system is free of contradictions. He hoped, and even conjectured, that this proof and general conclusion could be extended to all analysis. Kurt Godel's well known proof of the incompleteness theorem, completed a few years later (1931), showed that von Neumann's conjecture was wrong and that Hilbert's program to show the contradiction-free character of mathematics by intuitionist methods was hopeless.

An important consequence of von Neumann's familiarity with finite mathematical schemes was its close, if not direct, connection with numerical analysis. von Neumann, unlike the Bourbaki school of mathematics, had a deep personal interest in numerical results, as well as in qualitative results outside of pure mathematics. He strongly believed that numerical results could provide novel insights into many phenomena; insights which were not obtainable by exclusively analytical or abstract means. (He even believed that mathematical innovation itself had to originate—at least in part—from extra-mathematical sources: economic, biological, neurological, etc.) It was the confluence of these disparate factors, a knowledge of finite mathematical algorithms, and a deep interest in—and respect for—numerical results, that led to von Neumann's epoch making investigations of computers and automata.

It is perhaps a fortuitous but interesting coincidence that while in Princeton, von Neumann became well acquainted with Turing, who wrote his thesis on the "The Decision Problem," another one of Hilbert's problems in formal logic. von Neumann was clearly impressed by Turing: he asked Turing to be his assistant for the academic year 1938-1939. Although Turing did not accept the position, von Neumann was familiar with Turing's work; his general approach played an important role in von Neumann's later efforts to construct computers which could reproduce themselves. Thus, the succeeding explosive development of electronic computers is the curious progeny of a profound analysis of the logical foundations of mathematics on the one hand, and a highly personal interest in numerical results on the other. As unlikely (and presumably as incompatible) a lineage as one could possibly imagine! Yet these two factors were fundamental in starting the computer revolution and the emergence of CA. von Neumann used to say, "The computer changed intuitionistic mathematics from ideology to reality."

Although precursors of CA were studied in a rigorously mathematical context by Russian mathematician in the late 1920s and 1930s, CA, as such, were first introduced in discussions between Ulam and von Neumann in the fall of 1951. von Neumann was interested in finding a reductionist model for biological evolution. His ambitious scheme was to abstract a set of primitive local interactions necessary for the evolution of complex forms of organization essential for life. It was Ulam's felicitous suggestion to emphasize discrete systems and dynamics, which—since that time—is automatically included as a characterizing feature of CA and which initiated the explosive growth of the field.

During the succeeding summer of 1952, Fermi, Pasta and Ulam showed that the use of a computer, even when applied to a presumably well understood physical

situation in classical mechanics, can lead to unanticipated phenomena; phenomena that are not always easy to explain, even though the basic rules are simple. Using the rapidly increasing power of computers, many models could now be analyzed and discussed. Perhaps the best known model is Conway's *Life* game, a CA which, while based on almost absurdly simple rules, can exhibit extraordinarily complex and even bizarre behavior. Since the *Life* game can be played using rather modest computing facilities, it became very popular for a time—acquiring an almost cult-like following among computer “hackers” in the early 1970s. There was even a journal devoted exclusively to the publication of computer results (and their interpretations) of the *Life* game.^{||} Although this game did a great deal to publicize CA, the effect on the physics, mathematics and general scientific community was rather mixed. Whether causally related or not, the number of purely mathematical papers on CA dropped sharply after the publication of Conway's *Life* game in 1970.

For physicists, applied mathematicians, biologists, etc., the general popularity of the *Life* games raises an important question: *What do these games, or more generally, the processes generated by CA (in spite of their suggestive names), actually have to do with phenomena—physical or otherwise?* For actual applications and for the ultimate importance of CA as an autonomous scientific method, this is clearly a very basic question. Although a general answer to this question cannot yet be given, there are many indications that it is reasonable to hope that a thorough, deep understanding of CA may well lead to an alternative, possibly more profound, and more useful, formulation of the basic laws of nature. As a very minor hint, it has been observed by many physicists that CA are intimately related to discrete statistical models. Since these models are constructed to elucidate basic ideas and general principles of statistical mechanics, it is reasonable to expect that the corresponding CA possess a similar physical interpretation, and have similar physical relevance.

It is, of course, far from obvious that all or even most of the fundamental physics can be phrased in terms of discrete CA. In fact, in current particle and high energy physics, symmetries, gauge symmetries, groups, Lie groups, and differential geometry—all of which stress continuity and not discrete features—play increasingly important roles. Yet, even in fundamental physics, attempts are made (in fact, with surprising regularity!) to discretize space and time and to express the basic laws as difference equations. Even though none of these efforts have been spectacularly successful, it is still too early to categorically dismiss such attempts as being misdirected and necessarily pointless.

It is worth pointing out, that in one of the more successful areas of particle physics, *Quantum Chromodynamics* (QCD), where basic physical principles are

^{||}*Lifeline: A Quarterly Newsletter for Enthusiasts of John Conway's game of Life*, edited by Robert Wainwright, #'s 1-11, 1971-1973; available on the internet at URL address <http://members.aol.com/lifeline/life/lifepage.htm>. See also *Time* magazine, January 21, 1974: “The game of Life,” which is a lively account of hackers versus serious computer time.

presumably all known, the resulting equations are of such complexity that they can be explored only by using extensive computer simulations. In fact, the actual analysis is almost always performed in terms of a lattice gauge theory. The system is put on a lattice and treated numerically. This is not exactly a reduction to a problem in CA dynamics, but it is beginning to approach it. Certainly, many interpretation questions in lattice gauge theory contain elements CA theory. It is a highly nontrivial problem, for example, to decide whether solutions to the *discrete* problems—obtained numerically—are indeed legitimate (albeit approximate) solutions of the original *continuous* problems. The precise relation between a continuous problem and an approximate treatment of a related discrete problem is quite delicate and subtle. This, in spite of the claim made some time ago that the only problem remaining in strong interaction physics is to “get enough money for a supercomputer.” The precise arguments needed to assess the meaning of the results obtained by a numerical analysis of the discretized version of the theory, lead to discussions which involve many formal aspects of CA.

These two examples are just illustrations of the ubiquitous role of CA in many different, unrelated areas of physics. Through the important work of Wolfram [wolf83a], which strongly ignited the recent explosive development as far as physics is concerned, it has become clear that many highly complex phenomena are the result of the collective, cooperative dynamics of a very large number of—typically very simple—individual parts. In these emerging complex patterns, recognizable macroscopic features may appear that have no simple, visible, or immediate relation to the original microscopic rules. The mathematical analysis of these patterns and their underlying dynamics involves algebra, number theory, graph theory, logic, topology, as well as techniques originating from dynamical systems theory. (It is interesting, and a little ironic, that many of the questions arising from the study of such systems are closely related to the kind of problems von Neumann and Turing considered in their own studies of computability and the foundations of mathematics). Much of the current serious work with CA centers around the question of how simple rules produce complex patterns. It is certainly eminently reasonable to expect that these investigations will lead to important results. They already have. This alone would justify a serious systematic discussion.

But there still could be doubts. *Are CA merely an amusing form of computer graphics, a sophisticated computer game for scientists, or do they indeed herald a new beginning for a conceptually new and distinct approach to science generally and physics in particular?*

This book is intended to mitigate these doubts. There is already enough of a structure to the theory of CA to show that they provide an effective and practical basis for the treatment of specific, as well as general, questions. In this monograph, the physical, formal and mathematical framework will be systematized to such an extent, that the framework becomes the natural setting for an effective description of the natural world. Just to what extent the fundamental laws of physics can, or

should, all be phrased in terms of CA is impossible to say at this juncture. The subject is interesting enough, promising enough, and important enough, however, that a scientific field (or an individual scientist) ignores it at his or her own risk.

Chapter 1

Introduction: Preliminary Musings

Cellular automata (CA) are, fundamentally, the simplest mathematical representations of a much broader class of complex systems (where, for the moment, “complex system” means any dynamical system that consists of more than a few – typically nonlinearly – interacting parts). As such, CA have proven to be extremely useful idealizations of the dynamical behavior of many real complex systems, including physical fluids, neural networks, molecular dynamical systems, natural ecologies, military command and control networks, and the economy, among many others. Because of their underlying simplicity, CA are also powerful conceptual engines with which to study general pattern formation. They have already provided critical insights into the self-organization of chemical reaction-diffusion systems, crystal growth, pattern formation on seashells, and phase-transition-like phenomena in vehicular traffic flow, to name but a few examples. On a more practical side, CA may provide the basis for extremely powerful encryption algorithms, a subject about which there has recently been much heated debate. There is even some serious speculation that CA may provide the backbone of a radically new discrete fundamental physics (an idea that we will focus our attention on in Chapter 12). While the history of CA can be traced back to early *Systems’ Theory* ([bert68], [jant75]) and the rigorous (but almost impenetrably dry) mathematical analyses conducted primarily by Russian researchers in the 1930s and 40s, their more recent incarnation as simple models of complexity in nature can arguably be traced to a single landmark review paper published by Wolfram in the *Reviews of Modern Physics* in 1983 [wol83a]. Before embarking in earnest on our journey to explore some remarkable properties of CA in this book, we begin by giving in this introductory chapter a short historical overview and gentle first exposure to a few simple examples.

The fundamental challenge of physics has always been the understanding of the phenomenologically observed complexity in nature using a minimal set of simple principles. This reductionist program has historically—and for obvious reasons—concentrated mostly on studies of comparatively simple systems, deliberately avoiding more complex descriptions and phenomena.

Two powerful paradigms for studying natural systems have been provided by *statistical mechanics*, which deals with an infinite number of degrees of freedom and uses central limit theorems for computing desired observables, and *dynamical systems theory*, which deals with systems having only a relatively few degrees of freedom. During the last two decades there has been a veritable explosion of applications of nonlinear dynamics to physical systems. In particular, very simple dissipative deterministic classical systems have been shown to possess remarkable chaotic dynamical properties. Dynamical systems theory provides the tools for studying these systems, *provided* that their response to external probes is constrained to lie in some low-dimensional subspace of phase space. Neither traditional paradigm, however, is capable of dealing adequately with the collective behavior of *complex systems*, which—although consisting of large, often infinite, number of degrees of freedom—can behave in ways such that central limit theorems do not apply. In contrast to our understanding of irregular motions in continuous systems, a comprehensive analytical description of discrete complex systems, constructed out of large numbers of simple components undergoing nonlinear local interactions, is presently out of reach.

1.1 Complex Systems

What are complex systems? While difficult to define without first introducing a few technical concepts, we can see examples of complex systems just about everywhere we look in nature; from the turbulence in fluids to global weather patterns to beautifully intricate galactic structures to the complexity of living organisms. All such systems share at least this one property: they all consist of a large assemblage of interconnected, mutually (and typically nonlinearly) interacting parts. Moreover, their aggregate behavior is *emergent*. That is to say, the properties of the *whole* are not possessed by, nor are they directly derivable from, any of the *parts* – a water molecule is not a vortex, and a neuron is not conscious. A complex system must therefore be understood not just in terms of the set of components out of which it is constructed, but the topology of the interconnections and interactions among those components.

Gases, fluids, crystals, and lasers are all familiar kinds of complex systems from physics. Chemical reactions, in which a large number of molecules conspire to produce new molecules, are also good examples. In biology, there are DNA molecules built up from amino acids, cells built from molecules, and organisms built from cells. On a larger scale, the national and global economies and human culture as a whole are also complex systems, exhibiting their own brand of global cooperative behavior. One of the most far-reaching ideas of this sort is James Lovelock's controversial "Gaia" hypothesis, which asserts that the entire earth—molten core, biological ecosystems, atmospheric weather patterns and all—is essentially one huge, complex organism, delicately balanced on the edge-of-chaos [love79].

Perhaps the quintessential example of a complex system is the human brain, which, consisting of something on the order of 10^{10} neurons with 10^3 – 10^4 connec-

tions per neuron, is arguably the most *complex* complex system on this planet. Somehow, the cooperative dynamics of this vast web of “interconnected and mutually interacting parts” manages to produce a coherent and complex enough structure for the brain to be able to investigate its own behavior.

The emerging new sciences of complexity and complex adaptive systems explore the important question of whether (and/or to what extent) does the behavior of the many seemingly disparate complex systems found in nature—from the very small to the very large—stem from the same fundamental core set of universal principles.

References include monographs (Badii and Politi [badii97], Kauffman [kauff93], Holland [holl95], Mainzer [main93], Weisbuch [weis91]), popularizations (Lewin [lewin92], Waldrop [wald93], and Gell-Mann [gell94]), conference proceedings (Cowan [cowan94], Varela [varela92a], Yates [yates87a]) and a series of lecture notes from the Santa Fe Institute ([stein89], [jen90a], [nadel91], [nadel92], [nadel93], and [nadel95]). An eloquent exegesis of the complexity “worldview” is Kauffman’s *Investigations* [kauff00].

1.1.1 *Short History*

Whenever a new field emerges, many different individuals contribute to its development. This is of course also true of complex systems theory, yet three persons stand out as originating and shaping much of the field: *Alan Turing* [turing36], *John von Neumann* [vonN51], and *Stephen Wolfram* [wolf83a]. In addition, *Stanislaw Ulam* [ulam62] and *John Conway* [berk82] each made specific, original contributions of long-lasting fundamental significance. Table 1.1 shows a brief chronology of a few milestone events in the study of complex systems.

Turing, in 1936, published a landmark proof of what has come to be known as the Halting Theorem. Turing’s theorem fundamentally limits what one is able to know about the running of a program on a computer by asserting that there is in general no way to know in advance if an arbitrary program will ever stop running. In other words, there is, in general, no quick and dirty short-cut way of predicting an arbitrary program’s outcome; this is an example of what is called computational irreducibility. About five decades later, Wolfram suggested that computational irreducibility is actually a property not just of computers, but of many real physical systems as well [wolf85e].

Cellular automata were conceived in 1948 by John von Neumann, whose motivation was in finding a reductionist model for biological evolution [vonN51]. His ambitious scheme was to abstract the set of primitive logical interactions necessary for the evolution of the complex forms of organization essential for life. In a seminal work, completed by Burks, von Neumann followed a suggestion by Ulam to use discrete rather than continuous dynamics and constructed a two-dimensional automaton capable of self-reproduction. Although it obeyed a complicated dynamics and had a rather large state space, this was the first discrete parallel computational model formally shown to be a universal computer (which implies, in turn, that it is also computationally irreducible). Twenty years later, the mathematician John Conway introduced his well-known Life game, which remains among the simplest

Year	Researcher	Discovery
1936	Turing	Formalized concept of computability; universal turing machine
1948	von Neumann	Abstracted the logical structure of life; introduced self-reproducing automata as a means towards developing a reductionist biology
1950	Ulam	Proposed need for having more realistic models for the behavior of complex extended systems
1966	Burks	Completed and described von Neumann's work
1967	von Bertalanffy, <i>et al</i>	<i>System theory</i> applied to human systems
1969	Zuse	Introduced concept of "computing spaces," or digital models of mechanics
1970	Conway	Introduced two-dimensional cellular automaton Life rule
1977	Toffoli	Applied cellular automata directly to modeling physical laws
1983	Wolfram	Wrote a landmark review article on properties of cellular automata that effectively legitimized the field as research endeavor for physicists
1984	Cowan, <i>et al</i>	Santa Fe Institute founded, serving as a pre-eminent center for the interdisciplinary study of complex systems
1984	Toffoli, Wolfram	First cellular automata conference held at MIT, Boston
1987	Langton	First artificial life conference held at the Santa Fe Institute
1992	Varela, <i>et al</i>	First European conference on artificial life

Table 1.1 Some landmark historical developments in the study of cellular automata and complex systems.

known models proven to be computational universal [berk82].

Other important historical landmarks include the founding, in 1984, of the Santa Fe Institute,* which is one of the leading interdisciplinary centers for complex systems theory research; the first conference devoted solely to research in cellular automata (which is a prototypical mathematical model of complex systems), organized by Farmer, Toffoli and Wolfram at MIT in 1984 [farmer84]; and the first artificial life conference, organized by Chris Langton at Los Alamos National Laboratory, in 1987 [lang89].

*See the Santa Fe Institute's web site at <http://www.santafe.edu>.

1.2 Cellular Automata

Cellular automata (CA) are a class of spatially and temporally discrete, deterministic mathematical systems characterized by local interaction and an inherently parallel form of evolution. First introduced by von Neumann in the early 1950s to act as simple models of biological self-reproduction, CA are prototypical models for complex systems and processes consisting of a large number of identical, simple, locally interacting components. The study of these systems has generated great interest over the years because of their ability to generate a rich spectrum of very complex patterns of behavior out of sets of relatively simple underlying rules. Moreover, they appear to capture many essential features of complex self-organizing cooperative behavior observed in real systems.

Although much of the theoretical work with CA has been confined to mathematics and computer science, there have been numerous applications to physics, biology, chemistry, biochemistry, and geology, among other disciplines. Some specific examples of phenomena that have been modeled by CA include fluid and chemical turbulence ([d'Hum86], [gerh89]), plant growth [linde89] and the dendritic growth of crystals [kess90], ecological theory [phip92], DNA evolution, the propagation of infectious diseases [segel99], social dynamics [axtel96], forest fires [bak90], and patterns of electrical activity in neural networks [fran92]. CA have also been used as discrete versions of partial differential equations in one or more spatial variables. They have most recently been used to simulate some aspects of military combat (see [wood88] and [ilach97]).

The best sources of information on CA are conference proceedings and collections of papers, such as the one's edited by Boccara [bocc93a], Gutowitz [guto90a], Preston [prest84] and Wolfram ([wolf83b], [wolf94a]). An excellent review of how CA can be used to model physical systems is given by Toffoli and Margolus [marg87].

While there is an enormous variety of particular CA models—each carefully tailored to fit the requirements of a specific system—most CA models usually possesses these five generic characteristics:

- **Discrete lattice of cells:** the system substrate consists of a one-, two- or three-dimensional lattice of cells.
- **Homogeneity:** all cells are equivalent.
- **Discrete states:** each cell takes on one of a finite number of possible discrete states.
- **Local interactions:** each cell interacts only with cells that are in its local neighborhood.
- **Discrete dynamics:** at each discrete unit time, each cell updates its current state according to a transition rule taking into account the states of cells in its neighborhood.

There is a deceptive simplicity to these characteristics. In fact, as we shall see repeatedly in this book, such systems are capable of extremely complicated behavior. For example, although obeying local rules and having no intrinsic length scales other than the size of the neighborhoods about each site, CA can generate global patterns with very long-range order and correlation. CA are dynamically rich enough to be seriously considered as alternative mathematical models for a variety of physical systems.

While one is free to think of CA as being nothing more than formal idealizations of partial differential equations, their real power lies in the fact that they represent a large class of *exactly computable models*: since everything is fundamentally discrete, one need never worry about truncations or the slow accumulation of round-off error. Therefore, any dynamical properties observed to be true for such models take on the full strength of theorems [toff77a].

Exact computability in this sense, however, is achieved only at the cost of being able to obtain approximate solutions. Perturbation analysis, for example, is rendered virtually meaningless in this context. It is not surprising that traditional investigatory methodologies are not very well suited to studies of complex systems. Since the behavior of such models can generally be obtained *only* through explicit simulation, the computer becomes the one absolutely indispensable research tool.

1.2.1 CA & Computation

Since CA are totally discrete information processors, a useful analogy almost immediately presents itself between such models and conventional computers. Simply identify the initial state value specification in a CA with the initial *data* of a computer program, and identify the uniquely prescribed rule by which the sites evolve with the *program* itself. Running the program is equivalent to using the CA rule to evolve generations from the initial state, with successive configurations representing intermediate results of the computation. Unlike the serial computations making up the CPU cycles in conventional computers, however, CA process information in a fully parallel manner. Basic theoretical results have been obtained by exploiting this formal equivalence between CA and computers [wolf85e].

von Neumann's construction of a two-dimensional automaton capable of self-reproduction was the first discrete parallel computational model shown formally to be a *universal computer*. Twenty years later, John Conway introduced his (now, well studied) *Life* rule, which remains among the simplest known models proven rigorously to be a computationally universal system (see example # 2 below).

Computational universality is the ability to implement any finite algorithm and thus evaluate any computable function [wolf85e]. This property can be proven either by showing that the given system is formally equivalent to another system known to be a universal computer or by directly identifying the dynamics of intrinsically generated structures with the state transitions in a *Turing Machine* [garey79].

Apart from granting systems the same formal computational power as conventional digital computers, computational universality places a severe restriction on possible theoretical predictions of system behavior [toff77a]: because universal com-

puters all require the same order of magnitude times and data storage capacities to process particular algorithms, no computational method can exist with which a shortcut route is taken to a particular dynamical outcome. In the strongest possible terms, the long time behavior of computationally universal dynamical systems can be obtained only by direct simulation. No general predictive procedure is possible, even in principle. This implies, for example, that for systems such as von Neumann's self-reproducing automaton, there can neither be an analytical expression that exactly describes its asymptotic behavior nor an equation that defines the long-term behavior that itself can be solved in a time less than it would take the system to evolve (modulo a polynomial function of the number of iteration steps necessary for it to reach its final state). All such computationally irreducible systems share the property that their own evolution effectively defines the most efficient simulation of their behavior.

1.2.2 *Why Study CA?*

There are at least four partially overlapping motivations for studying CA, which we order according to increasing levels of theoretical significance:

- *As powerful computation engines*
- *As discrete dynamical system simulators*
- *As conceptual vehicles for studying pattern formation and complexity*
- *As original models of fundamental physics*

1.2.2.1 *CA as Powerful Computation Engines*

CA allow very efficient parallel computational implementations to be made of lattice models in physics and thus for a detailed analysis of many concurrent dynamical processes in nature. Indeed, dedicated hardware represents one of the most promising practical applications of CA modeling. With the help of such hardware, many heretofore intractable but technologically important problems such as fluid flow near and around airplane wings, are becoming computationally accessible for the first time. Weisbuch has aptly compared such dedicated CA processors to being the numerical equivalents of wind tunnels [weis91]. More ambitiously, Toffoli and Margolus foresee hardware implementations of CA systems as embodying the concept of *programmable matter* [toff91]; that is to say, a computationally amorphous "machine" that can be "programed" to act as a numerical wind tunnel one moment, or a sea of fermions the next. Their CAM-8 machine, a powerful new descendent of their earlier CAM-5 and CAM-6 CA simulators, comes close to realizing this exciting possibility.[†] The CAM-6, for example, which is still available commercially as a plug-in card for the PC, provides a 256-by-256 two dimensional array in which each site may contain up to four bits of data and the entire array is scanned, updated and displayed sixty times every second. Its speed is comparable in performance

[†]See MIT's *Information Mechanics Group* web page on the CAM-8 at <http://www.im.lcs.mit.edu/cam8/>.

to that of a CRAY-1 for this kind of application. A new generation of CA-based massively parallel computing machines is ushering in a new era in computational physics and applied mathematics.

1.2.2.2 CA as Discrete Dynamical System Simulators

CA allow systematic investigation of complex phenomena by embodying any number of desirable physical properties. Reversible CA,[‡] for example, can be used as laboratories for studying the relationship between microscopic rules and macroscopic behavior—exact computability ensuring that the memory of the initial state is retained exactly for arbitrarily long periods of time. The behavior of computationally universal reversible rules, such as Fredkin's *Billiard Ball* model [fredkin82], are of more than passing interest since they can conceivably avoid the fundamental lower bound on dissipation associated with the reversibility of logic elements in conventional computers [keyes70].

Suitably generalized discrete models have thus far been constructed and studied for dendritic crystal growth [kess90], spatial patterns generated by reaction-diffusion systems (such as the Belousov-Zhabotinsky reaction [madore83]; see example # 3 below), Ising models [creutz86], self-organization in neural networks [fran92], discrete multiple soliton-structure dynamics [aizawa90], and turbulence in hydrodynamical systems [chenh88]. Discrete models of turbulence are particularly impressive in that they clearly show that very simple finite dynamical implementations of local conservation laws (defined so that the discrete system is computationally universal) are capable of exactly reproducing continuum system behavior on the macroscale.

1.2.2.3 CA as Conceptual Vehicles for Exploring Pattern Formation

CA can be treated as abstract discrete dynamical systems embodying intrinsically interesting, and potentially novel, behavioral features. The central motivation is to abstract the general principles governing self-organizing structure formation. Haken ([haken77],[haken83]) has pioneered the interdisciplinary study of self-organization, coining the term *synergetics* to describe this emerging new discipline. Because of their underlying simplicity, CA offer a powerful theoretical and simulation research tool. Related interests include formal classification of the dynamical behavior of complex systems; a better understanding of the relationship between the dynamics of continuous and discrete systems; and the quantification of complexity—as a system property. All of these questions are particularly accessible through studying the generic behavior of CA systems.

[‡]Reversible CA are characterized by the property that each site value has a unique predecessor neighborhood configuration.

1.2.2.4 CA as Original Models of Fundamental Physics

CA allow studies of radically new discrete dynamical approaches to microscopic physics, exploring the possibility that nature locally and digitally processes its own future states. The entire last chapter of this book is devoted to a prolonged discussion of such potentially ground breaking models of physics. Using the fact that computationally universal systems are capable of arbitrarily complicated behavior (in the sense that they can mimic any computation performed by a conventional computer), the idea is to construct fundamentally discrete field theories to compete with existing continuous models. The emphasis in this class of models is emphatically *not* to construct a lattice-gauge-like theory; rather, in the same way as lattice-gas CA successfully reproduce continuous fluid flow despite never having heard of the Navier-Stokes equations, so the hope is to abstract a set of microphysical laws that reproduce known behavior on the macro scale. A number of interesting ideas have recently been explored. Fredkin [fredkin93] has arguably gone to the furthest extreme by asserting that the universe is, at its core, a CA! We will offer a few of our own speculations on this subject in the last chapter.

1.2.3 Example #1: One-dimensional CA

For a one-dimensional CA, the value of the i^{th} cell at time t – denoted by $c_i(t)$ – evolves in time according to a rule F that is a function of $c_i(t)$ and other cells that are within a range r (on the left and right) of $c_i(t)$:

$$c_i(t) = F(c_{i-r}(t-1), c_{i-r+1}(t-1), \dots, c_{i+r-1}(t-1), c_{i+r}(t-1)). \quad (1.1)$$

Since each cell takes on one of k possible values—that is, $c_i(t) \in \{0, 1, 2, \dots, k\}$ —the rule F is completely defined by specifying the value assigned to each of the k^{2r+1} possible $(2r+1)$ -tuple configurations for a given range- r neighborhood:

$c_{i-r}(t-1)$	$\dots$	$c_i(t-1)$	$\dots$	$c_{i+r}(t-1)$	$c_i(t)$
0		0		0	$F(0,0,\dots,0)$
0		0		1	$F(0,0,\dots,1)$
$\vdots$		$\vdots$		$\vdots$	$\vdots$
k		k		k	$F(k,k,\dots,k)$

Since F itself assigns any of k values to each of the k^{2r+1} possible $(2r+1)$ -tuples, there are a total of $k^{k^{2r+1}}$ possible rules, which is an exponentially increasing function of both k and r . For the simplest case of nearest neighbors (range $r=1$) and $k=2$ ($c_i = 0$ or 1), for example, there are $2^8 = 256$ possible rules. Increasing the number of values each cell can take on to $k=3$ (but keeping the radius at $r=1$) increases the rule-space size to $3^{3^3} \approx 7 \cdot 10^{12}$.

Figure 1.1 shows the time evolution of a nearest-neighbor (radius $r=1$) rule where c is equal to either 0 or 1. The row of eight boxes at the top of the figure shows the explicit rule-set, where – for visual clarity – a box has been arbitrarily colored

black if the value $c=1$ and white if $c=0$. For each combination of three adjacent cells in generation 0, the rule F assigns a particular value to the next-generation center cell of the triplet. Beginning from an initial state (at time=0) consisting of the value zero everywhere except the center site, that is assigned the value 1, F is applied synchronously at each successive time step to each cell of the lattice. Each generation is represented by a row of cells and time is oriented downwards. The first image shows a blowup of the first five generations of the evolution. The second shows 300 generations. The figure illustrates the fact that simple rules can generate considerable complexity.

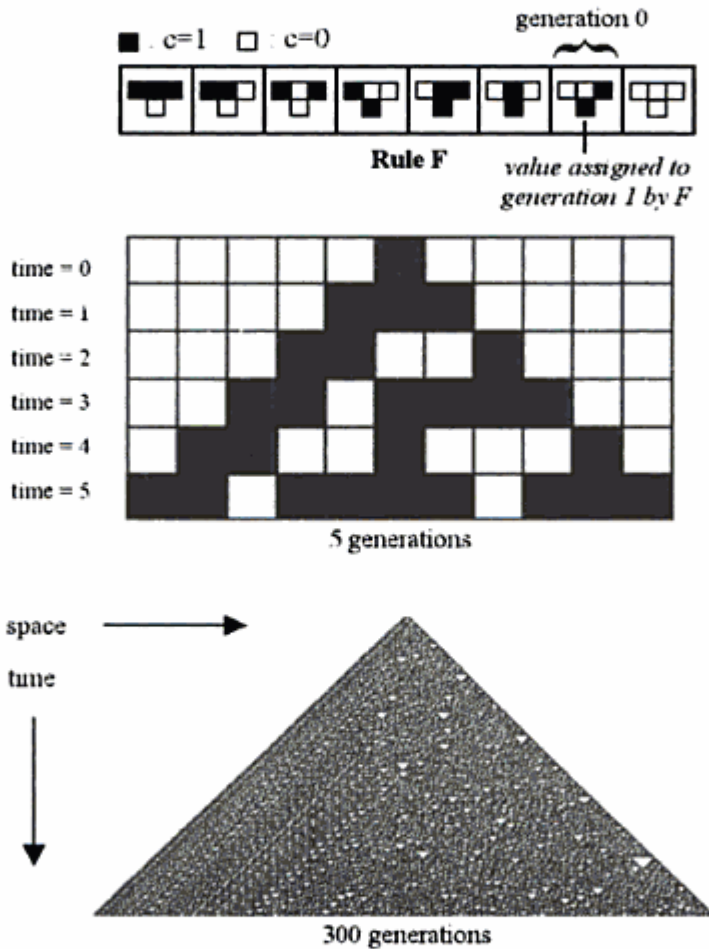


Fig. 1.1 Example of a one-dimensional CA starting from a single nonzero seed.

The space-time pattern generated from a single nonzero cell by this particular rule has a number of interesting properties. For example, it consists of a curious mixture of ordered behavior along the left-hand-side and what appears to be disordered behavior along the right-hand-side, separated by a corrugated boundary moving towards the left at a "speed" of about $1/4$ cells per "clock" tick. In fact, it can be shown that, despite starting from an obviously non-random initial state and evolving according to a fixed deterministic rule, the temporal sequence of ver-

tical values is completely random. Systems having the ability to deterministically generate randomness from non-random input are called autoplectic systems.

As another example, consider the rule shown at the top of figure 1.2. Its space-time evolution, starting from a random initial state, is shown at the bottom of the figure. Note that this space-time pattern can be described on two different levels: either on the cell-level, by explicitly reading off the values of the individual cells, or on a higher-level by describing it as a sea of particle-like structures superimposed on a periodic background. In fact, following a small initial transient period, temporal sections of this space-time pattern are always of the form "...BBBBPBB...BB...BBBP'BB...BBBP"BBB...", where "B" is a state of the periodic background consisting of repetitions of the sequence "10011011111000" (with spatial period 14 and temporal period 7), and the P's represent "particles." The particle pattern P = "11111000", for example, repeats every four steps while being displaced two cells to the left; the particle P = "11101011000" repeats every ten steps while being displaced two cells to the right.

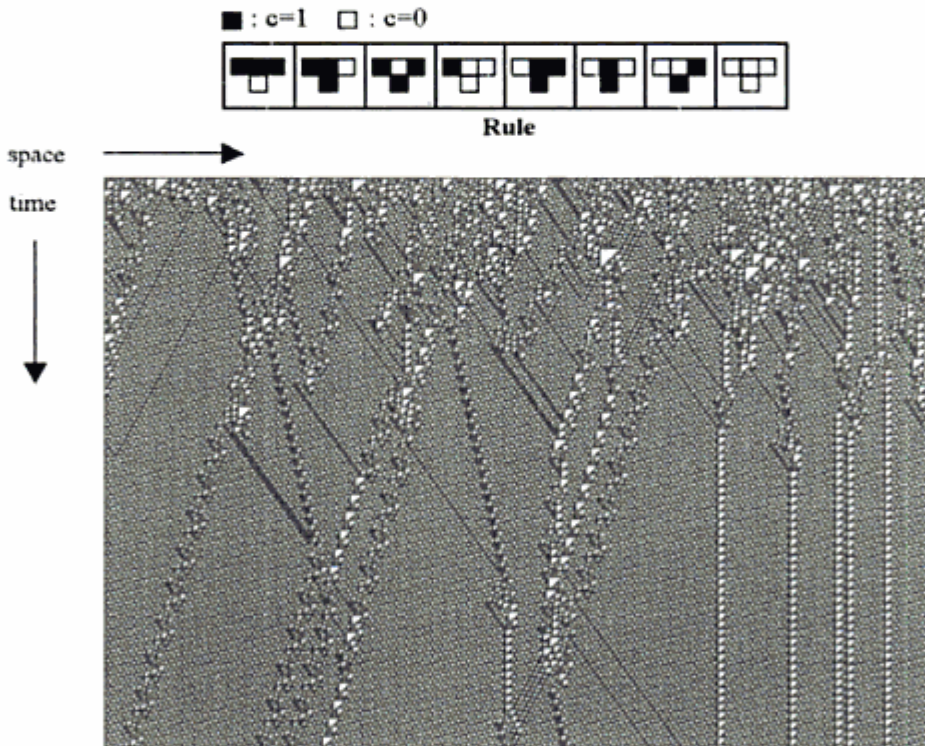


Fig. 1.2 Evolution of a one-dimensional CA starting from a random initial state.

Although the underlying dynamics describing this system is very simple, and entirely deterministic, there is an enormous variety, and complexity, of emergent particle-particle interactions. Such simple systems are powerful reminders that complex higher-level dynamics need not have a complex underlying origin. Indeed, suppose that we had been shown such a space-time pattern but were told nothing whatsoever about its origin. How would we make sense of its dynamics? Perhaps

the only reasonable course of action would be to follow the lead of any good experimental particle-physicist and begin cataloging the various possible particle states and interactions: there are N particles of size s moving to the left with speed v ; when a particle p of type P collides with q of type Q , the result is the set of particles $\{p_1, \dots, p_n\}$; and so on. It would take a tremendous leap of intuition to fathom the utter simplicity of the real dynamics.

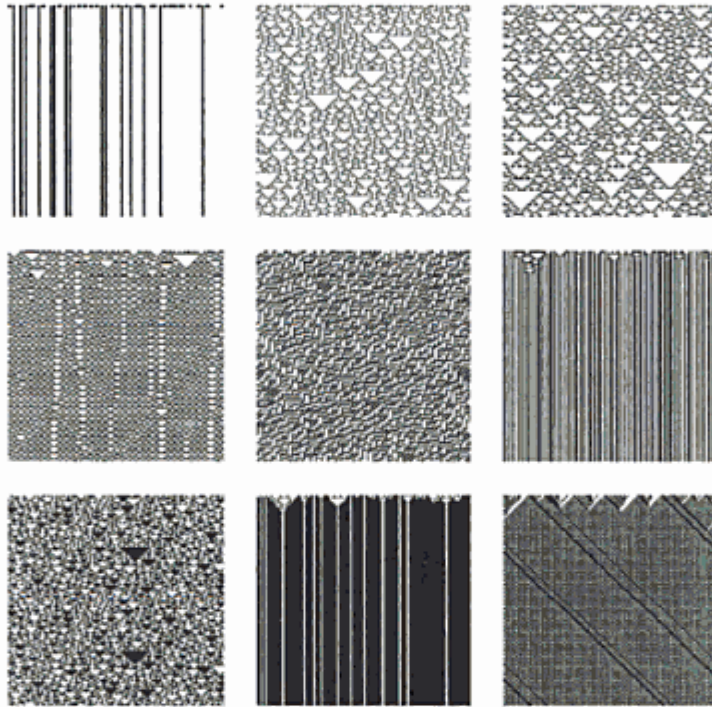


Fig. 1.3 Space-time evolution of nine different nearest neighbor one-dimensional CA starting from random initial states.

In general, the behavior of CA is strongly reminiscent of the kinds of behavior observed in continuum dynamical systems, with simple rules yielding steady-state behaviors consisting of fixed points or limit cycles, and complex rules giving rise to behaviors that are analogous to deterministic chaos. In fact, there is extensive empirical evidence suggesting that patterns generated by all (one-dimensional) CA evolving from disordered initial states fall into one of only four basic behavioral classes [wolf83a]:

- Class 1: *Evolution leads to a homogeneous state, in which all cells eventually attain the same value.*
- Class 2: *Evolution leads to either simple stable states or periodic and separated structures.*
- Class 3: *Evolution leads to chaotic nonperiodic patterns.*

- Class 4: *Evolution leads to complex, localized propagating structures.*

All CA within a given class yield qualitatively similar behavior. While the behaviors of rules belonging to the first three rule classes bear a strong resemblance to those observed in continuous systems – the homogeneous states of class 1 rules, for example, are analogous to fixed-point attracting states in continuous systems, the asymptotically periodic states of class 2 rules are analogous to continuous limit cycles and the chaotic states of class 3 rules are analogous to strange attractors – the more complicated localized structures emerging from class 4 rules do not appear to have any obvious continuous analogues (although such structures are well characterized as being soliton-like in their appearance).

Figure 1.3 shows a few examples of the kinds of space-time patterns generated by binary ($k = 2$) nearest-neighbor ($r = 1$) in one dimension and starting from random initial states.

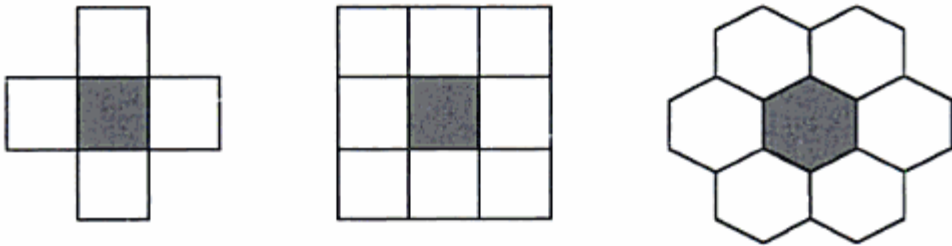


Fig. 1.4 Examples of CA neighborhoods in two dimensions.

Figure 1.4 shows examples of some commonly used neighborhood structures in two dimensions. These include the *von Neumann* neighborhood, which consists of the four cells that are horizontally and vertically adjacent to the center cell (left-most graphic appearing in figure 1.4), (2) the *Moore* neighborhood, that consists of all eight nearest-neighbor cells on a two-dimensional Euclidean lattice (center graphic in figure 1.4), and (3) the *Hexagonal* neighborhood, that consists of all nearest-neighbor cells on a hexagonal lattice (right-most graphic in figure 1.4).

1.2.4 Example #2: Conway's Life

"It's probable, given a large enough Life space, initially in a random state, that after a long time, intelligent self-reproducing animals will emerge and populate some parts of the space." – John H. Conway [berk82]

Perhaps the most widely known CA is the game of Life, invented by John H. Conway, and popularized extensively by Martin Gardner in his "Mathematical Games" department in *Scientific American* in the early 1970s (see, for example, [gardner70]).

Life is "played" using the 9-neighbor Moore neighborhood (see center graphic in figure 1.4), and consists of (1) seeding a lattice with some pattern of "live" and "dead" cells, and (2) simultaneously (and repeatedly) applying the following three

rules to each cell of the lattice at discrete time steps:

- **Birth:** replace a previously dead cell with a live one if exactly 3 of its neighbors are alive.
- **Death:** replace a previously live cell with a dead one if either (1) the living cell has no more than one live neighbor (i.e. it dies of isolation), or (2) the living cell has more than three neighbors (i.e. it dies of overcrowding).
- **Survival:** retain living cells if they have either 2 or 3 neighbors.

One of the most intriguing patterns in Life is an oscillatory propagating pattern known as the “glider.” Shown on the left-hand-side of figure 1.5, it consists of 5 “live” cells and reproduces itself in a diagonally displaced position once every four iterations.

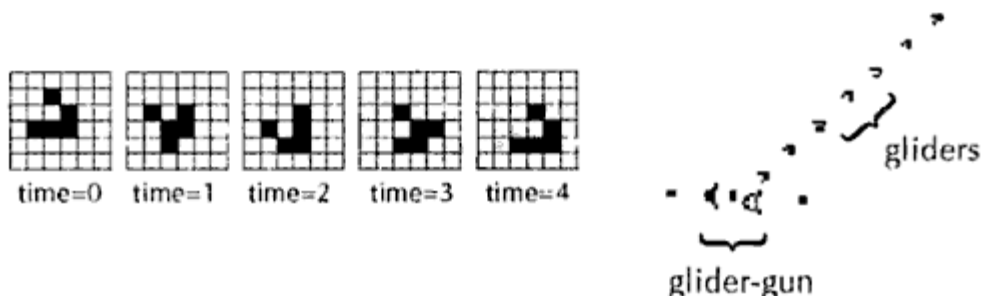


Fig. 1.5 Glider patterns in Conway's Life.

When the states of Life are projected onto a screen in quick succession by a fast computer, the glider gives the appearance of “walking” across the screen. The propagation of this pseudo-stable structure can also be seen as a self-organized emergent property of the system. The right-hand-side of figure 1.5 shows a still-frame in the evolution of a pattern known as a “glider-gun,” which shoots-out a glider once every 30 iteration steps.

What is remarkable about this very simple appearing rule is that one can show that it is capable of universal computation. This means that with a proper selection of initial conditions (i.e. the initial distribution of “live” and “dead” cells), Life can be turned into a general purpose computer. This fact fundamentally limits the overall predictability of Life's behavior.

The well known *Halting Theorem*, for example, asserts that there cannot exist a general algorithm for predicting when a computer will halt its execution of a given program [garey79]. Given that Life is a universal computer – so that the Halting Theorem applies – this means that one cannot, in general, predict whether a particular starting configuration of live and dead cells will eventually die out. No shortcut is possible, even in principle. The best one can do is to sit back and patiently await Life's own final outcome.

Put another way, this means that if you want to predict Life's long-term behavior with another “model” or by using, say, a partial differential equation, you

are doomed to fail from the outset because its long-term behavior is effectively unpredictable. Life – like all computationally universal systems – defines the most efficient simulation of its own behavior.

1.2.5 Example #3: Belousov–Zhabotinski Reaction

The Belousov-Zhabotinski (BZ) reaction is a chemical reaction consisting of simple organic molecules that is characterized by spectacular oscillating temporal and spatial patterns [zhabo64]. One variant of the BZ reaction involves the reaction of bromate ions with an organic substrate (typically malonic acid) in a sulfuric acid solution with cerium (or some other metal-ion catalyst). When this mixture is allowed to react exothermally at room temperature, interesting temporal and spatial oscillations (i.e. chemical waves) result. The system oscillates, changing from yellow to colorless and back to yellow about twice a minute, with the oscillations typically lasting for over an hour (until the organic substrate is exhausted).

These patterns are an example of what are sometimes called *dissipative structures*, which arise in many complex systems. Dissipative structures are dynamical patterns that retain their organized state by persistently dissipating matter and energy into an otherwise thermodynamically open environment.

Figure 1.6 shows a sample evolution of a CA model of this reaction, in which cells are identified with the reacting molecules, and are colored *black* if they are “active” and *white* if they are “inactive,” according to the reaction rules. The spatial and temporal patterns that emerge from the initially random mixture of states are also a good general example of how CA can be used to model self-organization. The rule shown here is due to Gerhardt and Schuster ([gerh89]; also see color plate 4 in the appendix to chapter three).

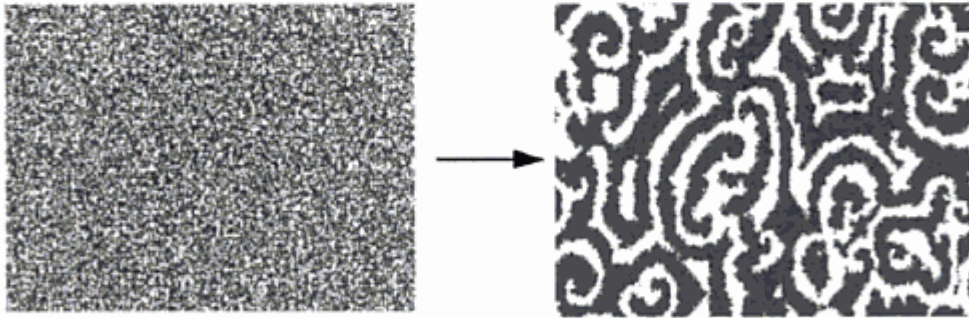


Fig. 1.6 Example of self-organization in a two-dimensional CA.

1.2.6 Example #4: Lattice Gases

Lattice gases are micro-level rule-based simulations of macro-level fluid behavior. Lattice-gas models provide a powerful new tool in modeling real fluid behavior ([doolen90], [doolen91]). The idea is to reproduce the desired macroscopic behavior of a fluid by modeling the underlying microscopic dynamics.

It can be shown that three basic ingredients are required to achieve an emergence of a suitable macrodynamics out of a discrete microscopic substrate [hass89]: (1) local thermodynamic equilibrium, (2) conservation laws, and (3) a “scale separation” between the levels at which the microscopic dynamics takes place (among kinetic variables living on a micro-lattice) and the collective motion itself appears (defined by hydrodynamical variable on a macro-lattice). Another critical feature is the symmetry of the underlying lattice.

While there are many variants of the basic model, one can show that there is a well-defined minimal set of rules that define a lattice-gas system whose macroscopic behavior reproduces that predicted by the Navier-Stokes equations exactly.⁵ In other words, there is critical “threshold” of rule size and type that must be met before the continuum fluid behavior is matched, and once that threshold is reached the efficacy of the rule-set is no longer appreciably altered by additional rules respecting the required conservation laws and symmetries.

Figure 1.7 shows a few snapshots of the evolution of a two-dimensional lattice gas starting from an initial condition in which there is a tightly packed region of particles at the center of the lattice. Notice how this central region expands rapidly outward, and is very reminiscent of the effect a dropped stone has on an initially stagnant pool of water. The most striking feature is the circular sound wave, which is circular despite the fact that the microscopic dynamics takes place on a square lattice. The lattice gas rules thus force a symmetry that is not present in the microscopic dynamics to emerge on the macro-scale.

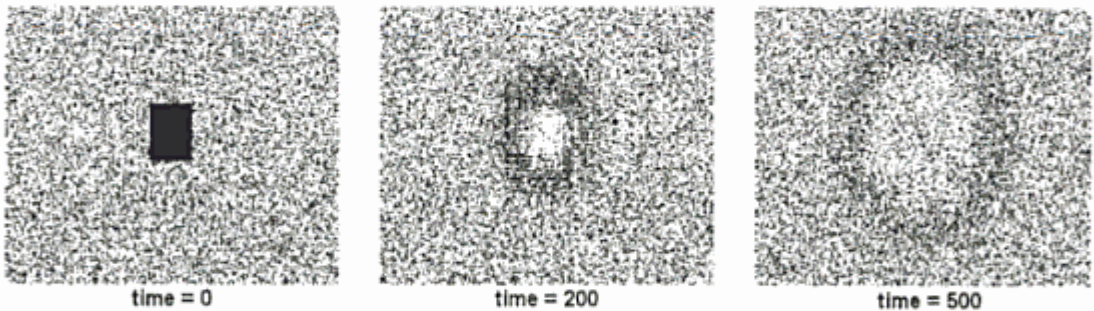


Fig. 1.7 Two-dimensional lattice-gas simulation of a fluid.

1.2.7 Example #5: Collective Behavior in Higher Dimensions

Chate and Manneville [chate92] have examined a wide variety of cellular automata that live in dimensions four, five and higher. They found many interesting rules that while being essentially featureless locally, nonetheless show a remarkably ordered global behavior.

Here again we see a pristine example of the three basic elements of emergence: (1) the global phenomenon (in this case the cell-value density) emerges out of an

⁵The Navier-Stokes equations are the fundamental equations describing incompressible fluid flow; see Chapter 9.

interaction of a large number of simple components (lattice cells of a cellular automaton), (2) there is no evidence of the global phenomenon on the local level, and (3) the global phenomenon obeys a separate dynamics (in this case, quasi-periodicity).

Figure 1.8, for example, plots the probability that a cell has value 1 at time $t+1$ – labeled P_{t+1} – versus the probability that a cell had value 1 at time t – labeled P_t – for a particular four dimensional cellular automaton rule. The rule itself is unimportant, as there are many rules that display essentially the same kind of behavior. The point is that while the behavior of this rule is locally featureless – its space-time diagram would look like noise on a television screen – the global density of cells with value 1 jumps around in quasi-periodic fashion. We emphasize that this quasi-periodicity is a *global* property of the system, and that no evidence for this kind of behavior is apparent in the local dynamics.

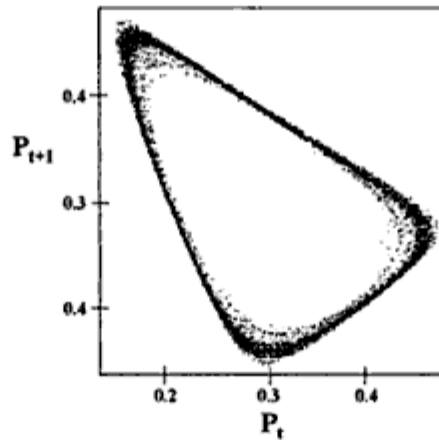


Fig. 1.8 Collective behavior of a four dimensional CA (after [chate92]).

1.2.8 Other Variants

There are at least as many variants of the basic CA algorithm as there are ways of generalizing the characteristics of a typical CA system. Here are a few general models:

Asynchronous CA. CA rules are typically defined so that all lattice sites update their values simultaneously throughout the lattice on each time step. A natural generalization is to lift this restriction by allowing *asynchronous* updates [inger84].

Coupled-map Lattices. Another obvious generalization is to lift the restriction that sites can take on only one of a few discrete values. Coupled-map lattices are CA models in which continuity is restored to the state space. That is to say, the cell values are no longer constrained to take on only the values 0 and 1 as in the examples discussed above, but can now take on arbitrary real values. First introduced by Kaneko [kaneko83]-[kaneko93], such systems are simpler than partial differential equations but more complex than generic CA. Coupled-map lattices are discussed in chapter 8.

Probabilistic CA. Probabilistic CA are cellular automata in which the deterministic state-transitions are replaced with specifications of the probabilities of the cell-value assignments. Since such systems have much in common with certain statistical mechanical models, analysis tools from physics are often borrowed for their study. Probabilistic CA are introduced in chapter 8.

Non-homogeneous CA. These are CA in which the state-transition rules are allowed to vary from cell to cell. The simplest such example is one where there are only two different rules randomly distributed throughout the lattice. Kauffman [kauff84] has studied the other extreme in which the lattice is randomly populated with all possible Boolean functions of k inputs.

Mobile CA. These are CA in which some (or all) lattice sites are free to move about the lattice. In effect, mobile CA are primitive models of mobile robots. Typically, their internal state space reflects some features of the local environment within which they are allowed to move and with which they are allowed to interact. An example of mobile CA used to model some aspects of military engagements is discussed in Chapter 12.

Structurally Dynamics CA. Most of the CA that we will encounter throughout this book (indeed, most that are currently being studied!) assume that the underlying lattice remains a passive and static object. The lattice is thus typically an arena for activity, not an active participant in the dynamics. What if the lattice were somehow made an integral part of the dynamics? That is to say, what if the topology – the sites and connections among sites – evolved alongside the value states? Structurally dynamic CA are discussed in Chapter 8.

1.3 Outline of Book

The remainder of the book is divided into eleven largely self-contained chapters. Chapter 2 introduces some basic mathematical formalism that will be used throughout the book, including set theory, information theory, graph theory, groups, rings and field theory, and abstract automata. It concludes with a preliminary mathematical discussion of one and two dimensional CA.

Chapter 3 provides a phenomenological introduction to generic CA. The narrative includes both a mathematical description of one, two and three dimensional CA along with guided-tour through a graphics-gallery of typical space-time patterns. Simple ways of parameterizing the space of CA rules are described, and a sketch of the proof of the computational universality of Conway's famous two-dimensional *Life*-rule is also provided.

Chapter 4 covers much of the same ground as chapter 3 but from a more formal dynamical systems theory approach. The discrete CA world is examined in the context of what is known about the behavior of *continuous* dynamical systems, and a number of important methodological tools developed by dynamical systems theory (i.e. Lyapunov exponents, invariant measures, and various measures of entropy and

dimension) are used to characterize the behavior of simple CA systems.

Chapter 5 provides some examples of purely analytical tools useful for describing CA. It discusses methods of inferring cycle-state structure from global eigenvalue spectra, the enumeration of limit cycles, the use of shift transformations, local structure theory, and Lyapunov functions. Some preliminary research on linking CA behavior with the topological characteristics of the underlying lattice is also described.

Chapter 6 is a short primer on CA and language theory, and provides a basic discussion of formal language theory, the relationship between CA and formal language theory, power spectra of regular languages and reversible computation.

Chapter 7 discusses a variety of topics all of which are related to the class of probabilistic CA (PCA); i.e. CA that involve some elements of probability in their state and/or time-evolution. The chapter begins with a physicist's overview of critical phenomena. Later sections include discussions of the equivalence between PCA and spin models, the critical behavior of PCA, mean-field theory, CA simulation of conventional spin models and a stochastic version of Conway's *Life* rule.

Chapter 8 describes a number of generalized CA models, including reversible CA, coupled-map lattices, quantum CA, reaction-diffusion models, immunologically motivated CA models, random Boolean networks, sandpile models (in the context of self-organized criticality), structurally dynamic CA (in which the temporal evolution of the value of individual sites of a lattice are dynamically linked to an evolving lattice structure), and simple CA models of combat.

Chapter 9 provides an introductory discussion of a research area that is rapidly growing in importance: *lattice gases*. Lattice gases, which are discretized models of continuous fluids, represent an early success of CA modeling techniques. The chapter begins with a short primer on continuum fluid dynamics and proceeds with a discussion of CA lattice gas models. One of the most important results is the observation that, under certain constraints, the macroscopic behavior of CA models exactly reproduces that predicted by the Navier-Stokes equations.

Chapter 10 covers another important field with a great overlap with CA: *neural networks*. Beginning with a short historical survey of what is really an independent field, chapter 10 discusses the Hopfield model, stochastic nets, Boltzman machines, and multi-layered perceptrons.

Chapter 11 contains a very brief introduction to what is rapidly becoming one of the central research areas in complex systems theory; namely, *artificial-life* (AL). Owing its origins to von Neumann's early explorations in self-reproducing automata, AL has blossomed in the last decade from consisting of a few toy worlds hardly more sophisticated than Conway's *Life*-rule universe to intricately rendered 3D artificial universes populated with interacting creatures undergoing an open-ended evolution. Topics include a brief survey of von Neumann's original work, Lindenmeyer systems, Langton's *vants* model, a short primer on genetic algorithms. The chapter concludes with a discussion of an artificial-life-like mobile CA model of land warfare.

The last chapter is a broad survey of a speculative proposition that CA just might one day prove to be even more profound in what they say about how our universe is organized than has heretofore been appreciated. The essence of the

proposition, borrowed from musings by Feynman [feyn82], Fredkin [fredkin90], Minsky [minsky82], Wheeler [wheel90] and others, is that the universe is fundamentally discrete and obeys, at its core, a simple CA-like dynamics. *Thus begin some final musings and a perhaps a glimpse of a new cosmogony!*

Appendix A provides a brief description of several existing hardware and software tools designed for CA research. Appendix B contains a useful list of CA and more general complexity-related information sources available on the World Wide Web (WWW), subject-sorted into a total of 91 WWW Universal Resource Locator (URL) links in 16 categories. The book is indexed and includes an extensive bibliography.

Chapter 2

Formalism

From a physicist's (or applied mathematician's) point of view, CA can be effectively thought of as being nothing more than very simple and elegant sets of rules that can be *played with* on a computer. However, a sincere understanding of their depth and elegance can come only from an appreciation of the great variety of different fields and mathematical formalisms to which they owe much of their history and substance. This introductory chapter briefly introduces some of the more important mathematical techniques that we will often use in our discussion. Specific formalisms will be subsequently developed in greater detail as needed in later chapters.

2.1 Mathematical Preliminaries

2.1.1 Set Theory

Sets

We shall often be dealing with *sets* of objects of some kind. A *set*, which we will label by capital letters $A, B, \dots$, is a collection of objects, denoted by lowercase letters $a, b, \dots$, which are *members* (or *elements*) of the set. Finite sets may be defined by explicitly listing all of their members: if the set A consists of the three elements a, b, c , for example, we would write $A \equiv \{a, b, c\}$. We also write $a \in A$ to mean that ' a ' belongs to the set A . Arbitrary sets may sometimes be more conveniently specified by some *property* $\mathcal{P}$, which is shared by all of their members. For example, the set

$$B \equiv \{x \mid x \text{ is an even integer} \}, \quad (2.1)$$

is the set consisting of all objects ' x ' such that ' x ' is an even integer. To indicate that a set C consists of all elements of some specific set S sharing the property $\mathcal{P}$, we can write $C = \{x \in S \mid \mathcal{P}(x)\}$.

A set A is a *subset* of B , written as $A \subset B$, if every element of A is also an element of B . One special kind of set is the *null* (or *empty*) set, which is "the set having no elements". The null set is the subset of every set A and is denoted by the symbol ϕ . The *power set* of A , $\mathcal{P}(A) = 2^A$, is defined as the set of all subsets of A : $\mathcal{P}(A) = \{B \mid B \subset A\}$. We observe that sets are *completely defined by their elements*: two sets A and B are *equal* if they have the exactly the same elements; i.e. $A = B$ if and only if $A \subset B$ and $B \subset A$.

Operations on Sets

From any two sets, one can form a third set by using a variety of set operations. The *union* of two sets A and B , for example, is the set C consisting of all elements in A or B or in both A and B ,

$$C = A \cup B \equiv \{x \mid x \in A \text{ or } x \in B\}, \quad (2.2)$$

and obeys the following properties:

$$\begin{aligned} \text{U1: } & A \cup B = B \cup A \\ \text{U2: } & A \cup A = A \text{ and } A \cup \phi = A \\ \text{U3: } & A \cup (B \cap C) = (A \cup B) \cap C \\ \text{U4: } & A \cup B = B \text{ if and only if } A \subset B \end{aligned} \quad (2.3)$$

A union of an arbitrarily large number of sets is handled in a straightforward manner: let $A_1, A_2, \dots, A_n$ be sets. Then

$$\bigcup_{i=1}^n A_i \equiv A_1 \cup A_2 \cup \dots \cup A_n = \{x \mid x \in A_i \text{ for at least one } i\}. \quad (2.4)$$

We can similarly form the *intersection* of A and B , which is the set C consisting of elements common to both:

$$C = A \cap B \equiv \{x \mid x \in A \text{ and } x \in B\} \quad (2.5)$$

The properties obeyed by intersection are analogous to those of the union:

$$\begin{aligned} \text{I1: } & A \cap B = B \cap A \\ \text{I2: } & A \cap A = A \text{ and } A \cap \phi = \phi \\ \text{I3: } & A \cap (B \cup C) = (A \cap B) \cup C \\ \text{I4: } & A \cap B = B \text{ if and only if } A \subset B, \end{aligned} \quad (2.6)$$

as is the definition of an arbitrary number of intersections:

$$\bigcap_{i=1}^n A_i \equiv A_1 \cap A_2 \cap \dots \cap A_n = \{x \mid x \in A_i \text{ for each } i = 1, 2, \dots, n\}. \quad (2.7)$$

The union and intersection are related by two distributive laws:

$$\begin{cases} A \cup (B \cap C) = (A \cup B) \cap (A \cup C) & \leftrightarrow \cup - \text{distributive} \\ A \cap (B \cup C) = (A \cap B) \cup (A \cap C) & \leftrightarrow \cap - \text{distributive} \end{cases} \quad (2.8)$$

A third operation on two sets A and B is the *difference*, $A - B$, consisting of elements of A which are not elements of B :

$$C = A - B \equiv \{x \mid x \in A \text{ and } x \notin B\}. \quad (2.9)$$

The difference operator has the following properties:

$$\begin{aligned} \text{D1: } & A - \phi = A \text{ and } A - A = \phi \\ \text{D2: } & A - B = \phi \text{ if and only if } A \subset B \\ \text{D3: } & A - B = A \text{ if and only if } A \cap B = \phi \\ \text{D4: } & A - B = A - C \text{ if and only if } A \cap B = A \cap C \\ \text{D5: } & A - (B \cap C) = (A - B) \cup (A - C) \\ \text{D6: } & A - (B \cup C) = (A - B) \cap (A - C) \end{aligned} \quad (2.10)$$

Properties **D5** and **D6** are sometimes referred to as the *DeMorgan Laws*.

Finally, we mention an important operation called the *cartesian* (or *direct*) product of two sets, $A \times B$, which is the set of ordered pairs of the form (a, b) , where $a \in A$ and $b \in B$:

$$C = A \times B \equiv \{(a, b) \mid a \in A \text{ and } b \in B\}. \quad (2.11)$$

Note that the cartesian product $A \times B$ is *not the same* as the product $B \times A$. A simple example is the two-dimensional coordinate plane $\mathcal{R} \times \mathcal{R}$, where $\mathcal{R}$ is the set of real numbers. Each point of the plane is specified by the ordered pair (x, y) of real numbers; $(x, y) = (y, x)$ if and only if $x = y$. Let $A_1, A_2, \dots, A_n$ be sets. Then

$$\mathbf{X}_{i=1}^n A_i \equiv A_1 \times A_2 \times \dots \times A_n = \{\vec{x} = (x_1, x_2, \dots, x_n) \mid x_i \in A_i\}, \quad (2.12)$$

where x_i is called the i^{th} *coordinate* of $\vec{x}$.

An important concept is that of the *size* of a set. Let $\mathcal{N}$ denote the set of *natural numbers*, and $\mathcal{N}_n$ denote the set $\{1, 2, \dots, n\}$. Then a set A is *finite* if $A = \phi$ or it is in one-to-one correspondence with $\mathcal{N}_n$, for some 'n'; in the latter case, the size (i.e. the number of elements) of A is equal to 'n': $|A| = n$. The following three properties are elementary:

$$\begin{aligned} \text{S1: } & |\mathcal{P}(A)| = 2^{|A|} \\ \text{S2: } & |A \cup B| + |A \cap B| = |A| + |B| \\ \text{S3: } & |A \times B| = |A| |B| \end{aligned} \quad (2.13)$$

A set which is not finite is called *infinite*. Although it is meaningless to speak of the 'number of elements' of such sets, we say that two infinite sets have the same *cardinality* if their respective elements can be put into a one-to-one correspondence.

In particular, sets for which there exists a one-to-one mapping to the set $\mathcal{N}$ are called *countable* (or *countably infinite*).

EXAMPLES: countable sets include the *integers* $\mathcal{Z}$ (simply use the 1 : 1 correspondence $f : \mathcal{N} \rightarrow \mathcal{Z}$, $f(n) = \lfloor n/2 \rfloor (-1)^n$, where $\lfloor x \rfloor$ is the greatest integer not exceeding x); *prime integers* (use $2 \leftrightarrow 1$, $3 \leftrightarrow 2$, $5 \leftrightarrow 3$, etc.) and the set of *rational numbers* $\mathcal{Q}$ of the form p/q , $p, q \in \mathcal{Z}$ (the easiest way to see this is to imagine an infinite square lattice array, each point of which represents a rational number, and to 'count' the points by following a zig-zag motion from the origin outwards).

Not every infinite set is countable, of course. For example, there can be no one-to-one correspondence between $\mathcal{N}$ and its power set $\mathcal{P}(\mathcal{N})$. That the set of reals, $\mathcal{R}$, is an also uncountable set can be demonstrated by using Cantor's *diagonal* argument: consider just the $\mathcal{R} \in [0, 1]$, and assume that each real in this interval can be put into one-to-one correspondence with an integer 'n'. We then have the matching $n \longleftrightarrow R(n)$. Representing each of the reals, $R(1)$, $R(2)$, $R(3)$, ..., by an infinitely long decimal expansion, we form another real, R^* , by the following prescription: its i^{th} digit is *any digit other than the one found in the i^{th} position of the decimal expansion of $R(i)$* . It should be clear that R^* cannot be an element of our presumably exhaustive set of reals, and therefore cannot be mapped to an integer: i.e. $\mathcal{R}$ is uncountable.

Topology

A *topology* $\mathcal{T}$ on a set X is defined to be a collection $\mathcal{T}$ of subsets of X with

$$\left\{ \begin{array}{l} \phi, X \in \mathcal{T} \\ \bigcup t_i \subset \mathcal{T}, \quad \forall t_i \in \mathcal{T} \\ \bigcap t_i \subset \mathcal{T}, \quad \forall t_i \in \mathcal{T}, \end{array} \right. \quad (2.14)$$

where $\phi \equiv$ empty set. A subset $U \subset X$ is an *open set* U of X if $U \in \mathcal{T}$. There are three distinct kinds of topologies of interest to us, and which will be used later to provide a topological characterization of CA: *discrete*, *product* and *metric* topologies.

A *discrete* topology is a collection of all subsets of X . To define the *product* topology we first introduce the notion of a basis for a topology: a basis β for a topology $\mathcal{T}$ on X is a collection of subsets of X such that

$$\left\{ \begin{array}{l} \forall x \in X, \exists \text{ at least one } b \in \beta \text{ containing } x \\ \text{if } x \subset (b_1 \cap b_2) \text{ then } \exists b_3 \text{ containing } x \mid b_3 \subset (b_1 \cap b_2) \end{array} \right. \quad (2.15)$$

Now, β can be used to generate a topology $\mathcal{T}(\beta)$: a subset U is *open* in X (i.e. $N \in \mathcal{T}(\beta)$) if $\forall x \in U \exists b \in \beta \mid x \in b \text{ and } b \subset U$. Then, the *product topology* on $X \times Y$ is the topology having as basis the collection β of all sets of the form $U \times V$, where U and V are open sets of X and Y , respectively.

In order to define the *metric* topology, we must first introduce the notion of *metric*: a function $\partial : X \times X \rightarrow \mathcal{R}$ is a metric on a set X if and only if it satisfies

the following three properties:

$$\begin{cases} \partial(x, y) \geq 0, \quad \forall x, y \in X; \quad \partial(x, y) = 0 \leftrightarrow x = y \\ \partial(x, y) = \partial(y, x) \\ \partial(x, y) + \partial(y, z) \geq \partial(x, z). \end{cases} \quad (2.16)$$

Using the ϵ -ball $b(x, \epsilon) \equiv \{y | \partial(x, y) < \epsilon\}$, we define the metric topology $\mathcal{T}_\partial$, induced by the metric ∂ , as the topology having as basis the collection $\{b(x, \epsilon) | \forall x \in X, \epsilon > 0\}$. That is, a set U is open in $\mathcal{T}_\partial$ if and only if $\forall u \in U \exists \delta > 0$ such that $b(u, \delta) \subset U$. Generally, topological spaces that arise from metric space are said to be *metrizable*.

A fundamental theorem states that a function $f : \mathcal{T}_1 \rightarrow \mathcal{T}_2$ between two metric topologies is *continuous* if and only if for all open sets $U \in \mathcal{T}_2$, the set $f^{-1}(U)$ is open in $\mathcal{T}_1$. In particular, if two different metrics, ∂_1 and ∂_2 , give rise to the same family of open sets then any function which is continuous under ∂_1 will also be continuous under ∂_2 .

EXAMPLES: (1) Consider the metric function

$$\partial(x, y) = \begin{cases} 1 & \text{if } x \neq y \\ 0 & \text{else.} \end{cases} \quad (2.17)$$

Then the basis elements are given by $b(x, 1) = x$ which defines the *discrete* topology.

(2) $\partial(x, y) = \{\sum_{i=1}^n (x_i - y_i)^2\}^{1/2} = \|\vec{x} - \vec{y}\|$ is the usual *Euclidean* metric on $\mathcal{R}^n$.

(3) If $\partial(x, y)$ is a metric and ' α ' is any positive real number, then $\partial_\alpha(x, y) \equiv \alpha\partial(x, y)$ is also a metric.

(4) A very useful distance measure between ordered sets of discrete valued elements is the *Hamming distance*, ∂_H . Given two sets, $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$,

$$\partial_H(\vec{x}, \vec{y}) \equiv \sum_{i=1}^n \chi_i, \quad (2.18)$$

where $\chi_i = 1$ if $x_i \neq y_i$ and $\chi_i = 0$ otherwise. Thus ∂_H indicates in how many positions two vectors are different.

Fractal Sets and Dimensions

Consider a subset $A \in X$ and an arbitrary metric ∂ . Let $N(A, \epsilon)$ be the smallest number of ϵ -balls needed to cover the set A ; i.e.,

$$N(A, \epsilon) = \text{smallest integer 'n' such that } A \subset \bigcup_{i=1}^n b(x_i, \epsilon), \quad (2.19)$$

for some distinct set of points $\{x_i, i = 1, 2, \dots, n\}$. If $N(A, \epsilon)$ increases as $N(A, \epsilon) \sim \epsilon^{-D}$ for $\epsilon \rightarrow 0$ then D is called the *fractal dimension* (sometimes also called the *capacity*) of the set A ; 'solving' for D , we find that

$$D_{\text{fractal}} = \lim_{\epsilon \rightarrow 0} \frac{\ln N(A, \epsilon)}{\ln (1/\epsilon)}. \quad (2.20)$$

That D_{fractal} gives the expected result for simple sets in Euclidean space is easy to see. If A consists of a single point, for example, we have $N(A, \epsilon) = 1, \forall \epsilon$, and thus that $D_{\text{fractal}} = 0$. Similarly, if A is a line segment of length L , then $N(A, \epsilon) = L/\epsilon$ so that $D_{\text{fractal}} = 1$. In fact, for the usual ' n ' dimensional Euclidean sets, the fractal dimension equals the topological dimension. There are more complicated sets, however, for which the two measures differ.

Consider the *triadic Cantor set* construction on the real line: let $x_0 = [0, 1]$ and x_1 be the set obtained from x_0 by deleting the open interval $(\frac{1}{3}, \frac{2}{3})$. Let x_2 be the set obtained from x_1 by deleting the 'middle thirds' $(\frac{1}{9}, \frac{2}{9})$ and $(\frac{7}{9}, \frac{8}{9})$. Continue in this fashion, letting $x_n = x_{n-1} - \bigcup_{i=0}^{\infty} (\frac{1+3i}{3^n}, \frac{2+3i}{3^n})$ (see figure 2.1). Then the Cantor set is the intersection $C = \bigcap_{n=0}^{\infty} x_n$; it is totally disconnected, compact, and uncountable.

Although the *length* of the Cantor set is zero –

$$L = 1 - \frac{1}{3} - \frac{2}{9} - \frac{4}{27} - \dots = 1 - \frac{1}{3} \sum_{i=0}^{\infty} \left(\frac{2}{3}\right)^i = 0, \quad (2.21)$$

– its fractal dimension is *greater* than zero: since at the n^{th} step of the construction $N(\epsilon) = 2^n$ balls of size $\epsilon = (1/3)^n$ are needed to cover the set, we see immediately that

$$D_{\text{fractal}}(\text{Cantor}) = \lim_{n \rightarrow \infty} \frac{\ln 2^n}{\ln 3^n} \sim 0.6309. \quad (2.22)$$

Although it is not the only such measure, the fractal dimension does quantify the intuitive belief that the Cantor set is somewhere 'in-between' a point and a line. We will consider generalizations of D_{fractal} as needed in later chapters.

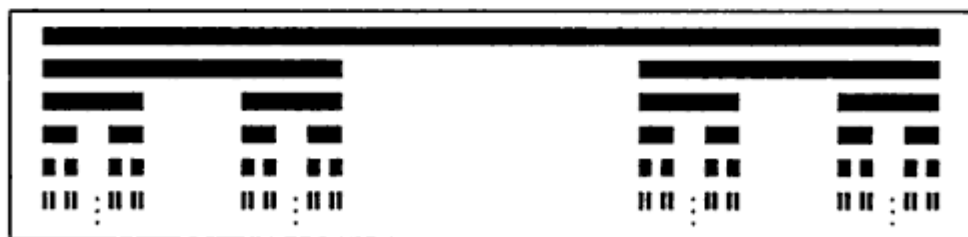


Fig. 2.1 First six steps of the construction of the triadic *Cantor Set*. The infinite-time limit point set has *fractal dimension* $D_{\text{fractal}} = \ln 2 / \ln 3$.

Consider a general sequence of transformations $\mathcal{T}$ applied to a set A ,

$$A_0 \rightarrow A_1 = \mathcal{T}A_0 \rightarrow A_2 = \mathcal{T}A_1 \rightarrow \cdots \rightarrow A_n = \mathcal{T}^n A_0, \quad (2.23)$$

where the scale of resolution at the n^{th} step is ϵ_n . If an arbitrary measurable quantity of interest Q (mass, area, volume, etc.), scales in self-similar fashion we can write

$$Q(A_{n+1}(\epsilon_{n+1})) = \left\{ \frac{\epsilon_n}{\epsilon_{n+1}} \right\}^D Q(A_n(\epsilon_n)), \quad (2.24)$$

where $Q(A_n(\epsilon_n))$ is quantity Q measured in units of ϵ_n . Since, in the general case, this relation may only be satisfied in the limit as $n \rightarrow \infty$ we obtain

$$D_{\text{fractal}} = \lim_{n \rightarrow \infty} \frac{\ln [Q(A_{n+1}(\epsilon_{n+1}))/Q(A_n(\epsilon_n))]}{\ln (\epsilon_n/\epsilon_{n+1})}. \quad (2.25)$$

Thus, whenever the set A has a manifest *self-similarity*, so that, like the Cantor set, it can be defined by a recursive geometric construction, D_{fractal} can be easily calculated from this relation. The *Koch Curve*, for example, the first three steps in the construction of which are shown in figure 2.2, has a length L which scales as

$$L_{n+1}(\epsilon_{n+1} = \epsilon_n/3) = 4 L_n(\epsilon_n), \quad (2.26)$$

so that $D_{\text{fractal}}(\text{Koch}) = \ln 4 / \ln 3 \sim 1.262$.

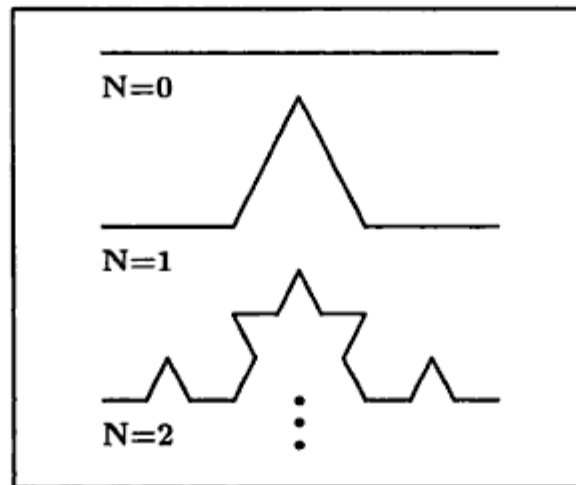


Fig. 2.2 First three steps in the construction of the *Triadic Koch Curve*. The fractal curve is obtained in the limit $N \rightarrow \infty$ and has a fractal dimension $D_{\text{fractal}} = \ln 4 / \ln 3 \sim 1.26$.

2.1.2 Information Theory

Like the physically 'primitive' notions of *spin* and *energy* of a particle, the *information content*, $\mathcal{I}$, of an arbitrary measurement or message composed of particular symbol sequences, is itself a primitive concept. While the roots of information theory extend back to the definition of the classical entropy of a physical system introduced by Clausius in 1864 and Boltzman's probabilistic re-interpretation of classical entropy in 1896, the mathematical formalism for measuring $\mathcal{I}$ is due largely to a seminal 1948 paper by Claude E. Shannon (see [shann49]). Within the context of sending and receiving messages in a communication system, Shannon was interested in finding a measure of the information content of a received message. His approach was to obtain a measure of the *reduction of uncertainty* given some *a-priori* knowledge of the symbols being sent.

Information Capacity

Suppose we are given a situation in which there are N different and *a-priori* equally likely possible outcomes. In the case of a roll of a single die, for example, $N = 6$ and the probability, $p_i = 1/6$ for $i = 1, \dots, 6$. The outcome of throwing the die may be interpreted as receiving a 'message'; heuristically, the larger the number N , the greater the uncertainty is in predicting the outcome and the greater the information gain upon receiving the message. A measure of this information gain, $\mathcal{I}$, is obtained by requiring that $\mathcal{I}$ is *additive for independent events*. That is to say, if there are two independent sets of outcomes, N_1 and N_2 , so that the total number of outcomes is $N = N_1 \cdot N_2$, it is required that

$$\mathcal{I}(N_1 \cdot N_2) = \mathcal{I}(N_1) + \mathcal{I}(N_2). \quad (2.27)$$

This requirement is *uniquely* satisfied by the function

$$\mathcal{I} = c \log N, \quad (2.28)$$

where 'c' is an arbitrary constant. The value of this constant is conventionally fixed by considering a binary sequence of length n ; by a binary sequence we mean one in which each symbol takes on one of only two values (*heads or tails, up or down, etc.*). By defining the information content of such a binary sequence to be equal to its *length*, n , we find $\mathcal{I} \equiv n = c \log N = c n \log 2 \implies c = \log_2 10$, where $N = 2^n$ is the total number of possible binary sequences of length n . With this value of 'c', equation 2.28 becomes

$$\mathcal{I} = \log_2 N \quad (\text{bits}), \quad (2.29)$$

where $\log_2$ is the logarithm base-2.

Average Information Gain

Equation 2.29, giving the maximum information content of a system with N equally likely possible outcomes, may be generalized to the case of N possible outcomes with

unequal probabilities. Consider a binary sequence of length N containing N_1 0's and N_2 1's, with $N = N_1 + N_2$. The total number of possible sequences that may be constructed, for fixed N_1 and N_2 , is given by $\mathcal{N} = N!/(N_1!N_2!)$. Using Stirling's approximation for factorials, $\log n! \approx n \log n - n$, we find that the *average information per symbol*, is

$$\begin{aligned} I &= \frac{\mathcal{I}}{N} = \frac{\log_2 \mathcal{N}}{N} \approx N(\log_2 N - 1) - N_1(\log_2 N_1 - 1) - N_2(\log_2 N_2 - 1), \\ &\approx \frac{N_1}{N} \log_2 \frac{N}{N_1} + \frac{N_2}{N} \log_2 \frac{N}{N_2}, \\ &\approx -(p_1 \log_2 p_1 + p_2 \log_2 p_2), \end{aligned} \quad (2.30)$$

where $p_i = N_i/N$, $i = 1, 2$, is the probability of finding each of the two possible symbols. The generalization of this result to a system with more than two symbols is Shannon's measure of average information gain: Given, *a-priori*, that a total of n possible events (or states) may occur with individual probabilities p_i , the *average information gained** by repeatedly measuring the outcome state of the system is given by

$$I^{(n)}(p_1, p_2, \dots, p_n) = -\sum_{i=1}^n p_i \log_2 p_i \quad (\text{bits/symbols}). \quad (2.31)$$

By extending $x \log_2 x$ to the origin by continuity, we define $p_i \log_2 p_i = 0$ if $p_i = 0$.

An increase in the accuracy of a measurement increases the information gain. Suppose we are measuring the position of a point along some line segment. This may be done by partitioning the segment into n equal intervals and noting which one contains the chosen point. Since the probability that it is in any of the segments is $p_i = 1/n$, the information gain of the measurement is $I^{(n)} = \sum_i \frac{1}{n} \log_2 n = \log_2 n$. Thus, as the resolution (i.e., n) increases, the information increases.

$I^{(n)}$ may be considered as being an average over the *self-information*, $I_i = -\log_2 p_i$ (bits), contained in the i^{th} outcome. Note that this definition is an 'intuitive' one: if we observe outcome ' i ', whose *a-priori* probability is known to be $p_i \sim 1$, we do not gain much information since we already expected to see it; if $p_i \sim 0$, on the other hand, the i^{th} outcome is a rare event an observation of which therefore yields a significant amount of information. If all N events are equally likely, $p_i = 1/N$ for all ' i ', and $I_i = I = \log_2 N$, consistent with the information content defined in equation 2.29 above.

Properties of $I^{(n)}$: We list a few basic properties of $I^{(n)}$ without proof; most are either obvious or straightforward to verify (for details see ([aczel75] and [guiasu77]).

P1. Since $\log_2 p_i \leq 0$ for $0 < p_i \leq 1$, $I^{(n)} \geq 0$. $I^{(n)} = 0$ if and only if all of the p_i except one are equal to zero.

*Also called the *uncertainty* or – because of its formal similarity to the entropy function used in statistical mechanics – *Shannon entropy*.

$$\mathbf{P2.} \quad I^{(n+1)}(p_1, p_2, \dots, p_n, 0) = I^{(n)}(p_1, p_2, \dots, p_n).$$

$\mathbf{P3.}$ For a given n , $I^{(n)}(p_1, p_2, \dots, p_n) \leq I^{(n)}(\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n}) = \log_2 n$. (This property is a simple consequence of the *convexity* property of the logarithm, $\log_2 x \leq x - 1$).[†]

$\mathbf{P4.}$ $I^{(n)}(\mathbf{p})$ is a *concave* function of $\mathbf{p}$.

$\mathbf{P5.}$ The average information is additive for *independent events*: $I^{(n)}(p_1, p_2, \dots, p_n) = \sum_{i=1}^n I^{(1)}(p_i)$. In general, $I^{(n)}(p_1, p_2, \dots, p_n) \leq \sum_{i=1}^n I^{(1)}(p_i)$.

2.1.3 Graph Theory

We shall extensively employ the notation of graph theory; it provides a powerful and elegant formalism for the description of both the 'structure' of the discrete lattices on which the CA live, and the complete 'dynamics' (*i.e.* the *global state transitions*) induced by those structures. Graph theory also allows the correspondence between CA configurations and the words of a regular language to be made in a very natural fashion.

Basic Terminology

A *graph* $G(N, M)$ (also called a *linear*, or *ordinary graph*), is a finite, nonempty set $V(G) = \{v_1, \dots, v_N\}$ of *vertices* together with (a possibly empty) set $E(G) = \{e_1, \dots, e_M\}$ of *edges*. Each edge $e = e(i, j) \in E(G)$, *connects* vertex ' i ' to vertex ' j '. If the edges represent *ordered* pairs of vertices, then G is a *directed* graph: each $e(i, j)$ defines an edge *directed from* ' i ' *to* ' j ', and is denoted by $e(i, j) = i\bar{j}$. If, on the other hand, $e_n(i_n, j_n) = e_n(j_n, i_n)$ for all ' n ', then G is an *undirected* graph, and all edges are denoted simply by $e(i, j) = ij = ji$. Two vertices, ' i ' and ' j ', are said to be *adjacent* if $e(i, j) \in E(G)$.

Intuitively, a graph can be realized geometrically in a three-dimensional Euclidean space: vertices are represented by *points* and edges are represented either by *lines* (in the case of undirected graphs) or *arrows* (in the case of directed graphs). In this book, we will be concerned with both kinds of graphs; *multiple edges* (*i.e.* when vertices are connected by more than one line or arrow), however, are not allowed.

The *order* of a graph G is the number of vertices of G : $|G| = |V(G)| = N$. The *size* of G is the total number of edges in G : $\|G\| = |E(G)| = M$. In principle, the order and size of G may both be infinite, but we will mostly consider the case in which they are both finite. Clearly, for every M , $0 \leq M \leq \binom{N}{2}$, there is a graph $G(N, M)$. The graph of order N and size $\binom{N}{2}$ is called a *complete N -graph*; it is

[†]A function f is called *convex* if a straight line between any two points of the graph of f never falls below the graph of f : *i.e.*, if

$$f(\alpha x_1 + (1 - \alpha)x_2) \leq \alpha f(x_1) + (1 - \alpha)f(x_2),$$

for all x_1, x_2 and all $0 < \alpha < 1$. A function f is *concave* if $-f$ is convex.

denoted by K_N .

A graph $G(N, M)$ is *labeled* if all of its N vertices are associated with N distinct labels in a one-to-one manner. An *edge-labeled* graph is defined in an analogous fashion.

It is very important to understand what is meant by two graphs being the 'same' or 'different'. For this purpose we introduce the notion of graph isomorphism. Two graphs, G_1 and G_2 , are *isomorphic*, which we write as $G_1 \cong G_2$, if there exists a bijection $\psi : V_1 \rightarrow V_2$ which preserves adjacency (i.e. such that $e(i, j) \in E_1$ if and only if $e(\psi(i), \psi(j)) \in E_2$). Isomorphic graphs necessarily must have the same order and size. It is easy to see that *isomorphism* is an *equivalence* relation on graphs: it divides the collection of all graphs into equivalence classes, for which any two member graphs must have the same structure.

Since all graphs in the same class are in this sense *topologically equivalent*, a representative member of each class, devoid of explicit vertex (or edge) labels, defines a unique *unlabeled graph*. Figure 2.3, for example, shows all of the undirected and unlabeled graphs of order 4.

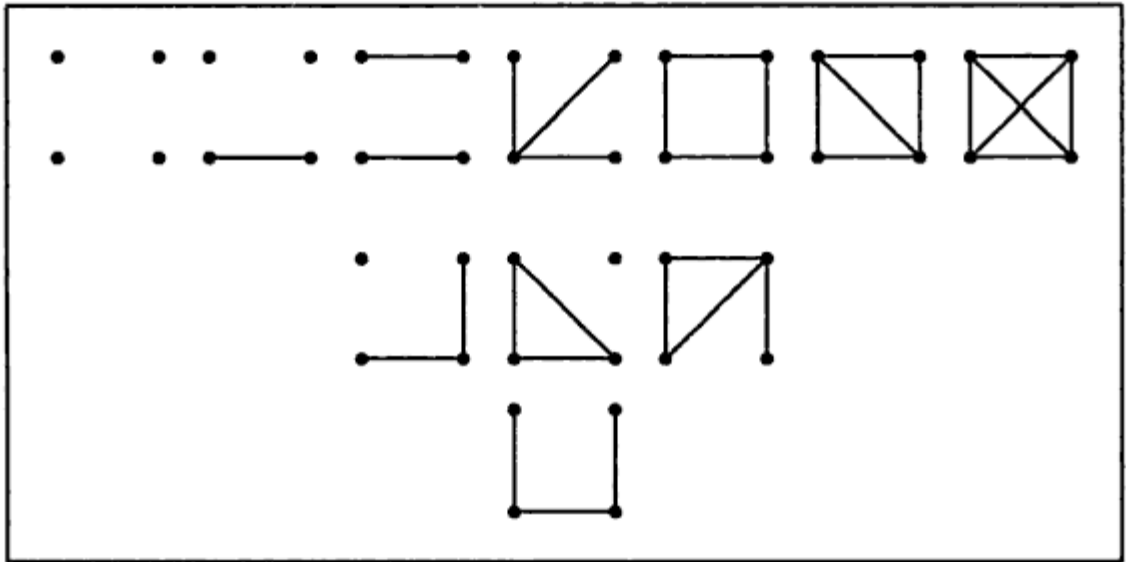


Fig. 2.3 All undirected, unlabeled graphs G of order $|G| = 4$.

Suppose π is a permutation of the N labels, $1, 2, \dots, N$ and G is a labeled graph of order N . Let $\pi(G)$ represent the graph obtained from G by relabeling each vertex ' i ' by ' $\pi(i)$ '. Then the set $\mathcal{A}(G)$, consisting of all permutations ' π ' such that G and $\pi(G)$ are identical graphs is called the *automorphism* group of G . Since any graph G can be labeled in any of $n!$ distinct ways, the order of the automorphism group, $|\mathcal{A}(G)|$, tells us how many of these labelings will be topologically equivalent: i.e.

the number of ways of labeling an unlabeled graph is given by

$$\alpha(G_{\text{unlabeled}}) = \frac{n!}{|\mathcal{A}(G_{\text{unlabeled}})|}.$$

It is easy to show that the number of graphs of order N , $\mathcal{G}_N = 2^{\binom{N}{2}}$, and the number of graphs of order N and size q , $\mathcal{G}_{N,q} = \binom{\binom{N}{2}}{q}$.

$\tilde{G} = (\tilde{V}, \tilde{E})$ is a *subgraph* of $G = (V, E)$, written $\tilde{G} \subset G$, if $\tilde{V} \subset V$ and $\tilde{E} \subset E$. If $\tilde{G}$ contains *all edges* of G that join two vertices in $\tilde{V}$, then $\tilde{G}$ is the *subgraph induced* (or *spanned*) by $\tilde{V}$, and is denoted by $G[\tilde{V}]$. A subgraph $\tilde{G}$ of G is an *induced subgraph* if $\tilde{G} = G[\tilde{V}(\tilde{G})]$. $\tilde{G}$ is a *spanning subgraph* of G if $\tilde{V} = V$.

The set of vertices adjacent to a vertex $i \in V(G)$ is denoted by $\Gamma(i)$. The *degree* of ' i ', $d(i)$, is defined to be the number of vertices adjacent to ' i ': $d(i) = |\Gamma(i)|$. Note that, for undirected graphs, the sum of the degrees is exactly *twice* the number of edges: $\sum_{i=1}^N d(v_i) = 2M$. We will denote the *minimum* degree of G by $\delta(G)$, and the *maximum* degree by $\Delta(G)$.

Examples of Graphs

A *walk* from the vertex v_1 to vertex v_{i+1} is a finite sequence of edges of the form $(v_1, v_2), (v_2, v_3), \dots, (v_i, v_{i+1})$ (also written as $(v_1, v_2) \rightarrow (v_2, v_3) \rightarrow \dots \rightarrow (v_i, v_{i+1})$). In general, a given vertex or edge can be visited any number of times. A walk in which each vertex is distinct is called a *path*. A *path of length n* is therefore a graph $\mathcal{P}_n$ consisting of the distinct sequence of vertices $\{v_1, \dots, v_n\}$ and edges $\{(v_1, v_2), (v_2, v_3), \dots, (v_{n-1}, v_n)\}$. If the edge (v_n, v_1) is added, the path becomes a *circuit of length n* , C_n . If we substitute the *arrows* (or *arcs*) $(v_i \rightarrow v_{i+1})$ for the lines (v_i, v_{i+1}) , the circuit becomes a *cycle of length n* , C_n . If a graph G contains at least one cycle which itself contains all of the vertices of G , then G is said to be *Hamiltonian*.

A graph G is *connected* if for every pair of distinct vertices in G there exists at least one path along existing edges. The connected (undirected) graph of order N which has the smallest size is called a *tree*. In fact, a tree T is equally well characterized by any of the following properties:

- $$\left\{ \begin{array}{l} \bullet \text{ } T \text{ contains no circuits and has } N - 1 \text{ edges} \\ \bullet \text{ } T \text{ is connected and has } N - 1 \text{ edges} \\ \bullet \text{ any two vertices of } T \text{ are connected by} \\ \quad \text{exactly one path} \\ \bullet \text{ } T \text{ contains no circuits; the addition of any} \\ \quad \text{new edge creates exactly one circuit.} \end{array} \right.$$

A *spanning tree* in G is an edge-subgraph of G which has $N - 1$ edges and contains no circuits.

If $\delta(G) = \Delta(G) = r$ (i.e. each vertex of G has the same degree $d = r$) then G is an *r -regular graph*. A *circuit*, for example, can be alternatively defined as a 2-regular connected graph.

Graph Matrices

Although most graphical properties are most easily distinguished by means of a diagram, there are many instances when a *matrix representation* of a graph is extremely helpful, particularly when a more formal analytic understanding is desired.

There are a variety of different matrices that can be defined; we mention two of the most important.

Adjacency Matrix: The adjacency matrix $A(G)$ of an order N graph G with $V(G) = \{v_1, v_2, \dots, v_N\}$ is an $N \times N$ matrix $[a_{ij}]$ with entries $a_{ij} = 1$ if $(v_i, v_j) \in E(G)$ and $a_{ij} = 0$ otherwise. $A(G)$ is therefore a symmetric $(a_{ij} = a_{ji})$ $(0, 1)$ -matrix with trace $\text{Tr}(A) = 0$ (i.e. A has all zeros on the diagonal).

Note that this is an exact correspondence: i.e. the set of all $N \times N$ matrices satisfying these properties represents the class of all (labeled) graphs G of order N .

The entries of the n^{th} power of $A(G)$ have a very simple interpretation: $[a_{ij}^{(n)}]$, $n \geq 1$ is the number of different walks from v_i to v_j of length ' n ' in G . In particular, $a_{ij}^{(2)}$, $i \neq j$ is the number of $v_i - v_j$ paths of length two and $a_{ii}^{(2)} = \deg v_i$.

While the rows and columns of A obviously depend on a particular choice of vertex labels, the generic structural properties of G must remain invariant under a permutation of rows and columns. Much of this structural information can in fact be extracted from the *spectrum* of G : the spectrum of a graph G ,

$$\text{Sp}(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_s \\ m(\lambda_1) & m(\lambda_2) & \cdots & m(\lambda_s) \end{pmatrix},$$

is the set of eigenvalues, λ_i of $A(G)$, together with their multiplicities, $m(\lambda_i)$. Since $A(G)$ is *real* and symmetric, we know that the eigenvalues λ_i must also be *real*. For example, the spectrum of the complete graph of order ' n ', $\text{Sp}(K_n) = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}$. Two non-isomorphic graphs, G_1 and G_2 , are *cospectral* if $\text{Sp}(G_1) = \text{Sp}(G_2)$.

The relationship between the topological properties of graphs and the set of eigenvalues of the adjacency matrix is an intensely studied field. For some questions, the spectrum yields a wealth of knowledge; for other questions, it may tell very little. Although it used to be believed that an arbitrary graph G is uniquely specified by $\text{Sp}(G)$, this conjecture was later shown to be very wrong. In 1973, for example, it was proven that the probability that an order N tree T belongs to a cospectral pair tends to *one* as $N \rightarrow \infty$; i.e. the probability that T is characterized by $\text{Sp}(T)$ approaches *zero* as $N \rightarrow \infty$.[†]

Some structural information about G can be obtained directly from the *characteristic polynomial* of $A(G)$:

$$\chi_G(\lambda) \equiv \det(A - \lambda I) = \sum_{i=0}^N a_i \lambda^{N-i}.$$

[†]A.J.Schwenk, in *New Directions in the Theory of Graphs*, ed. by F.Harary, Academic Press (1973), pp 275-307.

Since the coefficients a_i can be interpreted as sums of principal minors of $A(G)$, it is easy to check that (i) $a_1 = 0$, (ii) $a_2 = \text{the number of edges in } G$, and (iii) $a_3 = \text{twice the number of triangles in } G$. A more powerful version of this result will be presented and used in chapter 5.

Incidence Matrix: The incidence matrix $B(G)$ of an order N graph G with $V(G) = \{v_1, \dots, v_N\}$ and $E(G) = \{e_1, \dots, e_M\}$ is an $N \times M$ matrix $[b_{ij}]$ for which

$$b_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is the initial vertex of edge } e_j, \\ -1 & \text{if } v_i \text{ is the terminal vertex of edge } e_j, \\ 0 & \text{otherwise.} \end{cases}$$

$B(G)$ is often used to define the *complexity* of a graph G , $\kappa(G)$, equal to the number of spanning trees of G .[†] It turns out that

$$\kappa(G) = \det(J + BB^t) = \det(J + D - A),$$

where J is an $N \times N$ matrix all of whose entries are equal to one, D is an $N \times N$ diagonal matrix in which $[d_{ii}] = d(v_i)$, 'det' is the determinant and B^t is the transpose of B . Note that this result shows the simple relationship which holds between the adjacency and incidence matrices; namely, that $BB^t = D - A$.

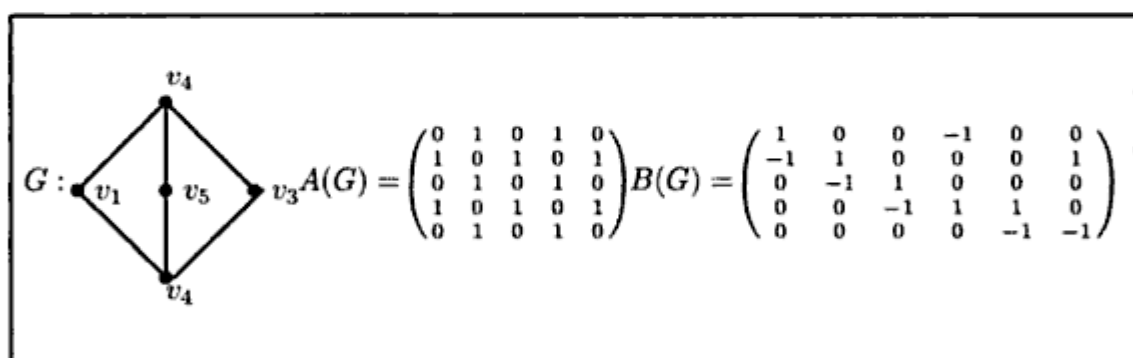


Fig. 2.4 The adjacency ($A(G)$) and incidence ($B(G)$) matrices of an order-5 directed graph G .

Random Graphs

The theory of random graphs—developed principally by Erdős and Rényi [erdos60]—offers an appropriate framework for posing questions about the general topological structures of computational systems and the expected mathematical behavior of certain random dynamical systems. The basic idea is to think of a graph as a living organism which develops by acquiring more and more edges and explore how its

[†]See H. Temperley, *Proc. Phys. Soc.* **83** (1964), 3.

various topological features emerge, often in a dramatically abrupt and unexpected fashion.

In order to show the emergence of some specific property $\mathcal{P}$ of a graph G , a probability space of graphs should first be formed, in which the probability that G has this property is positive. We define two frequently used models.

Model A: the sample space, Ω_A , consists of all order- N labeled graphs $G(N, M)$ of size M . The probability of G is given by

$$P(G) = \left(\binom{N}{2} \right)^{-1} \binom{M}{M},$$

so that each such graph is equally likely to occur.

Model B: the sample space, Ω_B , consists of all order- N graphs $G(N)$. If G has size M , then the probability of G is given by

$$P(G) = p^M (1 - p)^{\binom{N}{2} - M},$$

where ‘ p ’ is an independent probability, $0 \leq p \leq 1$, and is typically taken to be a function of N .

Note that **Model A** can be compared to the *microcanonical* ensemble in physics, in that it depends on the direct enumeration of possible configurations of a given graph; **Model B**, on the other hand, by assigning an independent probability to each edge, resembles the *canonical* ensemble. As for physical systems, these two models give the same results in the limit as $N \rightarrow \infty$. Depending on the problem at hand, the sample space can be generalized to include loops, multiple edges or even ensembles of graphs embedded in other topologies.

As alluded to earlier, as more and more edges are added to G (using **model A**), or the probability, ‘ p ’, of adding an edge is systematically increased (using **model B**), G successively passes through several well defined *structural* stages. If $M = cN$ in **model A** (or $p(N) = 2c/N$ in **model B**), for example, then an abrupt ‘phase transition’ occurs at $c = 1/2$: for $0 < c < 1/2$, G consists entirely of isolated points or small trees of order at most $\sim N \log N$; at $c = 1/2$, these small trees are suddenly replaced by a single tree spanning $\sim N^{2/3}$ vertices. An equally as dramatic a change occurs when $q = \frac{1}{2}cN \log N$ (or $p(N) = (c \log N)/N$): while G is almost always disconnected for $0 < c < 1$, for $c > 1$, G not only is almost always connected but is *hamiltonian* as well.

2.1.4 Groups, Rings and Fields

Groups

Let S be a set. A mapping $\phi : S \times S \rightarrow S$ is called a *binary* operation on S . A group $\mathcal{G} \equiv (G, \circ)$ is a set G together with a binary operation ‘ $\circ$ ’ on G such that the

following four properties hold:

$$\left\{ \begin{array}{ll} \text{Closure:} & \forall g_1, g_2 \in G, \quad g_1 \circ g_2 \in G \\ \text{Associativity:} & \forall g_1, g_2, g_3 \in G, \quad g_1 \circ (g_2 \circ g_3) = (g_1 \circ g_2) \circ g_3 \\ \text{Identity} & \exists e \in G, \text{ such that } \forall g \in G, \quad e \circ g = g \circ e = g \\ \text{Inverse:} & \forall g \in G \quad \exists g^{-1} \in G \text{ such that } g \circ g^{-1} = g^{-1} \circ g = e. \end{array} \right.$$

G is an *Abelian* group if, in addition to the above properties, for all $g_1, g_2 \in G$, $g_1 \circ g_2 = g_2 \circ g_1$.

Rings

The set R , together with the binary operations *addition* and *multiplication*, is a ring $\mathcal{R} \equiv (R, \circ, +)$ if it satisfies the following postulates:

$$\left\{ \begin{array}{ll} \text{Abelian:} & R \text{ is an abelian group with respect to '+'} \\ \text{Closure:} & \forall r_1, r_2 \in R, \quad r_1 \circ r_2 \in R \\ \text{Associativity:} & \forall r_1, r_2, r_3 \in R, \quad r_1 \circ (r_2 \circ r_3) = (r_1 \circ r_2) \circ r_3 \\ \text{Distributivity:} & \forall r_1, r_2, r_3 \in R, \quad r_1 \circ (r_2 + r_3) = r_1 \circ r_2 + r_1 \circ r_3 \\ & \forall r_1, r_2, r_3 \in R, \quad (r_1 + r_2) \circ r_3 = r_1 \circ r_3 + r_2 \circ r_3. \end{array} \right.$$

As for groups, R is a *commutative* ring if for all r_1, r_2 in R , $r_1 \circ r_2 = r_2 \circ r_1$. If there exists an integer n such that $nr = 0$ for all $r \in R$, then the least such integer n is called the *characteristic* of R . If no $n > 0$ exists then R is said to have characteristic 0. It is a simple exercise to show that if a ring $R \neq \{0\}$ which has an identity and no zero divisors (i.e. $ab = 0$ implies that either $a = 0$ or $b = 0$) has a positive characteristic, then it must have a prime characteristic.

Fields

Most of the analytical structure of the dynamics of linear CA systems emerges from their field-theoretic properties; specifically, those of finite fields and polynomials over fields. A brief summary of definitions and a few pertinent theorems will be presented (without proofs) to serve as reference for the presentation in subsequent sections.

A commutative ring $\mathcal{F}$ is called a *field* if, in addition to the properties given above, the following two postulates also hold true:

$$\left\{ \begin{array}{ll} \text{Identity:} & \exists \text{ an element } 1, \text{ such that } \forall f \in \mathcal{F}, \quad 1 \circ f = f \circ 1 \\ \text{Inverse:} & \forall \text{ nonzero } f \in \mathcal{F}, \quad \exists f^{-1} \text{ such that } f \circ f^{-1} = f^{-1} \circ f = 1. \end{array} \right.$$

Two simple examples of fields are the rational numbers, $\mathbb{Q}$ and the set of integers $Z_p = \{0, 1, \dots, p-1\}$, where p is prime and addition and multiplication are defined *modulo* p . The latter is an example of a *finite* field – that is, of a field containing only a finite number of elements. Since CA are almost always defined so that individual sites take on one of a finite number of values, if those values happen to be elements of a finite field then the dynamics can be well understood by using some of the general properties of that field. An elementary property of finite fields

with q elements, written $\mathcal{F}_q$, is that $\mathcal{F}_q$ must have prime characteristic. Moreover, if the characteristic of $\mathcal{F}_q$ is p , then the number of elements of $\mathcal{F}_q$ must be a power of p : $q = p^n$, for some positive integer n .

We will have occasion to use both polynomials and matrices defined over some finite field $\mathcal{F}_q$. In the case of a polynomial $f(x)$, what is meant is simply that

$$f(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_n x^n,$$

where $\alpha_i \in \mathcal{F}_q$. The set of all polynomials over $\mathcal{F}_q$ forms a ring, denoted by $\mathcal{F}[x]$. Similarly, a matrix over $\mathcal{F}_q$ is a matrix all of whose entries are elements of the field $\mathcal{F}_q$.

The *degree* of $f(x)$, denoted by $\partial[f]$, is the highest power of x with a nonzero coefficient; this coefficient is called the *leading coefficient* of $f(x)$. If the leading coefficient is '1', then $f(x)$ is called a *monic polynomial*. For any two polynomials, $f_1(x)$ and $f_2(x)$, one can uniquely write $f_1(x) = q(x)f_2(x) + r(x)$, where $0 \leq \partial[r] < \partial[f_2]$ or $r(x) = 0$. If $r(x) = 0$ then $q(x)$ is a *divisor* of $f_1(x)$. A polynomial $f(x)$ is *irreducible* if its only divisors are α and $\alpha f(x)$, where $\alpha \in \mathcal{F}$.

The *prime factorization theorem* states that any polynomial $f(x)$ can be written in the following form:

$$f(x) = [p_1(x)]^{\nu_1} [p_2(x)]^{\nu_2} \cdots [p_n(x)]^{\nu_n},$$

where ' $p_i(x)$ ' are distinct irreducible polynomials and $[p_i(x)]^{\nu_i}$ are the *prime factors* of $f(x)$. The factorization is unique up to a constant multiplier and the order in which the prime factors appear.

It is easy to show that every polynomial $f(x)$ (not divisible by x) over a finite field $\mathcal{F}_q$ is a factor of $1-x^n$, for some power ' n '. The *order* (sometimes also called the *period* or *exponent*) of $f(x)$, denoted by $\text{ord}(f)$, is the least such ' n '. If $f(x) = p(x)$ is an irreducible polynomial (other than x) with $\partial[f] = n$ then $\text{ord}(f)$ must divide $p^n - 1$. There are two important theorems concerning the orders of prime factors and products of relatively prime polynomials over $\mathcal{F}_q$:

Theorem 1: let $p(x) \in \mathcal{F}_q$, $p(0) \neq 0$, be irreducible, $\text{ord}(p)=n$, and $f(x) = [p(x)]^m$, with m a positive integer. Then $\text{ord}(f)=np^t$, where t is the smallest integer with $p^t \geq m$.

Theorem 2: Let $f_1, f_2, \dots, f_k$ be pairwise relatively prime nonzero polynomials over $\mathcal{F}_q$, and $f = \prod_i f_i$. Then $\text{ord}(f) = \text{lcm}(\text{ord}(f_1), \dots, \text{ord}(f_k))$.

The set of all polynomials over $\mathcal{F}_q$ which satisfies the property that any two polynomials, $f_1(x)$ and $f_2(x)$, are equal if and only if $f_1(x) - f_2(x) = \alpha a(x)$, where $\alpha \in \mathcal{F}_q$, constitutes a ring called the *ring of polynomials over $\mathcal{F}_q$ modulo $a(x)$* . The ring of polynomials over $\mathcal{F}_q$ modulo $p(x)$, where $p(x)$ is an irreducible polynomial, is also a field. If $\partial[p] = k$, then this field is represented by the set of all p^k polynomials of degrees $k-1$ or less over $\mathcal{F}_q$ and is called the *Galois field of order p^k* . Every finite field $\mathcal{F}_q$ is isomorphic (*i.e.* can be put into a one-to-one correspondence) with some

Galois field of order p^k .

2.1.5 Abstract Automata

Alphabets and Strings

Just as *points* and *lines* are formally undefined geometrical objects, a *symbol* represents an abstract undefined object. Typical representations include *letters* and *digits*. An *alphabet* is then simply a finite nonempty set A of symbols. An n -tuple of symbols of A is defined to be a *string* on A (also called a *word* on A). If $A = \{a_1, a_2, \dots, a_n\}$, for example, then we would write the string $s(A) = a_1 a_2 \cdots a_n$; the *length* of the string is the number of symbols of which it is composed, and is written $|s(A)| = n$. The *null* string, s_0 , is a unique string consisting of zero symbols (so that $|s_0| = 0$). Letting S^* denote the set of all strings, we introduce a binary *concatenation* operator: if $s_1, s_2 \in S^*$, then the concatenation $\overline{s_1 s_2}$ is obtained by placing the string ' s_2 ' after the string ' s_1 '. For example, if $s_1 = a_1 a_2 a_3$ and $s_2 = b_1 b_2$ then

$$\overline{s_1 s_2} = a_1 a_2 a_3 b_1 b_2 \neq \overline{s_2 s_1} = b_1 b_2 a_1 a_2 a_3. \quad (2.32)$$

It is clear that $\overline{s\phi} = \overline{\phi s} = s$. If ' s ' is a string and $n \in \mathcal{N}$, $n > 0$ then we write $s^{[n]} = \underbrace{ss \cdots s}_n$. By convention, $s^{[0]} = \phi$.

Define the set $S(A)$ to be the set of all subsets on A . Then a *language on A* (or a *language with alphabet A*) is any subset of $S(A)$. The set of all strings over a fixed finite alphabet A , for example, is a language; it is denoted by $\mathcal{L}(A)$. If $A = \{0, 1\}$, then $\mathcal{L}(A) = \{\phi, 0, 1, 00, 01, 10, 000, \dots\}$.

Formal Languages

Formal languages are subsets of $S(A)$ formed according to definite grammatical rules. It is easy to see that sets of CA configurations can be considered to be formal languages; in chapter 6, we will in fact exploit the correspondence between the *words* and *configurations* by using the *finite* set of grammatical rules to analyze the *infinite* set of CA configurations.

A computer can be used to implement the grammatical rules to generate (or recognize) the strings in the formal language; different *types* of languages being distinguished by the required size of memory in the computer. The simplest example of an idealized computer is the abstract automaton:

DEFINITION: A finite automaton $\mathcal{M}$ is specified by three sets A , Σ and Σ^* and a state-transition function $\phi : \Sigma \times A \rightarrow \Sigma$, where

$$\begin{cases} A & = \{a_1, \dots, a_n\} \text{ is a finite input alphabet,} \\ \Sigma & = \{\sigma_1, \dots, \sigma_m\} \text{ is a finite set of states,} \\ \Sigma^* \subset \Sigma & \text{is the set of output (or accepting) states.} \end{cases}$$

Given an automaton $\mathcal{M}$ that starts in state σ_1 , and any finite string $s \in A^*$, $\phi^*(\sigma, s)$ will represent the final output state that $\mathcal{M}$ will enter after having processed s , one symbol at a time, from left to right. $\mathcal{M}$ is said to *accept* the word s if $\phi^*(\sigma_1, s) \in \Sigma^*$; the word s is *rejected* if and only if it is not accepted. Finally, we may define the *language* $\mathcal{L}(\mathcal{M})$ accepted by $\mathcal{M}$ as the set of all words $s \in A^*$ that are accepted by $\mathcal{M}$. A language $\mathcal{L}$ is called *regular* if there is a finite automaton $\mathcal{M}$ that accepts it.

The *grammars* for regular languages can be conveniently specified by *finite state transition graphs* for the finite automata that recognize them. The vertices of the graph represent the the system states $\sigma_i \in \Sigma$ and the arcs represent the possible input states $a_i \in A$. The arrows point to the next state that will result from the initial state when the input on the arc is applied.

EXAMPLE: Consider an automaton $\mathcal{M}$ with alphabet $A = \{0, 1\}$, state space $\Sigma = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4\}$ and transition rule ϕ given by

$$\left\{ \begin{array}{llll} \phi(\sigma_1, 0) = \sigma_2, & \phi(\sigma_1, 1) = \sigma_4, & \phi(\sigma_2, 0) = \sigma_2, & \phi(\sigma_2, 1) = \sigma_3, \\ \phi(\sigma_3, 0) = \sigma_4, & \phi(\sigma_3, 1) = \sigma_3, & \phi(\sigma_4, 0) = \sigma_4, & \phi(\sigma_4, 1) = \sigma_4. \end{array} \right\}$$

Assume that the initial state is σ_1 and that the accepting set is $\Sigma^* = \{\sigma_3\}$. It is easy to see that $\mathcal{M}$ will reject the strings $s_1 = 00110$ and $s_2 = 10011$ (since $\phi^*(\sigma_1, s_1) = \phi^*(\sigma_1, s_2) = \sigma_4$), and accept $s_3 = 00111$ (since $\phi^*(\sigma_1, s_3) = \sigma_3 \in \Sigma^*$). In fact, $\mathcal{M}$ accepts the regular language

$$\mathcal{L} = \{0^{[n]}1^{[m]}, n, m \geq 0\}.$$

The state transition graph for this example is given in figure 2.5.

Finite automata such as these are the simplest kind of computational model, and are not very powerful. For example, no finite automaton can accept the set of all *palindromes* over some specified alphabet. They certainly do not wield, in abstract terms, the full computational power of a conventional computer. For that we need a suitable generalization of the these primitive computational models. Despite the literally hundreds of computing models that have been proposed at one time or another since the beginning of computer science, it has been found that each has been essentially equivalent to just one of four fundamental models: *finite automata*, *pushdown automata*, *linear bounded automata* and *Turing machines*.

Each one of these four models can be thought of as defining the response of a black-box to a tape of symbols that is fed to it, cyclically, one cell at a time. During each cycle, the black-box reads the symbol at the appropriate cell, responds to that symbol according to a set of model-specific rules, and then moves the tape forward by one cell. What type of computational model the black-box represents depends on its general response. Although a more detailed discussion of each of these types will be given in chapter 6, we mention here that the four models make up what is conventionally called the *Chomsky hierarchy*[†]. Each type of computational

[†]Named after the linguist and philosopher of language, Noam Chomsky.

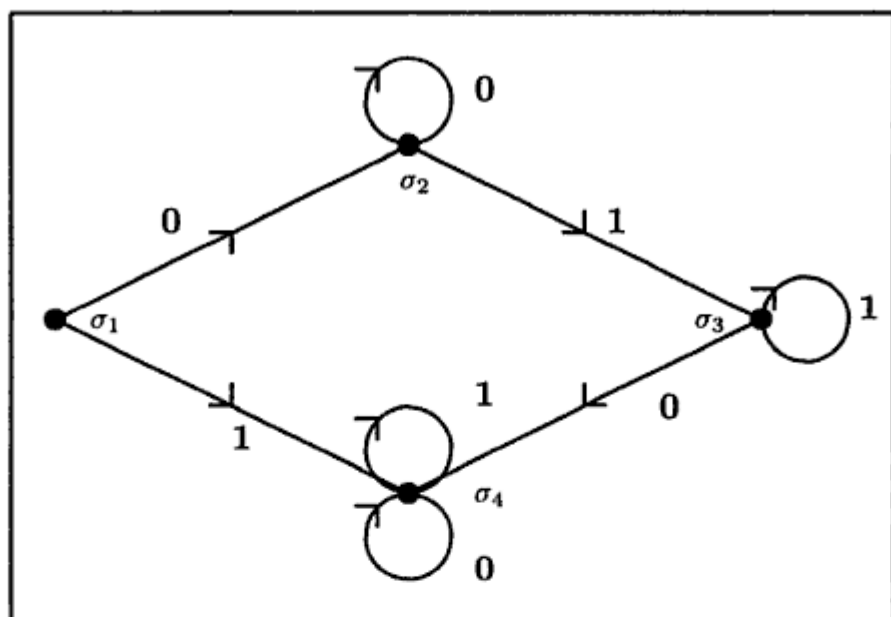


Fig. 2.5 State Transition graph for the regular language $\mathcal{L} = \{0^{[n]} 1^{[m]}\}$.

Level	Language Class	Class of Accepting Automata	Memory
0	Unrestricted	Universal computer	arbitrarily large
1	Context-Sensitive	linear-bounded	$\sim s_{\text{input}} $
2	Context-Free	pushdown	fixed length
3	regular	finite	none

Table 2.1 Chomsky Language Hierarchy.

model determines a particular language class, and, since each is more general than its predecessor, each language class must include the one that comes before it. Each level of the hierarchy is characterized by the amount of memory needed in an automaton that accepts it (see table 2.1).

2.2 Dynamical Rules: Notation and Definitions

Although there is an incredibly rich variety of specific CA systems, each of which is carefully defined or selected to fit the requirements of a particular model, the definition of any of these specific systems requires the specification of each of the following four generic characteristics:

Discrete Cellular State Space $\mathcal{L}$: the discrete lattice of cells or sites upon which CA ‘live’, and their dynamics unfolds. $\mathcal{L}$ can be one-dimensional, two-dimensional

(either rectangular or hexagonal), three-dimensional, or even random.

Local Value Space Σ : each cell of $\mathcal{L}$, indexed by the elements of the $\mathcal{L}$'s symmetry group, can assume only one of a finite number of different values:

$$\sigma_{\vec{i} \in \mathcal{L}}(t) \in \Sigma \equiv \{0, 1, 2, \dots, k-1\}, \quad (2.33)$$

where $\sigma_{\vec{i}}$ is the value of the $\vec{i}^{\text{th}}$ cell at time ' t ', and Σ is any finite commutative ring (usually taken to be the integers *modulo* ' k ', $\mathbb{Z}_k$). If the CA evolves on a finite lattice of N cells, then the total number of *global* states is also finite, and is given by k^N .

Boundary Conditions: although CA are assumed to live on infinitely large lattices, computer simulations must necessarily be run on finite sets. For a one dimensional lattice with N cells, it is common to use *periodic boundary conditions*, in which σ_{N+1} is identified with σ_1 . Alternatively, all cells to the left and right of a finite block of N cells may be arbitrarily defined to possess value '0' for all time, so that their dynamics remains uncoupled with that taking place within the block. Similarly, in two dimensions, it is usual to have the dynamics take place on a *torus*, in which $\sigma_{i,M+1} = \sigma_{i,1}$ and $\sigma_{N+1,j} = \sigma_{1,j}$. As we will see later it turns out that boundary conditions often play an important role in shaping the form of the resulting dynamics.

Dynamical Rule ϕ : $\overbrace{\Sigma \times \Sigma \times \dots \times \Sigma}^n \longrightarrow \Sigma$, where ' n ' specifies the number of cells needed to define the *neighborhood* of a given cell. Defining $\mathcal{N}\{\vec{i}\}$ to be the neighborhood about cell $\vec{i}$, the transition rule is most generally written as

$$\sigma_{\vec{i}}(t+1) = \phi(\sigma_{\vec{j}} \in \mathcal{N}\{\vec{i}\}). \quad (2.34)$$

State transitions are therefore *local* in both space and time: individual cells evolve iteratively according to a fixed, and usually deterministic, function of the current state of that cell and its neighboring cells. One *iteration step* of the dynamical evolution is achieved after the simultaneous application of the rule ϕ to each cell in the lattice $\mathcal{L}$.

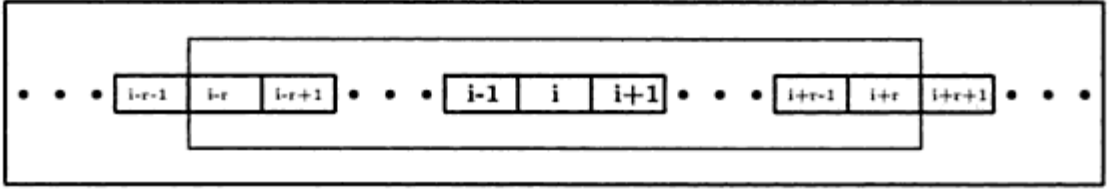
2.2.1 One-dimensional CA

An arbitrary *range- r* one-dimensional rule can be written as follows:

$$\sigma_i(t+1) = \phi(\sigma_{i-r}(t), \dots, \sigma_i(t), \dots, \sigma_{i+r}(t)), \quad \phi : S^{2r+1} \longrightarrow S, \quad (2.35)$$

where the range ' r ' specifies the size of the neighborhood for each site.

Since each site can take one any of ' k ' values, ϕ is completely defined by specifying the value assigned to each of the k^{2r+1} possible $(2r+1)$ -tuple configurations for a given neighborhood:

Fig. 2.6 One-dimensional *range-r* neighborhood of center site 'i'.

$\sigma_{i-r}(t)$	$\dots$	$\sigma_i(t)$	$\dots$	$\sigma_{i+r}(t)$	$\longrightarrow$	$\sigma_i(t+1)$
0		0		0		$\phi(0,0,\dots,0)$
0		0		1		$\phi(0,0,\dots,1)$
0		0		2		$\phi(0,0,\dots,2)$
$\vdots$		$\vdots$		$\vdots$		$\vdots$
k		k		k		$\phi(k,k,\dots,k)$

For example, let $k = 2$ (so that $\sigma_i \in \{0, 1\}$) and range $r = 1$, and consider the rule $\phi : \{0, 1\}^3 \rightarrow \{0, 1\}$ defined by

$$\phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)) = \sigma_{i-1}(t) \oplus_2 \sigma_{i+1}(t), \quad (2.36)$$

where ' $\oplus_2$ ' is addition *modulo* 2. The explicit form of the dynamics is given by listing, for each of the eight possible local states that three adjacent cells can be in at time ' t ', the corresponding state at time ' $t+1$ ' that is assigned by ϕ to the central cell of this 3-tuple:

111	110	101	100	011	010	001	000
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
0	1	0	1	1	0	1	0

After choosing some specific initial global state

$$\vec{\sigma}(t=0) = (\sigma_1(0), \sigma_2(0), \dots, \sigma_N(0)), \quad (2.37)$$

the temporal evolution of this CA is then given by the simultaneous application of ϕ to each of the N lattice cells. After four iterations are applied to a size $N = 17$ lattice with periodic boundary conditions, and initial state $\vec{\sigma}(t=0) = '010111010110101'$, for example, we find that $\vec{\sigma}(t=0)$ evolves into $\vec{\sigma}(t=4) = '1000001101111000'$:

time (t)	$\vec{\sigma}(t)$															
0	0	1	0	1	1	1	0	1	0	1	1	0	1	0	1	0
1	0	0	0	1	0	1	0	0	0	1	1	0	0	0	0	0
2	0	0	1	0	0	0	1	0	1	1	1	1	0	0	0	0
3	0	1	0	1	0	1	0	0	1	0	0	1	1	0	0	0
4	1	0	0	0	0	0	1	1	0	1	1	1	1	1	0	0

Rule Composition

Rules may be combined by *composition*: i.e., two rules, ϕ_1 and ϕ_2 , may be combined to form the rule $\tilde{\phi} \equiv \phi_1\phi_2$. The set of rules obtained in this way is closed under composition, although the number of sites in the neighborhood will typically have to be increased. If a rule is composed with itself, then $\tilde{\phi} = (\phi\phi)$ generates patterns consisting of alternate time steps of the patterns of ϕ . In general, composition is noncommutative: $\phi_1\phi_2 \neq \phi_2\phi_1$.

Higher Order Time Dependence

Equation 2.35 defines an arbitrary range- r rule that is 1st-order in time. n^{th} -Order rules, for which a particular site value at time ' t ' depends on the r -neighborhood site values for the previous ' n ' iteration steps, may, of course, also be constructed:

$$\sigma_i(t) = \phi^{(n)} \left(\begin{array}{ccccccc} \sigma_{i-r}(t-n+1), & \dots, & \sigma_i(t-n+1), & \dots, & \sigma_{i+r}(t-n+1), \\ \vdots, & & \vdots & & \vdots \\ \sigma_{i-r}(t), & \dots, & \sigma_i(t), & \dots, & \sigma_{i+r}(t) \end{array} \right) \quad (2.38)$$

By defining 'effective' site values $\tilde{\sigma} \equiv \sum_{j=0}^{n-1} k^j \sigma(t-j)$, and allowing for a larger neighborhood radius, an equivalent 1st-order rule, $\tilde{\phi}^{(1)}$, may always be constructed from a given n^{th} -order rule.

Figure 2.7, for example, shows how a 2nd-order radius $r = 1$ rule ϕ may be converted into a 1st-order radius $r = 2$ rule $\tilde{\phi}$. Effective values $\tilde{\sigma} \in \{0, 1, \dots, k^2\}$ define the states of the single remaining cell of a two-state collapse in time, and extra sites are added on to either side of the original neighborhood.

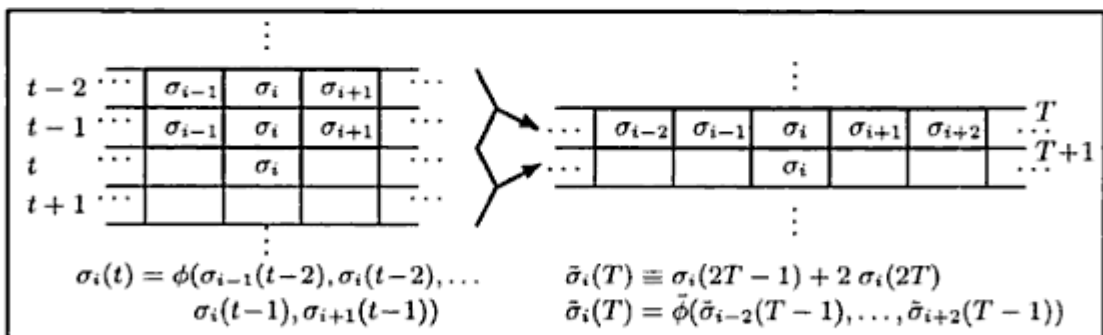


Fig. 2.7 Construction of equivalent radius $r = 2$ rule, $\tilde{\phi}$, that is 1st-order in time from a radius $r = 1$, 2nd-order rule, ϕ .

In general if a radius- r rule ϕ is n^{th} order in time, an equivalent 1st order rule will be defined on a neighborhood with radius $r' = nr$; if $\sigma \in \{0, 1, \dots, k\}$, then $\tilde{\sigma} \in \{0, 1, \dots, k^n\}$.

Rule Codes

Rather than being defined by lengthy explicit listings of their local action, rules are instead conventionally identified by a compact *code*. If the bottom eight binary digits of the $r = 1 \bmod 2$ rule in the example cited above are interpreted as the binary representation of a decimal number, then the code, $R[\oplus_2]$, is given by that base-10 equivalent:

$$\begin{aligned} R[\oplus_2] &= 0 \cdot 2^0 + 1 \cdot 2^1 + 0 \cdot 2^2 + 1 \cdot 2^3 + 1 \cdot 2^4 + 0 \cdot 2^5 + 1 \cdot 2^6 + 0 \cdot 2^7 \\ &= 90 \end{aligned} \quad (2.39)$$

This rule can then be alternatively referred to in the text as **R90**.

More generally, for an arbitrary rule ϕ of the form given in equation (2.3), we define the code

$$R[\phi] \equiv \sum_{\{\sigma_{i-r}, \dots, \sigma_{i+r}\}} \phi[\sigma_{i-r}, \dots, \sigma_{i+r}] k^{\sum_{j=-r}^r k^{r-j} \sigma_{i+j}}. \quad (2.40)$$

Since each explicit listing of the local action on each of the k^{2r+1} possible range- r neighborhoods defines a unique rule, and since there are $k^{k^{2r+1}}$ such distinct explicit listings, we find that there are, in general, $k^{k^{2r+1}}$ possible range- r rules (see table 2.1).

'Legal' and Other 'Simplifying' Forms of Rules

Because of the rather large total number of possible rules, it is frequently convenient to deal with more restricted classes. As we will later see, however, it is rather fortuitous that most, if not *all*, of the characteristic behavior of generic CA rules is nonetheless retained.

Legal Rules: Legal rules are those for which the following two properties hold:

$$\begin{cases} \text{Null state quiescence: } \phi(0, 0, \dots, 0) = 0 \\ \text{Reflection Symmetry: } \phi(\sigma_{i-r}, \dots, \sigma_{i+r}) = \phi(\sigma_{i+r}, \dots, \sigma_{i-r}). \end{cases} \quad (2.41)$$

Imposition of these 'legality' conditions for $r = 1$ reduces the set of 256 general rules to a set of 32 legal rules of the form

$$\begin{aligned} 111 \rightarrow a, \quad 110 \rightarrow b, \quad 101 \rightarrow c, \quad 100 \rightarrow d, \\ 011 \rightarrow b, \quad 010 \rightarrow e, \quad 001 \rightarrow d, \quad 000 \rightarrow 0, \end{aligned} \quad (2.42)$$

where $a, b, c, d, e \in \{0, 1\}$.

Totalistic Rules: Totalistic (**T**) rules, ϕ_{tot} , are functions of the *sums* of values of all sites in a particular neighborhood: $\phi_{\text{tot}} = \phi_{\text{tot}}(\sum_{j=-r}^r \sigma_{i+j})$. Here we define the totalistic code

$$\mathbf{T}[\phi_{\text{tot}}] \equiv \sum_{i=0}^{(2r+1)(k-1)} k^i \phi_{\text{tot}}(i). \quad (2.43)$$

k	r	TOTAL	LEGAL	TOTALISTIC	OUTER TOTALISTIC	ADDITIVE
2	1	256	32	8	8	8
2	2	$4 \cdot 10^9$	524288	32	32	32
2	3	$3 \cdot 10^{38}$	$2 \cdot 10^{21}$	128	128	128
3	1	$8 \cdot 10^{12}$	129140163	64	48	27
3	2	10^{116}	10^{64}	1024	768	243
.	.	.	.	.	.	.
k	r	$k^{k(2r+1)}$	$k^{k^{r+1}(k^r+1)/2-1}$	$2^{(k-1)(2r+1)}$	$k2^{2r(k-1)}$	k^{2r+1}

Table 2.2 Number of possible rules of a specific type for a given 'k' and range 'r'.

If $r=1$, $k=2$ and $\sigma_i(t+1) = 1 \iff \sigma_{i-1}(t) + \sigma_i(t) + \sigma_{i+1}(t) \in \{1, 3\}$, for example, then $T = 2^1 + 2^3 = 10$ and we would cite the rule ϕ_{tot} as **T10**.

Outer-Totalistic Rules: Outer-totalistic (OT) rules, $\phi_{\text{out-tot}}$, are functions of both the value of a given site and the sum of values of all *remaining* sites in the neighborhood of that site. Thus, $\phi_{\text{out-tot}} = \phi_{\text{out-tot}}(\sigma_i, \sum_{j=-r}^r \sigma_{i+j} - \sigma_i)$, with general code given by

$$\text{OT}[\phi_{\text{out-tot}}] \equiv \sum_{i=0}^{2r(k-1)} \sum_{j=0}^{k-1} k^{ki+j} \phi_{\text{out-tot}}(j, i). \quad (2.44)$$

Additive Rules: Rules belonging to the special class of *additive* rules, ' ϕ_{add} ', are linear functions of neighborhood sites:

$$\phi_{\text{add}} = \sum_{j=-r}^r \alpha_j \sigma_{i+j} \pmod{k}, \quad \alpha_j \in S. \quad (2.45)$$

The eight additive $r=1$, $k=2$ rules, for example, are of the general form

$$\begin{aligned} 111 \rightarrow a, \quad 110 \rightarrow b, \quad 101 \rightarrow 0, \quad 100 \rightarrow c, \\ 011 \rightarrow b, \quad 010 \rightarrow a, \quad 001 \rightarrow c, \quad 000 \rightarrow 0, \end{aligned} \quad (2.46)$$

where $a, b, c \in \{0, 1\}$ and $c = (a + b) \text{ modulo } 2$.

By exploiting the fact that such rules obey an additive superposition principle – namely, that if Φ_{add} is the *global* transition function, then $\Phi(\vec{\sigma}_A + \vec{\sigma}_B) = \Phi(\vec{\sigma}_A) + \Phi(\vec{\sigma}_B)$ – virtually all of the fundamental dynamical behavior of CA obeying this type of a rule can be obtained. We will discuss various methodologies for performing exact algebraic analyses of such systems, including the interesting question of the dynamical relationship between such rules and the underlying lattice topology, in chapter 5.

Feedback Shift Registers: Feedback shift registers are essentially one-dimensional finite state machines consisting of a linear array of sites $i = 1, 2, \dots, n$, with each site i carrying value σ_i . At each time step, the system evolves according to the following

two rules (see figure 2.8): (1) all of the sites are shifted one site to the right, $\sigma'_i = \sigma_{i-1}$, and (2) $\sigma'_0 = f(\sigma_{n-m+1}, \sigma_{n-m}, \dots, \sigma_n)$, where sites $i = n-m+1, n-m, \dots, n$ label the positions of the “taps” on the shift-register. A feedback shift register is called *linear* if f is a linear function:

$$f(\sigma_{n-m+1}, \sigma_{n-m}, \dots, \sigma_n) = \alpha_0 \sigma_{n-m+1} \oplus_2 \alpha_1 \sigma_{n-m} \oplus_2 \dots \oplus_2 \alpha_m \sigma_n, \quad (2.47)$$

where $\alpha_i \in \{0, 1\}$ and *oplus*₂ is addition *modulo-two*.

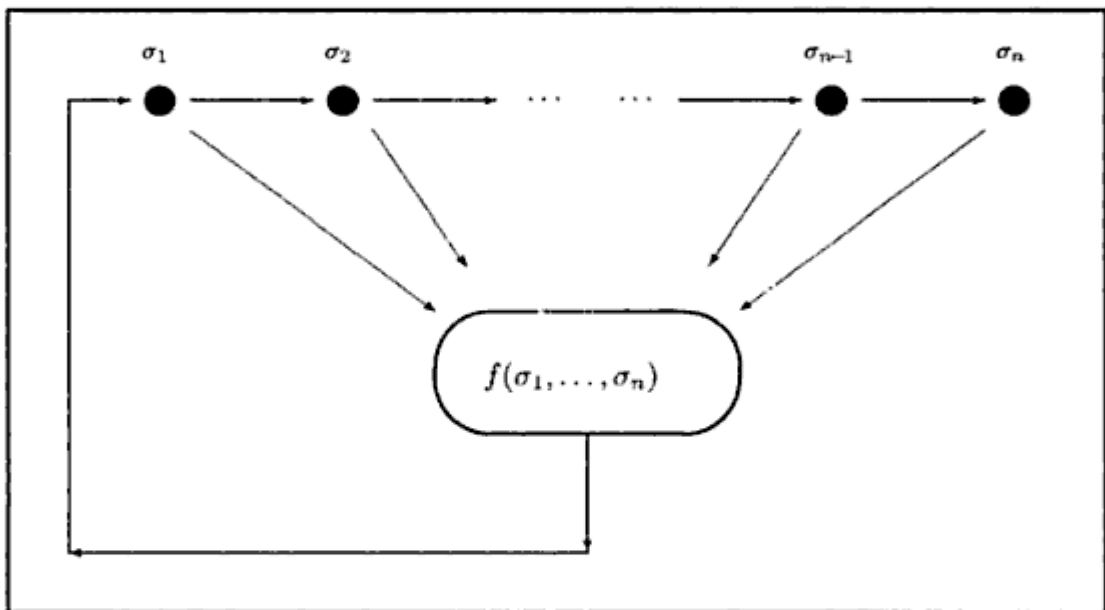


Fig. 2.8 Schematic diagram of a length- n feedback shift register.

It is easy to see that an elementary size- n one-dimensional CA rule ϕ is equivalent to a size- n feedback shift register with $\sigma \in \{0, 1\}$, taps at positions $n-2$, $n-1$ and n , and $f = \phi$. The only difference is that it takes n “shift-register” time-steps to reproduce a single “CA” time step.

Topological Characterization of Cellular Automata

Labeling each cell of the one-dimensional ‘lattice’ by $i \in \mathcal{Z}$, where $\mathcal{Z}$ is the set of integers, the collection of all *configurations* $\vec{\sigma}$ defines the CA *phase space*, and is denoted by $\Gamma \equiv \Sigma^{\mathcal{Z}}$.

If we give Σ the discrete topology and Γ the product topology, then Γ becomes a compact metric space homeomorphic to the Cantor set under the metric

$$\partial(\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}) = \sum_{i=-\infty}^{\infty} k^{-|i|} |\vec{\sigma}_i^{(1)} - \vec{\sigma}_i^{(2)}|, \quad \vec{\sigma}^{(1)}, \vec{\sigma}^{(2)} \in \Gamma. \quad (2.48)$$

Two configurations are *close*, under ‘ ∂ ’, if their components $\vec{\sigma}_i^{(1)}$ and $\vec{\sigma}_i^{(2)}$ are the same for $|i| < N$ for large N .

Open sets ‘ $\mathcal{O}$ ’ are defined as unions of n -cylinders: $\mathcal{O} \equiv \bigcup_i c_i^{(n)}$, where $c_i^{(n)} \equiv \{\vec{\sigma} \mid \vec{\sigma}_i = c_i, \dots, \vec{\sigma}_{i+n-1} = c_{i+n-1}\}$. Each n -cylinder may be put into a one-to-one correspondence with an n -block $B_n^{(i)} \equiv \{b_1 = c_i, b_2 = c_{i+1}, \dots, b_n = c_{i+n-1}\}$, each of which is simply an explicit list of a specified sequence of states.

We define two maps:

1. the *shift* operator $\gamma : \Gamma \rightarrow \Gamma$, such that for any $\vec{\sigma} \in \Gamma$, $(\gamma\vec{\sigma})_i = \vec{\sigma}_{i+1}$. ‘ γ ’ is clearly a homeomorphism of Γ , and
2. the *dynamical* map $\Phi : \Gamma \rightarrow \Gamma$, defined by

$$[\Phi(\vec{\sigma})]_i = \phi(\sigma_{i-r}, \sigma_{i-r+1}, \dots, \sigma_{i+r-1}, \sigma_{i+r}), \quad (2.49)$$

where $\phi : \Sigma^{2r+1} \rightarrow \Sigma$ is a *range- r* local function.[†]

We see that (i) if $\vec{\sigma}^{(1)}$ is close to $\vec{\sigma}^{(2)}$, then $\Phi[\vec{\sigma}^{(1)}]$ will be close to $\Phi[\vec{\sigma}^{(2)}]$, so that ‘ Φ ’ is *continuous*, and (ii) the commutator $[\Phi, \gamma] = 0$. That the converse is also true—i.e. that if $\phi : \Gamma \rightarrow \Gamma$ is a continuous map which commutes with ‘ γ ’, then it must be of the above form—was shown by Hedlund in 1969 [hedl69]. Specifically, he showed that the set of shift-commuting functions on $\Sigma^{\mathbb{Z}}$ which are continuous with respect to the metric ‘ ∂ ’, is identical to the set of cellular automata. Cellular automata can, therefore, be viewed as discrete dynamical systems whose temporal evolution is given by some continuous mapping of a Cantor set to itself; the dynamics of such maps can then be compared to the continuous dynamics of iterated maps $f : \mathcal{R}^n \rightarrow \mathcal{R}^n$.

Observing that $\Phi\Gamma \subseteq \Gamma$, the fundamental problem is to describe the limit set $\Lambda_\Gamma \equiv \lim_{n \rightarrow \infty} (\Phi^n \Gamma)$. Such mappings have been studied previously as *shift-dynamical systems*, but largely without reference to any underlying physical motivation. It was only following the pioneering study of Wolfram in 1983 [wolf83a], that such dynamical systems were first brought to the full attention of the physics community.

Finite Lattice Dynamics

Although CA are most often assumed to *live* on infinitely large lattices, we can equally well consider lattices that are finite in extent (which is done in practice regardless, since all CA simulations are ultimately restricted by a finite computer memory). If a lattice $\mathcal{L}$ has N sites, there are clearly a finite number, k^N , of possible global configurations. The global dynamical evolution can then be represented by a finite *state transition graph* $G_{\mathcal{L}}$, much like the one considered in the description of an abstract automaton in section 2.1.4.

[†] ϕ is more formally defined by first choosing an arbitrary operator mapping $B_{2r+1} \rightarrow B_1$, and then extending it, via the shift-operator γ , to a map $B_{2r+i} \rightarrow B_i$, for any ‘ i ’. ϕ is then made to act on configurations ‘ $\vec{\sigma}$ ’ by infinite extension by ‘ γ ’.

The nodes of $G_{\mathcal{L}}$ represent specific global states, $\vec{\sigma}_i$, in $\mathcal{L}$, and there is a directed link from $\vec{\sigma}_i$ to $\vec{\sigma}_j$ if and only if $\Phi[\vec{\sigma}_i] = \vec{\sigma}_j$. Since there are a finite number of possible states, all finite systems must enter *cycles* – wherein a fixed subset of configurations is repeatedly visited – in a time $t \leq k^N$. We represent these subsets – or *attracting* states of the finite system – by a formal *cycle sum decomposition*

$$C[\mathcal{L}] \equiv \sum_i^{N_{\max}} [n_i, \ell_i] = [n_1, \ell_1] + [n_2, \ell_2] + \cdots + [n_m, \ell_m] + \cdots + [n_{N_{\max}}, \ell_{N_{\max}}], \quad (2.50)$$

where n_i = number of cycles of length ℓ_i . Vertices corresponding to cyclic states may be roots of *trees*, which represent all *transient* configurations of the system. Whenever directed trees are present, we have a manifest irreversibility: although there is exactly one outwardly oriented link at each tree-vertex, a given vertex can have an arbitrary number of predecessor vertices. Peripheral vertices, or those having no incoming links, represent so-called *garden-of-eden* configurations which can occur only as initial states, and thus can never be generated in the course of the evolution.

Figure 2.9 shows a typical $G_{\mathcal{L}}$ topology, computed for a one-dimensional lattice consisting of four vertices and evolving according to totalistic rule **T2**.

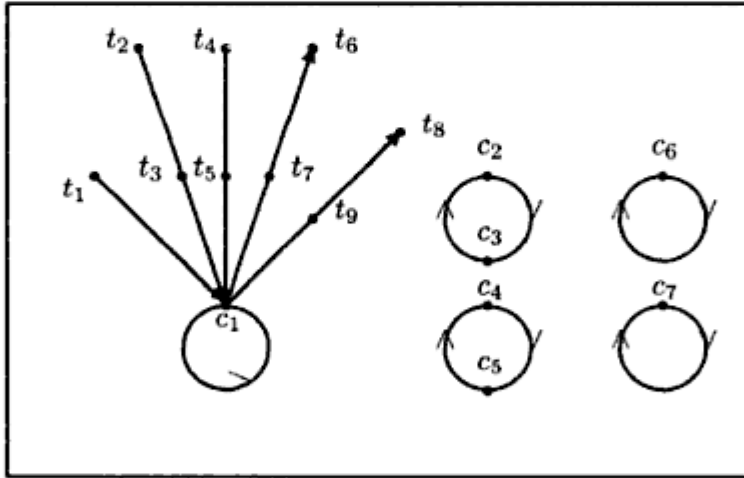


Fig. 2.9 The state transition graph $G_{\mathcal{L}}$, computed for a 1-dim lattice consisting of $N = 4$ points (with periodic boundary conditions), and totalistic rule **T2**. The vertices labeled ' t_i ' represent transient configurations; those labeled ' c_i ' represent cyclic states, and give rise to the formal cycle cum decomposition $C[\mathcal{L}] = [3, 1] + [2, 2]$.

The explicit form of the $G_{\mathcal{L}}$ topology is analytically accessible for only a very few specific systems, most notably those defined by *additive* rules and relatively simple lattices. The method of calculation of these topologies will be presented in some detail in chapter 5.

2.2.2 Two-dimensional CA

There are a variety of different lattices and neighborhood structures that can be used by two-dimensional CA (see figure 2.10). The *von-Neumann* neighborhood, consisting only of the four cells which are horizontally and vertically adjacent to the center cell of interest, and the *Moore* neighborhood, consisting of all eight cells which are immediately adjacent to the center site, are both defined on a regular Euclidean lattice and have been studied most extensively. Their explicit forms are given as follows:

$$\left\{ \begin{array}{ll} \text{von-Neumann:} & \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i,j}^{(t)}, \sigma_{i-1,j}^{(t)}, \sigma_{i+1,j}^{(t)}, \sigma_{i,j-1}^{(t)}, \sigma_{i,j+1}^{(t)}) \\ \text{Moore:} & \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i-1,j-1}^{(t)}, \sigma_{i,j-1}^{(t)}, \sigma_{i+1,j-1}^{(t)}, \sigma_{i-1,j}^{(t)}, \sigma_{i,j}^{(t)}, \\ & \sigma_{i+1,j}^{(t)}, \sigma_{i-1,j+1}^{(t)}, \sigma_{i,j+1}^{(t)}, \sigma_{i+1,j+1}^{(t)}) \end{array} \right. \quad (2.51)$$

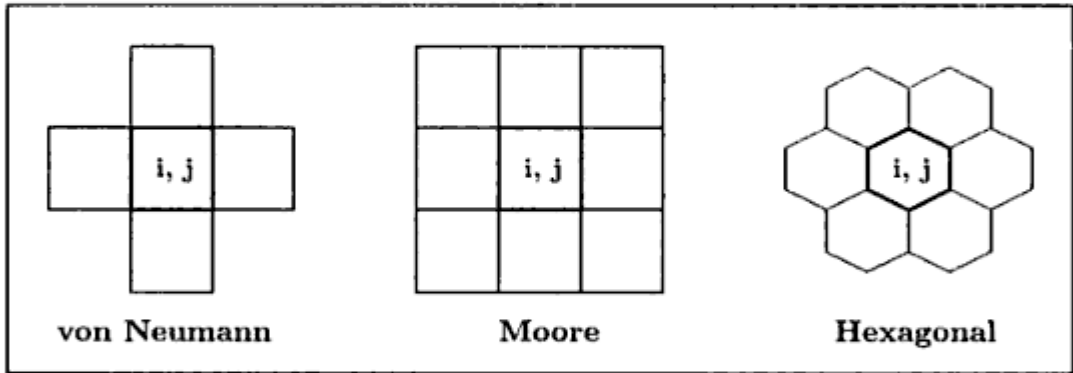


Fig. 2.10 Examples of possible two-dimensional neighborhoods of site 'i, j'.

Triangular and hexagonal lattices (which, along with the *von-Neumann* neighborhood, may be considered as special cases of the nine-neighbor *Moore* neighborhood), can also be used. *Totalistic*, *outer-totalistic*, and *additive* rules are defined exactly as in the one-dimensional case, while *legal* rules may now be generalized to include rotation, reflection, and completely symmetric rules. The various numbers of such two-dimensional rules, for $k = 2$, are given in table 2.2.

The extension of generic CA systems to two dimensions is significant for two reasons: first, the extension brings with it the appearance of many new phenomena involving behaviors of the boundaries of, and interfaces between, two-dimensional patterns that have no simple analogs in one-dimension. Secondly, two-dimensional dynamics permits easier (sometimes direct) comparison to real physical systems. As we shall see in later sections, models for dendritic crystal growth, chemical reaction-diffusion systems and a direct simulation of turbulent fluid flow patterns are in fact specific instances of 2D CA rules and lattices.

Rule Type	<i>von-Neumann</i>	<i>Moore</i>	<i>Hexagonal</i>
General	$4 \cdot 10^9$	10^{154}	$3 \cdot 10^{38}$
Reflection symmetric	$2 \cdot 10^7$	$5 \cdot 10^{86}$	10^{22}
Rotation symmetric	4096	10^{42}	$2 \cdot 10^{19}$
Completely symmetric	4096	$5 \cdot 10^{30}$	$3 \cdot 10^8$
Outer-Totalistic	1024	$3 \cdot 10^5$	16384
Totalistic	32	512	128

Table 2.3 Numbers of possible rules of various types for $k = 2$ two-dimensional CA with specified neighborhood structures.

Generalizations

The explicit forms of rules introduced thus far in this chapter have been essentially generic, in that they arguably represent the simplest possible form of a discrete dynamics. Although, as we will see very shortly, such generic systems already possess an impressive variety of complex behaviors, extensions and generalizations of these primitive systems must be made if one hopes to capture the essence of the actual patterns and structures underlying specific physical (or even social and behavioral) systems. We provide a general list here of what are some of the more important generalizations of the basic CA systems that have appeared in the literature, and indicate the corresponding chapters of this book in which more detailed accounts can be found.

Reversible Rules: almost any random rule that one writes down will give rise to *non-invertible* dynamics, in the sense that it will be impossible to determine what local configuration of site values at the *previous time step* gave rise to a particular value at the current step. Since real physical dynamical laws are *microscopically reversible* any honest attempts at simulating real physical systems can be made only if the underlying CA is itself reversible. Following a suggestion first made by Fredkin [fredkin82], it turns out to be fairly straightforward to write down a general form for such rules:

$$\sigma_{\vec{r}}^{(t+1)} = \phi(\sigma_{\vec{r}}^{(t)} \in \mathcal{N}\{\vec{i}\}) \ominus_k \sigma_{\vec{r}}^{(t-1)}, \quad (2.52)$$

where ‘ $\ominus_k$ ’ is the *modulo- k* difference, and ϕ is completely arbitrary. It should be clear that for such rules, any preceding or succeeding value of $\sigma_{\vec{r}}$ can be determined if the values at site $\vec{r}$ are known for two consecutive time steps; *i.e.*, the total information contained in the initial state is preserved for all time. Moreover, it turns out that reversible rules can be universal, which in turn leads to the intriguing new concept of *reversible computation*. These, and other issues, of reversible rules are discussed in chapters 4.3 and 6.3. *Ballistic Computation* – a CA implementation of Fredkin’s billiard-ball model of computation (BBMC) – is introduced in chapter 3.2.4.

Probabilistic CA (PCA): deterministic state-transitions may be replaced with

specifications of the *probabilities* of cell-value assignments. That is to say, rules ϕ are replaced by probabilities

$$\text{prob} \left\{ \sigma_i^{(t+1)} = \alpha, \text{ given the values } (\sigma_{i-1}^{(t)}, \sigma_i^{(t)}, \sigma_{i+1}^{(t)}) \text{ in } \mathcal{N} \right\}, \quad (2.53)$$

where $\alpha \in \Sigma$. Instead of studying particular evolutions of arbitrary initial states, such rules require that *ensembles* of CA trajectories be considered. An important application of PCA is to the well-studied *Ising model*; Domany and Kinzel [domany84], for example, have constructed an explicit mapping of a d -dim PCA onto an Ising model in $(d+1)$ -dimensions. Chapter 7.2.2 discusses the general relationship existing between PCA and statistical mechanical models.

Non-Homogeneous CA: a characteristic feature of all CA rules defined so far has been that of *homogeneity* – each cell of the system evolves according to the *same* rule ϕ . Hartman and Vichniac [hart86] were the first to systematically study a class of inhomogeneous CA (INCA), in which the state-transition rules are allowed to vary from cell to cell. The simplest such example is one where there are only two different ϕ 's, which are randomly distributed throughout the lattice. Kauffman has studied the other extreme in which the lattice is randomly populated with all 2^{2^k} possible boolean functions of k inputs. The results of such studies, as well as the relationship with the dynamics of *random mappings*, are covered in detail in chapter 8.3.

Coupled-Map Lattices: these are models in which continuity is restored to the state space:

$$x_i^{(t+1)} = \varepsilon f(x_i^{(t)}) + (1 - \varepsilon) (x_{i-1}^{(t)} + x_{i+1}^{(t)}); \quad x \in \mathcal{R}_{[0,1]}, \quad (2.54)$$

where $f(x) : \mathcal{R}_{[0,1]} \rightarrow \mathcal{R}_{[0,1]}$ is an arbitrary continuous function and ε is a coupling term. First introduced by Kaneko [kaneko83], they are simpler than partial differential equations, but more complex than generic CA. Their behavior is analyzed in chapter 8.

Structurally Dynamic CA: the only generalizations mentioned so far were generalizations of either the rules or state space. Another intriguing possibility is to allow for the lattice $\mathcal{L}$ itself to become a full participant in the dynamical evolution of the system, much as the classically 'static' physical space-time arena becomes a bona-fide dynamic element in general relativity. The idea is to study the behavior of systems evolving according to both value and local structure rules:

$$\begin{cases} \sigma^{(t+1)} &= \phi \left[\sigma^{(t)} \in \mathcal{N}, a_{i,j}^{(t)} \in A^{(t)}(\mathcal{L}) \right] \\ a_{i,j}^{(t+1)} &= \psi \left[\sigma^{(t)} \in \mathcal{N}, a_{i,j}^{(t)} \in A^{(t)}(\mathcal{L}) \right], \end{cases} \quad (2.55)$$

where $A^{(t)}(\mathcal{L}) = [a_{i,j}^{(t)}]$ is the adjacency matrix of the lattice at iteration step ' t '. The kinds of lattice structures that emerge in such fully dynamic systems is examined in detail in chapter 8.1.

Quantum Cellular Automata (QCA): in order to address the possibly very fundamental role CA-like dynamics may play in the microphysical domain, some form of quantum dynamical generalization to the basic rule structure must be considered. One way to do this is to replace the usual time evolution of what may now be called classical site values σ_i , by unitary transitions between k -component complex probability- amplitude states, $|\sigma\rangle_i$ – defined in such a way as to permit superposition of states. As is standard in quantum mechanics, the absolute *square* of these amplitudes is then interpreted to give the probability of observing the corresponding classical value. Two independently defined models – both of which exhibit much of the typically quantum behavior observed in real systems – are discussed in chapter 8.2.

Chapter 3

Phenomenological Studies of Generic CA

The renaissance of CA research following Wolfram's pioneering review [wolf83a] would arguably not have occurred were it not for the existence of, and easy access to, affordable personal computers and graphics workstations. Most of the important but excessively technical mathematics of what were called tessellation-automata had already been published years before ([yamad69], [ostr71], and [amoro72]); it was not until the dynamics could be observed directly, however, that anything approaching an *intuition* for the behavior of these systems could finally be obtained. As has already been alluded to repeatedly, except for special-case rules, the behavioral properties of even the simplest CA systems can be exceedingly difficult to establish by direct mathematical analysis. Not surprisingly, the most prudent course of action has proven to be a direct phenomenological study of the systems in question: a particular CA rule and initial state are selected and the dynamical evolution—with an emphasis given to any observable generic properties—is traced directly by computer simulation. Such an approach, also used widely in the general study of continuous chaotic systems, is gaining a considerable respectability and really constitutes a fundamentally new experimental branch of mathematics. This chapter introduces the generic behavior of the simplest one and two dimensional CA systems by way of a guided-tour through a graphics gallery of their dynamical evolutions.

3.1 One-dimensional Systems

We recall from chapter 2 (section 2.1.1) that the general form of a range 'r' one-dimensional rule ϕ is given by

$$\sigma_i(t+1) = \phi(\sigma_{i-r}(t), \sigma_{i-r+1}(t), \dots, \sigma_{i+r-1}(t), \sigma_{i+r}(t)), \quad (3.1)$$

where $\sigma_j \in \{0, 1, \dots, k-1\}$, and ϕ is explicitly defined by assigning values to each of the k^{2r+1} possible $(2r+1)$ -tuple configurations for a given neighborhood. In the following, specific rules will be referred to more compactly by using the simple code given in equation 2.7.

3.1.1 Space-Time Patterns

Simple Seeds

We begin with the simplest CA of all; namely those whose site variables take on only one of two values and evolve according to rules which depend only on the previous values of a given site and those of its immediate left and right neighbors:

$$\sigma_i(t+1) = \phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)), \quad \sigma \in \{0, 1\}. \quad (3.2)$$

We recall, from equations 2.8 and 2.9, that only 32 so-called *legal* rules (out of the 256 total possible rules that can be defined), leave the zero-state $\vec{\sigma} = 0$ unchanged and are such that reflection-symmetric local states – ‘100’ and ‘001’, for example – yield the same values. We now examine the patterns generated by these types of rules.

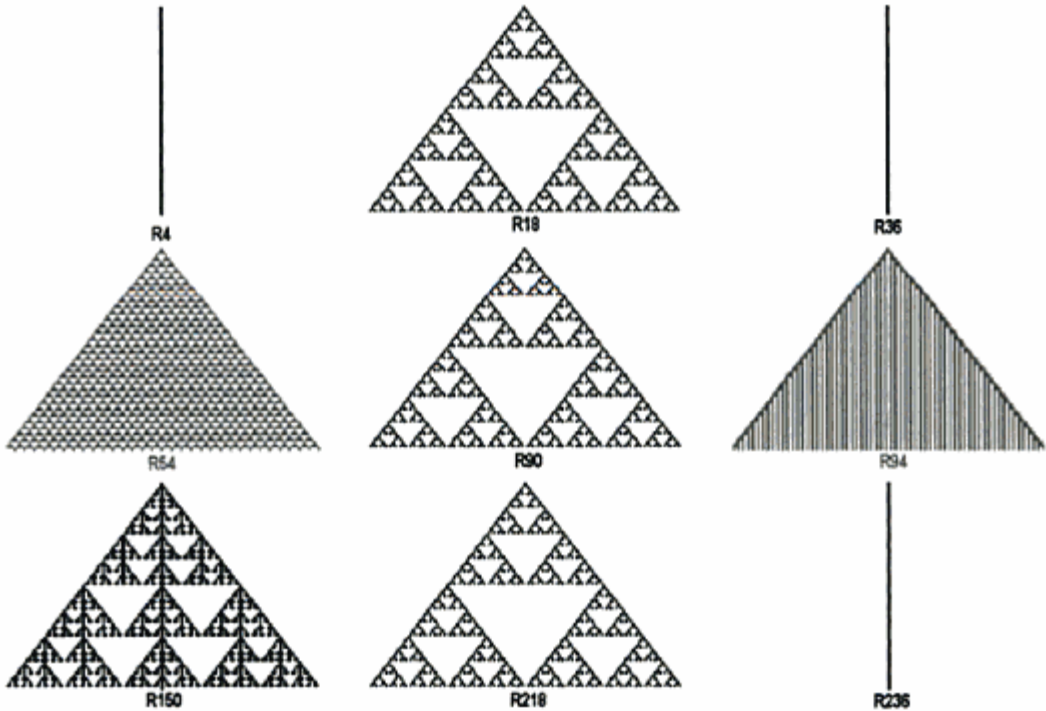


Fig. 3.1 Space-time patterns of a few elementary *legal* rules ($k = 2$, $r = 1$).

Figure 3.1 shows the evolution of a few legal rules, starting from an initial state consisting of a single nonzero value at the center site. In each case, and all such one-dimensional *space-time* patterns appearing in this book, the time axis runs from top to bottom and sites with value $\sigma_i = 1$ are colored *black*.

Several distinct classes of patterns, or behaviors, are evident:

- (i) the initial state remains unchanged for all time (**R4**, **R36**),

- (ii) the region of nonzero sites expands symmetrically to the right and left of the center value to produce essentially uniform structures (**R54**, **R94**), and
- (iii) the symmetrically expanding nonzero region forms a nontrivial complicated pattern of zero's and one's (**R18**, **R90**, **R150**, **R218**).

By virtue of being *local*, CA rules can define neither an intrinsic 'length' scale other than the size of the local neighborhood nor any intrinsic 'time' scale other than the discrete interval between successive configurational states. Since an initial state consisting of a single nonzero site itself defines no intrinsic length scale, the CA configurations appearing in figure 3.1 should also not exhibit an intrinsic scale, at least in the infinite time limit. While some rules yield obviously scale-invariant *uniform* final patterns, the scale invariance of the more complex patterns is more subtle.

Patterns of this third class in fact demonstrate a complex form of scale-invariance by their *self-similarity*; in the infinite time limit, different magnifications observed at the same resolution are indistinguishable. The pattern generated by rule **R90**, for example, matches that of the successive lines in Pascal's triangle: $\sigma_i(t)$ is given by the coefficient of x^i in the expansion of $(1+x)^t$ *modulo-two* (see figure 3.2).

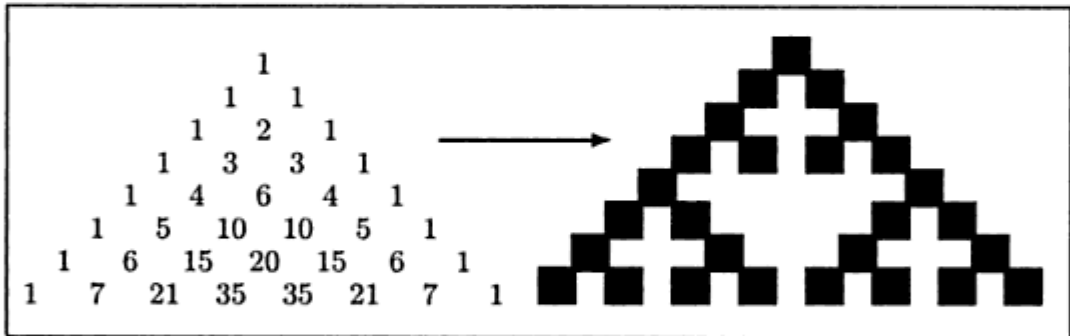


Fig. 3.2 Algebraic construction for the single-seed evolution under **R90**. The left side gives the values of the coefficients of x^n in the expansion of $(1+x)^n$; the right, which matches that of **R90**, are those same values *modulo-two*.

The resulting large-time limit pattern can be obtained by a simple recursive geometrical construction (see figure 3.3), and its manifest self-similarity can be quantitatively characterized by the *Hausdorff-Besicovitch* (or *fractal*) dimension defined in the previous chapter. We see that at each successive stage in the construction the number of triangles increases by a factor of three while their base-length decreases by a factor of two. Thus, defining $T(n)$ to be the number of triangles with base-length ' n ' ($n = 2^k$),

$$T(n/2) \sim 3 T(n) \implies D_{\text{fractal}}(\mathbf{R90}) = \frac{\ln 3}{\ln 2} \sim 1.5849. \quad (3.3)$$

While the patterns generated by rules **R18** and **R218** are essentially the same as

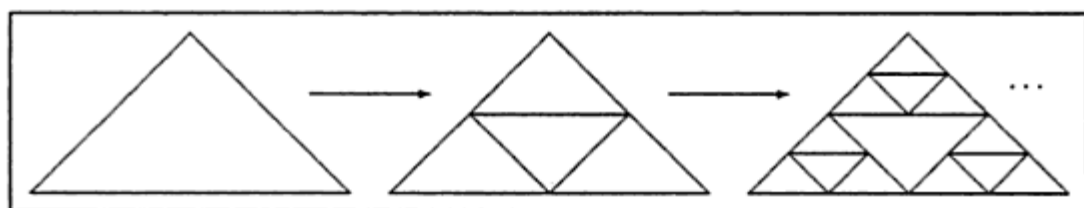


Fig. 3.3 First three steps in the recursive geometric construction of the large-time pattern induced by **R90** when starting from a simple nonzero initial state. The actual final pattern would be given as the infinite time limit of the sequence shown here, and is characterized by a *fractal dimension* $D_{\text{fractal}} = \ln 3 / \ln 2$.

the one resulting from **R90**, the single-seed pattern induced by **R150** can be shown to be equal to the sequence of coefficients of x^i in the expansion of $(1 + x + x^2)^t$ *modulo-two*, and can be geometrically constructed according to the scheme shown in figure 3.4. In this case, $T(n)$ satisfies a *two-term* recurrence relation

$$\begin{aligned} T(n = 2^k) &= 2T(2^{k-1}) + 4T(2^{k-2}), \quad T(2) = 4, \quad T(4) = 12, \\ &= \frac{(5+3\sqrt{5})(1+\sqrt{5})^k}{10} + \frac{(5+3\sqrt{5})(1-\sqrt{5})^k}{10}, \end{aligned} \quad (3.4)$$

so that, as $k \rightarrow \infty$, $T(n) \sim n^{-\log_2(1+\sqrt{5})} \Rightarrow D_{\text{fractal}}(\mathbf{R150}) \sim 1.6942$.

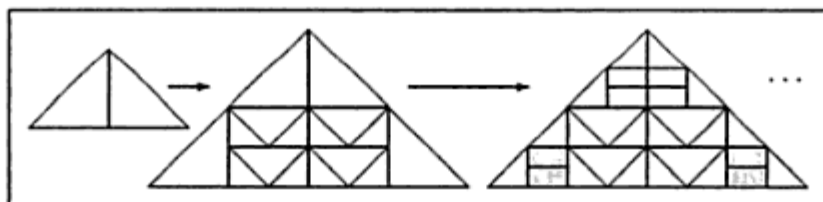


Fig. 3.4 First three steps in the recursive geometric construction of the large-time pattern induced by **R150** when starting from a simple nonzero initial state. The infinite time limit pattern is characterized by a *fractal dimension* $D_{\text{fractal}} \sim 1.69$.

In general, when starting from a single seed and independent of the value of the nonzero site, sum *modulo-k* rules for k equal to a *prime*,

$$\sigma_i(t+1) = \sum_{j=i-r}^{i+r} \sigma_j(t) \pmod{k}, \quad (3.5)$$

generate self-similar fractal patterns with fractal dimension given by

$$D_{\text{fractal}}(\oplus_k; \text{single-seed}) = \log_k \sum_{i=1}^k i = 1 + \log_k \left(\frac{k+1}{2} \right). \quad (3.6)$$

Figure 3.5 shows the time evolution of a few asymmetric (*i.e.*, *illegal*) $k=2$, $r=1$ rules. Doing away with the quiescence condition produces patterns in which $\bar{\sigma}$

alternates between $\bar{1}$ or $\bar{0}$ in successive time-steps; removing reflection symmetry, on the other hand, tends to 'shift' local patterns. Although self-similarity is still evident it is also sheared by shifting. With the one possible exception of rule **R30**, therefore – whose pattern is really a complicated mixture of periodicity and randomness and about which we will have more to say in a later section of this chapter, illegal rules generally do not appear to introduce any dramatically new qualitative dynamical features.

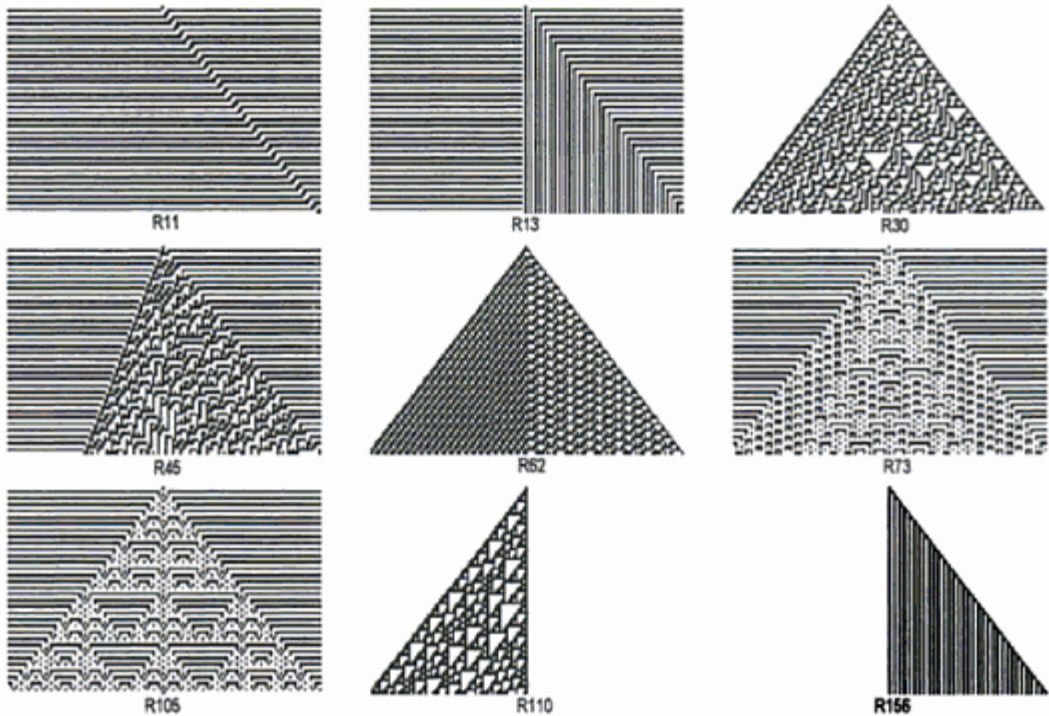


Fig. 3.5 Space-time patterns of a few asymmetric (i.e. *illegal*) $k = 2$, $r = 1$ rules.

Figure 3.6 shows the same legal rules appearing in figure 3.1 but starting from an initial state with nonzero sites occupying only a small central region.

For some rules (such as **R4** and **R94**) the patterns obtained from single seeds are stable under the addition of further nonzero sites. For other rules (such as **R218**) the pattern is unstable. Although the patterns for **R18** and **R150** retain much of their fractal structure, some of the details appear to be washed away. A similar contrast between the evolutionary behaviors of single and small nonzero region seeded rules can be observed for the $r = 2$ totalistic rules shown in figures 3.7 and 3.8.

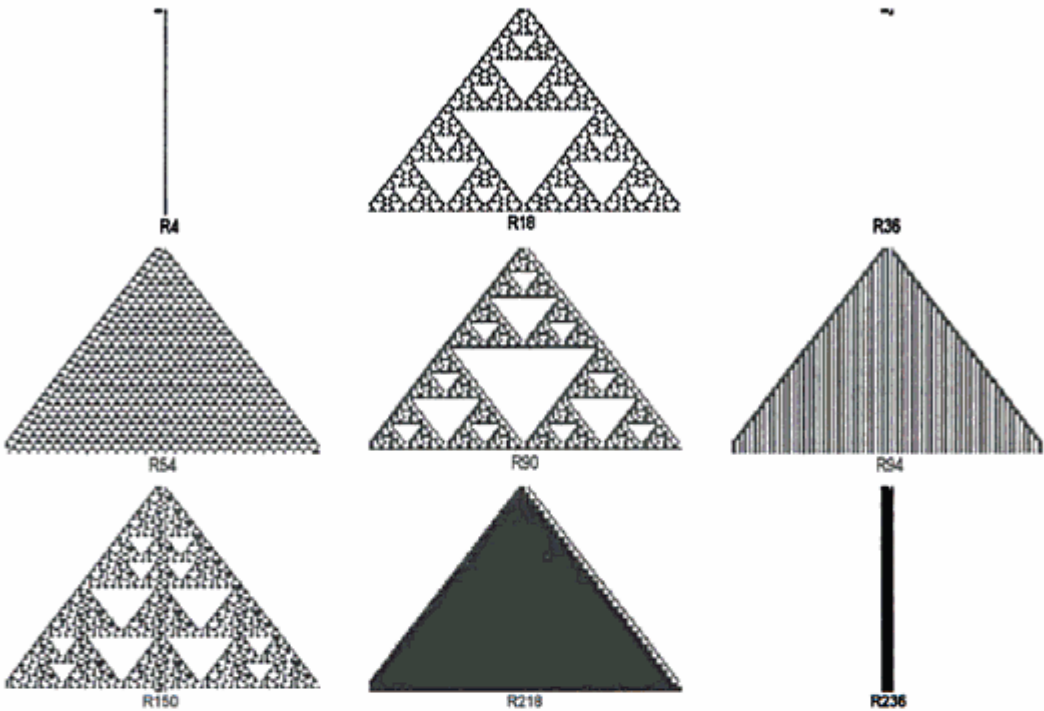


Fig. 3.6 Space-time plots of the same legal rules appearing in figure 3.5 but starting from an initial state with nonzero sites occupying only a small central region.

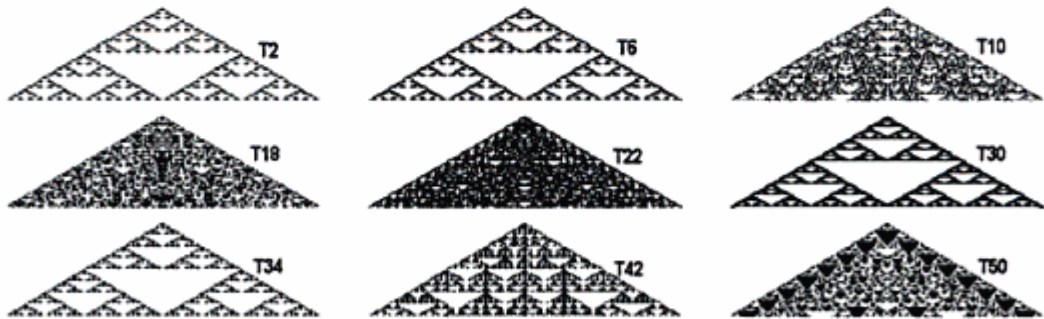


Fig. 3.7 Space-time plots $r = 2$ totalistic rules. The lattice consists of 256 sites and each rule is iterated 64 times. The initial condition, in each case, is a single non-zero site at the center.

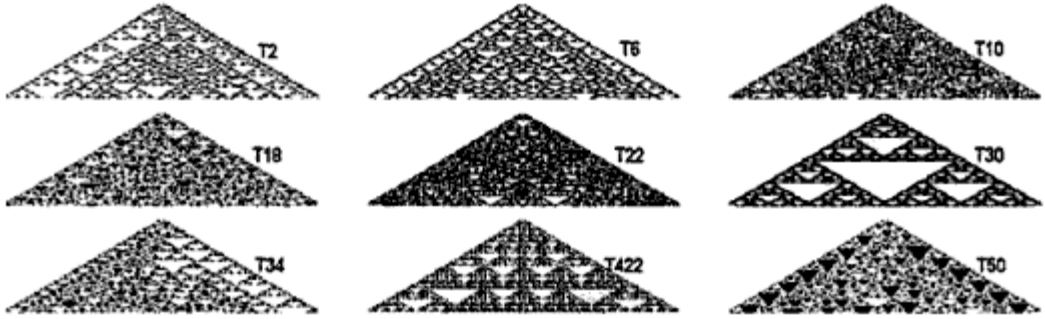


Fig. 3.8 Space-time plots $r = 2$ totalistic rules. The lattice consists of 256 sites and each rule is iterated 64 times. The initial condition, in each case, consists of five nonzero sites near the center.

It is important to point out that except for the obvious *necessary* two conditions that either

$$\begin{cases} \phi(\sigma_{i-r}, \sigma_{i-r+1}, \dots, \sigma_{i-1}, 0, \dots, 0) \neq 0, & \text{or} \\ \phi(0, \dots, 0, \sigma_{i+1}, \sigma_{i+2}, \dots, \sigma_{i+r}) \neq 0, \end{cases} \quad (3.7)$$

must be satisfied for some set of σ_i in order for there to be unbounded growth, there is no known simple general criterion by which the type of pattern to emerge can be predicted directly from ϕ . Similarly, a *necessary*, but not *sufficient*, condition for self-similar pattern formation is to have some sort of *growth inhibition*: the presence of nonzero site configurations must sometimes cause ϕ to yield zero.

Irregular Growth: Although, as we have seen, the nonzero region of most space-time patterns evolving from simple seeds propagates outward at a fixed speed of $c \leq r$ sites per time step, there exist rules for which the growth is much more irregular. Figure 3.9, for example, shows the evolution of the initial state $\vec{\sigma}(0) = \dots 0042400 \dots$ according the $k = 5$, $r = 1$ totalistic rule **T985707700**. The nonzero region, or *light-cone*, undergoes a series of alternating growths and decays, with an average expansion rate of about ~ 0.2 sites per time step.

Random Seeds

Figures 3.10-3.14 show the time evolution of a variety of $r = 1$, $r = 2$ and $r = 3$ rules for both $k = 2$ and $k = 3$ and all starting from a disordered or random configuration. The configurations are defined by randomly and independently assigning each site the value $\sigma = 0$ or $\sigma = 1$ with equal probability: $\text{prob}(\sigma=0) = \text{prob}(\sigma=1) = \dots = \text{prob}(\sigma=k-1) = 1/k$.

We again see a variety of behaviors, including both uniform and complicated patterns. Generally speaking, rules for which fractal patterns emerge from single or simple seeds produce chaotic patterns when grown from larger seeds. The most interesting feature, however, is the fact that many rules destroy the independence of

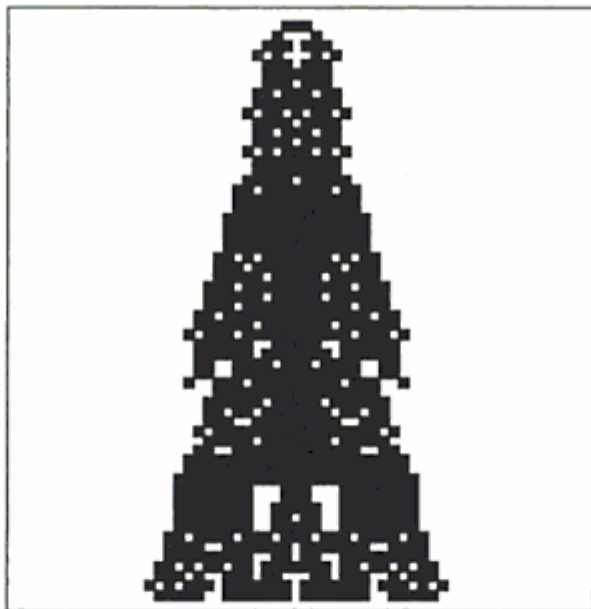


Fig. 3.9 Example of a slow *diffusive*-like growth from a simple seed. The initial state $\vec{\sigma} = \dots 0042400 \dots$ evolves according to the $k = 5$, $r = 1$ totalistic rule **T985707700**. All sites with $\sigma > 0$ are colored black.

the initial configuration and dynamically generate correlations between (often very far) separated sites.

Local regularities within random appearing patterns are associated with *invariants* of a given rule. For example, because the null configuration is invariant under all *legal* rules, any finite string of contiguous zeros can only be reduced in size by nonzero values propagating inward from the sides. Finite strings of zeros thus lead to the triangular clearings seen in the figures.

We have already seen that most CA rules are irreversible: a particular global configuration may have a number of different predecessors, so that the global mapping Φ is not one-to-one. Moreover, there also exist configurations (the so called *garden-of-eden* states) for which there are no predecessors, so that Φ is not onto. The contractive nature of most rules, therefore, implies that only some subset of the space of all possible configurations may occur at large times. What we are thus seeing these figures is rather dramatic (albeit crude) evidence of the phenomenon of *self-organization*, in which an initially random state evolves to a state exhibiting long-range correlations and whose overall space-time patterns contain manifestly *nonlocal* structure. The manifest irreversibility of a given rule results in a long time behavior which is effectively determined by the properties of some limit set consisting of a special subset of all possible states. It is the *universality* of the properties of these special subsets that we turn to next.

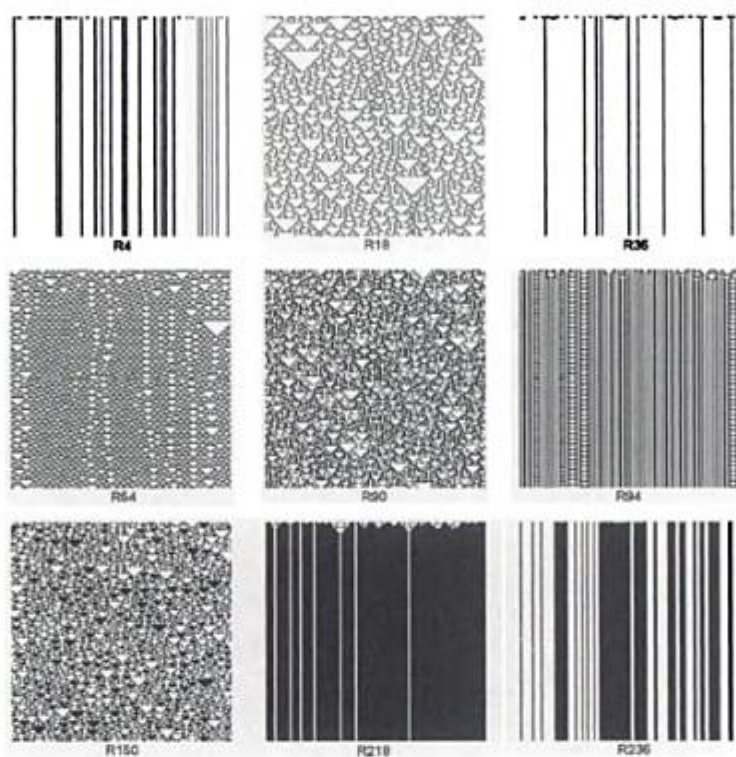


Fig. 3.10 One-dimensional $k = 2$, $r = 1$ rules starting with random initial conditions.

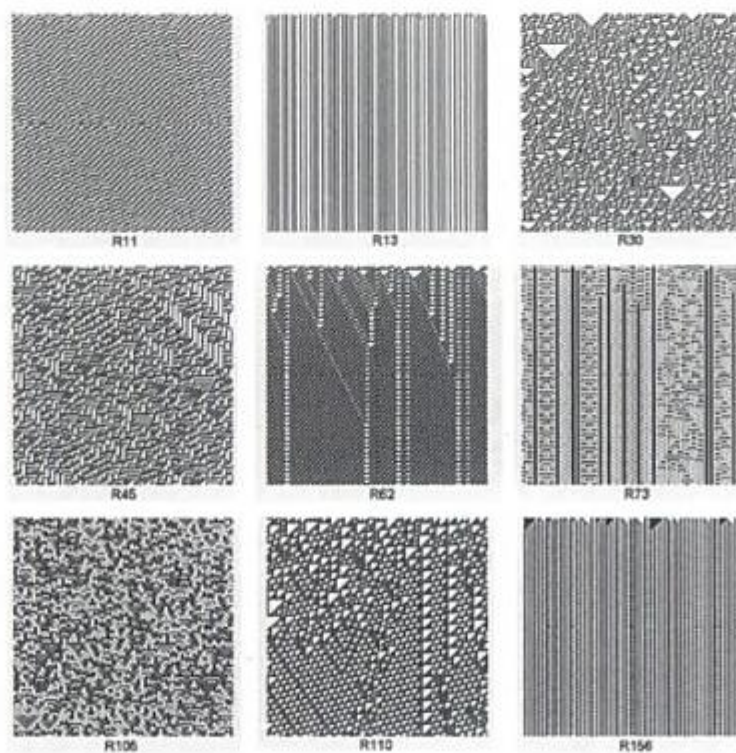


Fig. 3.11 One-dimensional $k = 2$, $r = 1$ rules starting with random initial conditions.

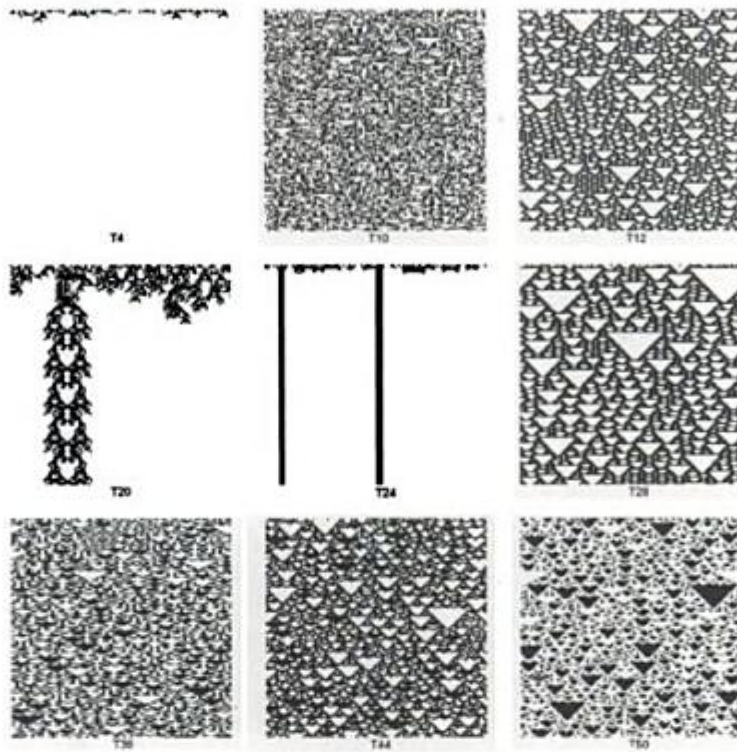


Fig. 3.12 Totalistic $d = 1$, $k = 2$, $r = 2$ rules; starting from random initial conditions.

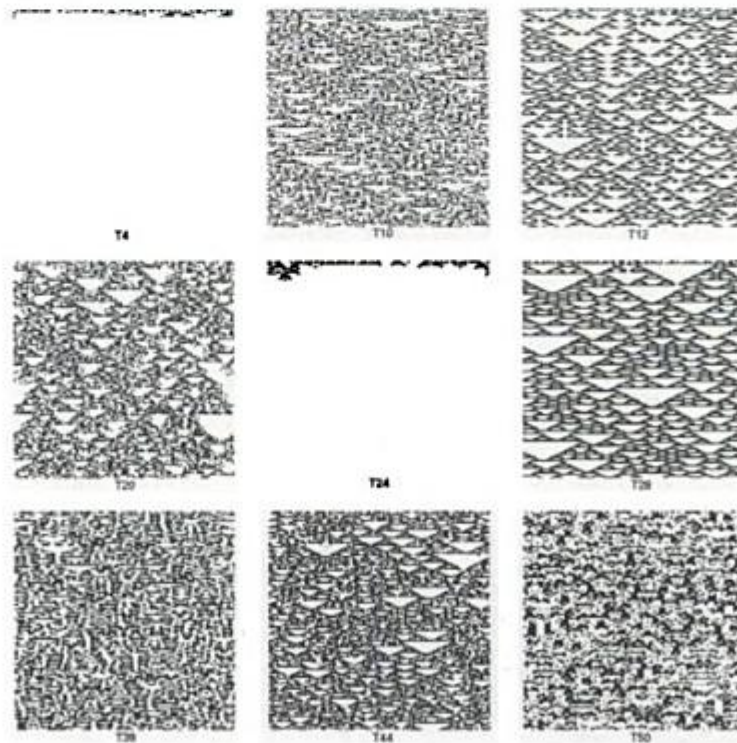


Fig. 3.13 Totalistic $d = 1$, $k = 2$, $r = 3$ rules; starting from random initial conditions.

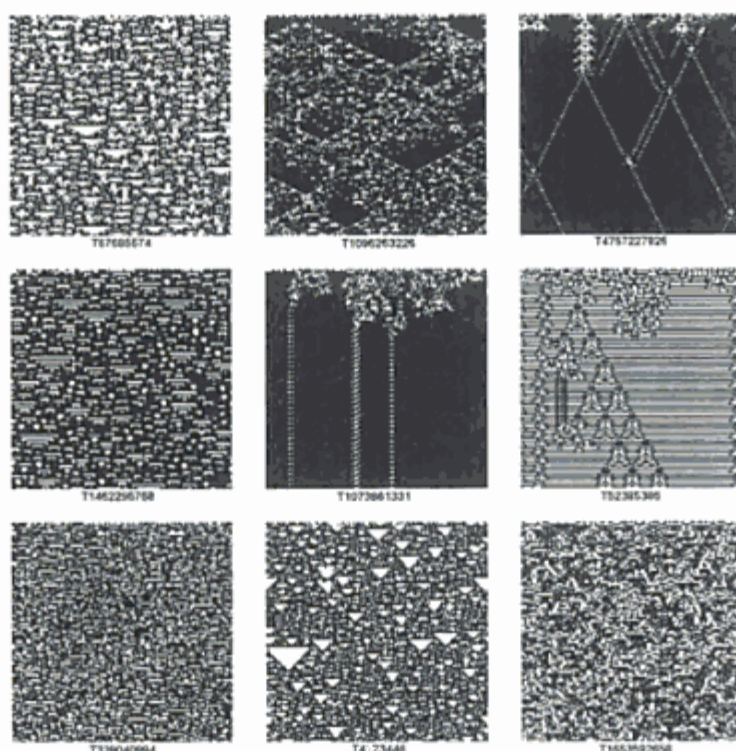


Fig. 3.14 Totalistic $d = 1$, $k = 3$, $r = 2$ rules; starting with random initial conditions.

3.1.2 Behavioral Classes

Although different initial configurations typically give rise to patterns which differ in the *details* of their appearance (see figures 3.10-3.11, for example), the gross overall characteristics of a given pattern appear unchanged: each particular rule yields its own unique and easily recognizable space-time pattern*. Indeed, there is extensive empirical evidence to support the conjecture that the patterns generated by *all* (one-dimensional) CA rules evolving from disordered initial states fall into one of only four basic qualitative behavioral classes ([wolf85b], [wolf85f]) :

Class c1: *All sites eventually attain the same value.*

Class c2: *Simple stable states or periodic and separated structures emerge.*

Class c3: *Chaotic nonperiodic patterns are generated.*

Class c4: *Complex, localized, propagating structures are formed.*

All CA within a given class, regardless of the precise specification of the evolution rule, yield qualitatively similar behavior. Except for rules in the **c4** class, the

*Exceptional initial states yielding distinctly different patterns from the same rule may exist but with low or zero probability.

behaviors bear a strong resemblance to those observed in continuous systems. The homogeneous final states occurring for all **c1** rules, for example, are essentially the same as a *fixed point* attracting final state. Similarly, the asymptotically periodic final states of all **c2** rules are analogous to continuous *limit cycles*, while the chaotic states generated by **c3** rules are analogous to the *strange attractors* appearing in continuous dynamical systems (see chapter 4.2 for details). The more complicated localized structures emerging from **c4** class rules, on the other hand, do not appear to have any obvious continuous analogs, although many are best described as being *soliton-like* in their appearance.

Alternative classification schemes are of course possible. Culik and Dube [culik89a], for example, provide an empirical refinement to class **c3** for $k = 2$, $r = 2$ totalistic rules, based on observations of evolutions starting from random finite initial configurations[†]; they observed that such rules actually form an almost continuous spectrum when classified on the basis of fractal-generation ability. A more formal approach based on observations of behavior starting from finite configurations is taken by Culik and Yu [culik88]. Among the several important, and unexpected, results reported there, are (i) it is undecidable whether all the finite configurations of a given CA eventually become quiescent, and (ii) it is undecidable to which class a given CA belongs, *even when choosing between the simplest two classes*.

3.1.2.1 Difference Patterns

Although the question of the quantitative characterization of these classes is taken up in earnest in chapter 4, we can here mention that an important tool will be a discrete *Green function*. Green functions measure *changes* in patterns generated by a given rule resulting from a small change in the initial state, and give the average probability that sites a given distance away from the small area of differing initial values will be changed after a certain number of iteration steps. We can get a glimpse of the form of these Green functions for a selected rule by plotting various *difference patterns*.

Difference patterns are space-time patterns of the difference between two evolutions of the same rule starting from two different initial states. For example, the i^{th} site at the n^{th} step of a difference pattern for ($k = 2$ global) rule Φ in which the two different initial global states $\vec{\sigma}_1(0)$ and $\vec{\sigma}_2(0)$ differ only at a single site (see figure 3.15), is defined to be

$$\Delta_i^{[1]}(n) = \Phi^n [\vec{\sigma}_1(0)]_i \oplus_2 \Phi^n [\vec{\sigma}_2(0)]_i. \quad (3.8)$$

The rate of growth of such patterns – which gives an idea of the speed with which various features in a CA pattern may propagate through the lattice – provides one quantitative measure that can be used to distinguish between the behaviors of different classes.

[†]By a *finite* initial configuration we mean one in which all but a finite number of sites in an infinite lattice are in the same quiescent state.

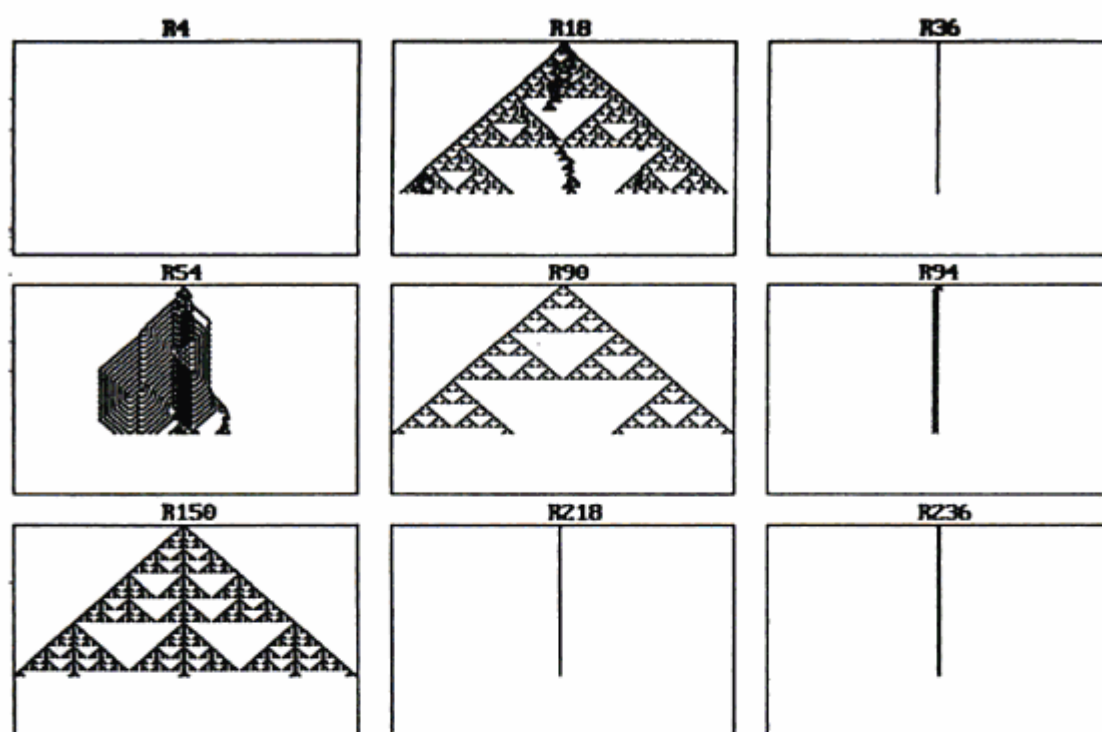


Fig. 3.15 *Difference patterns for a few elementary $k = 2$, $r = 1$ rules; see text.*

Class **c1** rules, for example, have unique final states which are unaffected by any change to the initial state. Similarly, **c2** rules are such that small changes in the initial state only affect a fixed finite region around the area in which the values were changed. A change in the value of even a single site for **c3** rules, on the other hand, affects a linearly increasing region of sites; given enough time, therefore, infinitely large lattices would have arbitrarily large regions affected by a minimal perturbation to the initial state.

The same structural irregularity of the space-time patterns of **c4** rules appears also in their difference patterns. While some perturbations on some initial configurations appear to propagate arbitrarily far, others die out rather quickly. Unlike the first three classes of rules, for which statistical averages of propagation speeds are easily obtained, the behavior of **c4** rules is so irregular that meaningful averages cannot be obtained. In particular, this means that Green functions cannot be properly defined for **c4** rules.

Table 3.1 (taken from reference [wolf86b]) gives the approximate fractions of a variety of legal totalistic rules belonging to each of the four behavioral classes. We see that rules generally become more likely to exhibit **c3** or **c4** behavior for larger ' k ' and ' r ', and that **c4** behavior does not appear at all in any of the *elementary* $r = 1$, $k = 2$ rules.

Since the speed of information propagation is, as we shall see in chapter 4, related to the Lyapunov exponent for the CA evolution, and is a direct measure of the sensitivity to initial conditions, it should not be surprising to learn that various rules can also be distinguished by the *degree of predictability* for the outcome of

CLASS	k=2, r=1	k=2, r=2	k=2, r=3	k=3, r=1
c1	0.50	0.25	0.09	0.12
c2	0.25	0.16	0.11	0.19
c3	0.25	0.53	0.73	0.60
c4	0.00	0.06	0.06	0.07

Table 3.1 Approximate fraction of legal totalistic rules belonging to each of the four behavioral classes.

CLASS	FINITE SEED	RANDOM SEED	DIFFERENCE PATTERN	PREDICTABILITY
c1	pattern disappears	all sites attain same value	no change	completely predictable
c2	evolves to fixed finite size	simple stable or periodic structures	changes only over finite region	locally predictable from local initial state
c3	grows indefinitely	chaotic aperiodic behavior	changes over ever expanding region	behavior depends on ever increasing initial region
c4	alternating growth and decay	complex localized structures	irregular changes	effectively unpredictable

Table 3.2 Characteristics of the four behavioral classes.

their evolution. Table 3.2 summarizes the qualitative differences among the four behavioral classes.

What has not yet been discussed is the reason for this behavioral universality. A possible mechanism may be provided by the apparently ubiquitous phenomenon of attractive rule simulation in *blocking transformation* networks, a description of which we turn to next.

3.1.2.2 Blocking Transformations

' T ' iterations of rule ' ϕ_1 ' are often *simulated* by ' nT ' ($n > 1$) iterations of another rule ' ϕ_2 ', provided that individual site values of the first system are replaced with particular blocks of sites in the second:

$$\begin{cases} 0 \longrightarrow B_0, \\ 1 \longrightarrow B_1. \end{cases} \quad (3.9)$$

As a simple example of this, consider the elementary rules **R18** and **R90**:

RULE	111	110	101	100	011	010	001	000
	↓	↓	↓	↓	↓	↓	↓	↓
R18	0	0	0	1	0	0	1	0
R90	0	1	0	1	1	0	1	0

Notice that any initial configuration that does not contain any '110' or '011' blocks will evolve in the same way under the two rules.

Provided that *two time steps* under **R18** are carried out for every *one time step* of rule **R90**, it is in fact easy to show that under the block transform

$$\begin{cases} 0 \rightarrow '00' \\ 1 \rightarrow '10', \end{cases} \quad (3.10)$$

the evolution of arbitrary starting configurations under **R90** is reproduced, or *simulated*, by **R18**.

Consider the global state $\vec{\sigma}_1 = '0011000'$, for example, which evolves into $\vec{\sigma}_2 = '0111100'$ under **R90**. $\vec{\sigma}_2$ could equally well be obtained by applying two iterations of **R18** to the block-transformed starting state $B(\vec{\sigma}_1) = '00001010000000'$:

$$\begin{aligned} \Phi_{\mathbf{R18}} [\Phi_{\mathbf{R18}} (B(\vec{\sigma}_1))] &= '00101010100000' \\ &= B(\vec{\sigma}_2) \\ &= B(\Phi_{\mathbf{R90}}[\vec{\sigma}_1]). \end{aligned} \quad (3.11)$$

Simulation of ϕ_1 by ϕ_2 implies the existence of a set $\lambda \subseteq \Lambda$ for which the evolution under the two rules ϕ_1 and ϕ_2 is the same. Since most CA rules are irreversible it may happen that *only the one subset of blocks corresponding to some particular simulated rule* will continue being generated at large times. If this happens, then it may be said that the behavior of the first rule is *attracted* to that of the second. Rule **R18**, for example, is attracted to rule **R90** in precisely this manner (see below).

Many, possibly all, rules appear to generate asymptotic states which are block-related to configurations evolving according to one of only a small subset of the set of all rules, members of which are left invariant under all block transformations. That is, the infinite time behavior appears to be determined by evolution towards *fixed point rule* behavior, and the statistical properties of all CA rules can then, in principle, be determined directly from the appropriate block transformations necessary to reach a particular fixed point rule.

Block-Defined 'Phases' of Behavior: The simulation of **R90** by **R18** also illustrates the appearance of distinct *phases* of behavior, separated by domain walls. Each phase corresponds to a particular set of configurations, such as those for which the given rule simulates some other rule.

We first observe that any random initial configuration '*S*' can be decomposed into two distinct sets:

$$S = \left(\bigcup_i S_i^{\text{even}} \right) \cup \left(\bigcup_j S_j^{\text{odd}} \right), \quad (3.12)$$

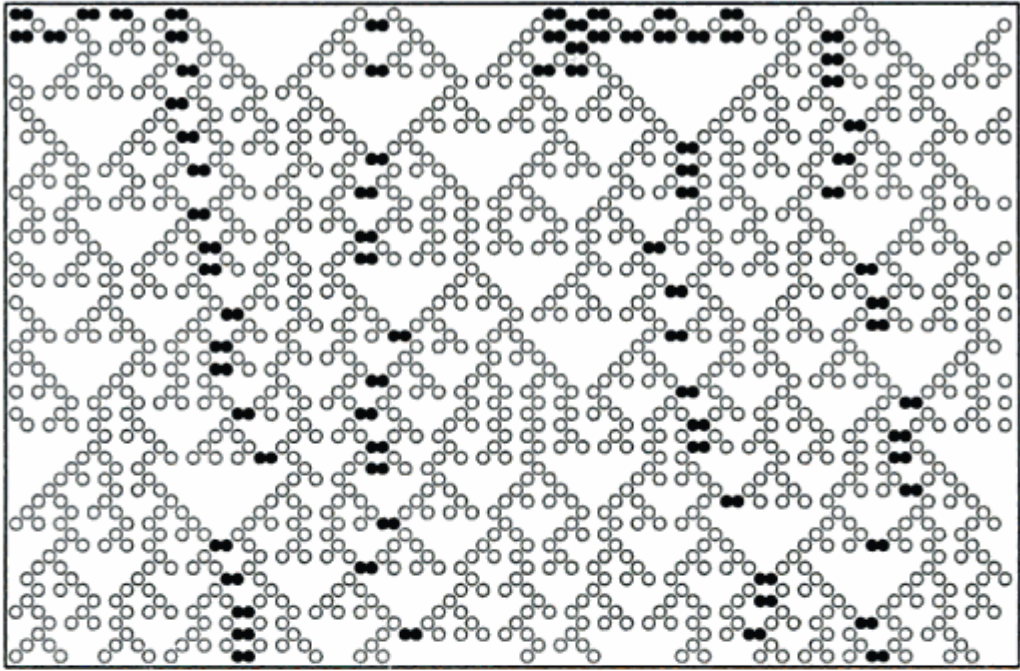


Fig. 3.16 Space-time pattern of $k = 2$, $r = 1$ rule **R18**; *kink*-sites (i.e. neighboring $\sigma = 1$ sites) are indicated in solid black. Notice the stochastic-like kink trajectories, despite the strictly deterministic rule.

where S^{even} and S^{odd} are configurations in which all *even* and all *odd* sites are zero, respectively. It is easy to see that

1. Both of the sets, S^{even} and S^{odd} , are *invariant* under **R18**, and
2. Each set, or *phase*, has the correct blocking form to simulate evolution under rule **R90**.

The domain walls (or *kinks*, consisting of pairs of sites with value $\sigma = 1$) that define the boundary between the two sets, however, *do not* evolve as they would under **R90** but instead undergo pairwise annihilating random walks (see figure 3.16). Indeed, numerical analysis [grass84a] has shown that, as $t \rightarrow \infty$, their density decreases like

$$\rho_{\text{kink}} \sim (4\pi t)^{-1/2}. \quad (3.13)$$

A similar kind of ‘kink-annihilation’ exists for rules **R122**, **R126**, **R146**, and **182**.[†]

[†]One may speculate on the fundamental importance of the following obvious, but no less intriguing, point: despite a fundamentally deterministic evolution taking place on the lower *site* level, a nondeterministic stochastic dynamics unexpectedly appears on the higher *kink* level. We are at least reminded once again that neither complex nor random behavior need have a complex

As time increases, S^{even} and S^{odd} take up arbitrarily large regions of the lattice. The behavior of rule **R18** thus approaches that of **R90** arbitrarily closely; i.e., rule **R18** is *attracted*, to rule **R90**, via the block transformation defined by equation 3.10.

Rule $\mathcal{R}_1$	(Simulates) $\rightarrow \mathcal{R}_2$	$0 \rightarrow 'B_0'$	$1 \rightarrow 'B_1'$	Simulation Steps
22	0	11011000	11111000	4
	90	0000	1000	4
	146	00	01	2
58	0	101	100	3
	128	00	10	2
	170	11010	10110	5
	240	1100	1110	8
60	60	00	10	2
90	90	00	10	2
110	0	110100	101100	9
	170	10011000	11111000	16
	240	111000	100110	9
122	0	1010	1000	2
	90	00	11	2
	128	00	10	2
	204	11100	11110	2

Table 3.3 Block-Transformation Simulations for a few selected elementary rules.

Table 3.3 lists blocking transformations and equivalent simulation time steps for a few other rules.[†] Notice that some rules, like **R60** and **R90**, remain invariant under certain blocking transformations and can thus be considered *fixed points* of the transform. Essentially all rules whose blocking transformation properties have been studied thus far have been found to follow an attractive simulation path to one of the few fixed point rules. It has been suggested that the large time behavior of *all rules* tends towards that of the fixed point rules ([wolf83a], [wolf85a], [wolf85d]). If true then the set of fixed point rules accounts for the phenomenologically observed behavioral universality of CA: all class **c1** rules tend towards the null rule; all class **c2** rules are attracted towards the identity rule, and all class **c3** rules are attracted to the class **c3** fixed point rules.

We have just seen that rule **R18** has essentially one phase that takes two different forms. A general rule typically supports many different phases, each corresponding to simulations of different rules. Not all of these phases will be *stable* however. For example, of the two **R122** phases defined by block transforms $\mathcal{T}_1 = \begin{pmatrix} 0 \rightarrow 00 \\ 1 \rightarrow 11 \end{pmatrix}$ (for dynamical origin.

[†]More complete tables of blocking transformations appear in [wolf83a] and in the appendix of reference [wolf85c].

which **R122** simulates the class **c3** rule **R90**) and $\mathcal{T}_2 = \begin{pmatrix} 0 \rightarrow 11100 \\ 1 \rightarrow 11110 \end{pmatrix}$ (for which **R122** simulates the class **c2** rule **R204**), only the former is stable.

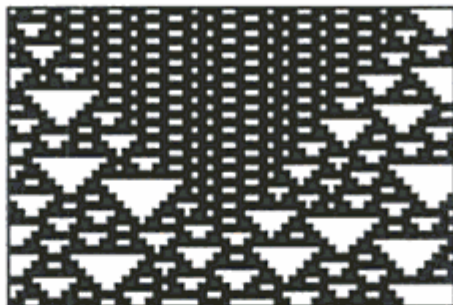


Fig. 3.17 Stable (class **c3**) and unstable (class **c2**) phases of rule **R122**.

Figure 3.17 shows the evolution of an initial state consisting only of blocks '11100' and '11110', except for two 'defects', '00' and '10', placed at the end (periodic boundary conditions are used). Starting from these defects, the stable class **c3** behavior expands approximately linearly in time to eventually dominate the overall pattern.

Blocked Space-Time Patterns: The intrinsic phase structure of a rule can sometimes be directly observed by graphing its *blocked pattern*. We can describe the space-time sets of the two ordered states of rule **R18** by

$$\begin{cases} \sigma_n^I(t) & \longleftrightarrow & n + t = \text{even} \\ \sigma_n^{II}(t) & \longleftrightarrow & n + t = \text{odd} \end{cases} \quad (3.14)$$

The two sets may thus be effectively disjoined from one another by plotting only *every-other* site, both spatially and temporally. Higher order blocked patterns may also prove useful. Various phases for systems with $k > 2$, on the other hand, are often evident even without resorting to blocked patterns.

Block-Transform Generation of Fractal Patterns: Blocking transformations provide an elegant 'explanation' of the self-similar, or scale-invariant, fractal patterns generated by rules such as **R90** and **R218** (see figure 3.1). If the (inverse) blocking transform $\mathcal{T} \equiv \begin{pmatrix} 00 \rightarrow 0 \\ 01 \rightarrow 1 \end{pmatrix}$ were applied to either of these two rules, for example, the resulting blocked-pattern would be reproduced by the same rule; *i.e.*, rules **R90** and **R218** are *fixed points* of $\mathcal{T}$. Since the rule and initial configuration are both invariant under $\mathcal{T}$, the resulting space-time pattern must also be; hence, the scale-invariance of the final figure. Similarly, any rule that simulates one of these rules using another block transform $\mathcal{T}'$ will also produce scale-invariant patterns when their initial states consist solely of the blocks in $\mathcal{T}'$.

3.1.3 General Properties of Elementary CA

Figures 3.10-3.15 present some qualitative evidence for the *self-organization* of space-time patterns emerging out of initial configurations of uncorrelated sites. In this section we introduce some of the quantitative characterizations of self-organization in elementary $r = 1$, $k = 2$ rules by examining these systems from two different points of view:

1. the local statistical properties of individual configurations, and
2. the global statistical properties of the ensemble of all possible configurations.

More general methodology applicable to a wider variety of complex rules is introduced in chapters 4 and 5.

3.1.3.1 Local Properties

As alluded to earlier, a given configuration may be considered *disordered* (or essentially random) if the values of different sites are statistically uncorrelated. Deviations of statistical measures from those obtained for disordered configurations signify the appearance of *order* and therefore mark the appearance of correlations between values of separated sites. While a completely disordered configuration is completely specified by a single parameter ' p ', representing the probability that a given site has value '1', the specification of ordered configurations requires additional parameters.

Density: The simplest statistical measure that can be used to characterize a configuration is the *density* $\rho_1(t)$, defined to be the *average fraction of sites with value $\sigma = 1$ at time t* . For a disordered configuration, for example, $\rho_1 = p$.

Consider, first, the density $\rho_1(t = 1)$, obtained from an initially disordered configuration by evolution for one time step. For a disordered configuration, $p = \rho_1 = 1/2$, so that all eight possible 3-tuple local neighborhoods occur with equal probability. The fraction of sites with value ' $\sigma = 1$ ' after one iteration of rule ' ϕ ' is given by the fraction of the eight possible neighborhoods that yield the value '1' according to the ' ϕ ':

$$\rho_1(1) = \frac{\#_1(\phi)}{\#_1(\phi) + \#_0(\phi)} = \frac{\#_1(\phi)}{8}, \quad (3.15)$$

where $\#_1(\phi)$ is the number of occurrences of the digit '1' in the binary representation of the rule ' ϕ '. The binary representation of **R122**, for example, is given by '01111010' so that $\#_1(\mathbf{R122}) = 5$ and, consequently, the density $\rho_1(1) = 5/8$ for an infinitely large configuration.

The generalization of this simple formula to the case when $p \neq 1/2$ is straightforward. In this case, each of the eight possible 3-tuple neighborhoods $\vec{\sigma} = \sigma_1\sigma_2\sigma_3$

must first be weighted by a factor

$$p(\vec{\sigma}) = p^{\#_1(\vec{\sigma})} (1-p)^{\#_0(\vec{\sigma})}, \quad (3.16)$$

where $\#_1(\vec{\sigma})$ is the number of occurrences of the digit '1' in the 3-tuple $\vec{\sigma}$. The density after one time step is then given by adding the probabilities for all $\vec{\sigma}$ which yield value '1' under ' ϕ ':

$$\rho_1(1) = \sum_{\{\vec{\sigma} \mid \phi(\vec{\sigma})=1\}} p(\vec{\sigma}). \quad (3.17)$$

Obtaining $\rho_1(t)$ for $t > 1$ is more difficult because of the correlations that are inevitably generated in the course of a typical evolution. In particular, since the independence assumption underlying the above derivation of $\rho_1(1)$ is generally invalid, derivations must usually be tailored to particular rules. An exception is the class of *additive rules*, which we recall obey the property of the *additive superposition*: configurations obtained by evolution from arbitrary initial states are given by adding (*modulo 2*) the evolutions of initial configurations having a single nonzero cell. Consider, for example, the additive rule **R90**.

An examination of figures 3.1 and 3.2 reveals that the number of sites with value '1' at time ' t ' obtained by an evolution of an initial state containing a single nonzero site according to rule **R90** is given by

$$N_1(t) = 2^{\#_1(t)}, \quad (3.18)$$

where $\#_1(t)$ is the number of occurrences of '1' in the binary representation of ' t '. The value of a site at time ' t ' is the sum *modulo 2* of the initial values of $N_1(t)$ sites, each of which has a probability $\rho_1(0)$ of having the value $\sigma = 1$. Since a site can have value $\sigma = 1$ only if the predecessor 3-tuple neighborhood had an *odd* number of sites with value '1', we merely have to calculate the probability, p_{odd} , that the sum of values of the sites is *odd*. If each of a set of ' k ' sites has value '1' with probability ' p ', then p_{odd} is given by

$$p_{\text{odd}} = \sum_{\{i \text{ odd}\}} \binom{k}{i} p^i (1-p)^{k-i} = \frac{1}{2} [1 - (1-2p)^k], \quad (3.19)$$

so that $\rho_1(t)$, obtained from an initially disordered state with density $\rho_1(0)$ according to **R90** is

$$\rho_1(t) = \frac{1}{2} \left[1 - (1-2\rho_1(0))^{2^{\#_1(t)}} \right]. \quad (3.20)$$

Note that for large ' t ', $\#_1(t) = \mathcal{O}(\log_2 t)$ except at a set of measure zero, so that $\rho_1(t) \rightarrow 1/2$ at $t \rightarrow \infty$ for almost all ' t '.

Asymptotic results obtained for additive rules can often be almost immediately extended to certain non-additive rules, by exploiting 'blocking-transformation' relationships. We recall from the discussion in the last section, for example, that the complex rule **R18** *simulates* **R90** under a transformation which associates with

each site an additional zero valued cell. This transformation thus effectively ‘dilutes’ the patterns evolving according to **R90**; specifically, if no kinks were present, $\rho_{1,\mathbf{R18}}(t)$ would equal $\frac{1}{2} \cdot \rho_{1,\mathbf{R90}}(t)$. Assuming that the system has evolved long enough according to **R18** to allow most of the *kinks* to annihilate, we may conclude that the asymptotic density $\rho_{1,\mathbf{R18}}(t \rightarrow \infty) = 1/4$.

For general rules, a first-order statistical approximation for limiting densities $\rho_1(t \rightarrow \infty)$ can be obtained by a method akin to the *mean-field* theory in statistical mechanics (more sophisticated approaches will be introduced in chapter 4).

Mean Field Approximation: as a first order approximation, we will ignore all correlations between values at different sites and parameterize configurations purely in terms of the average density at time ‘ t ’, ρ . The time evolution of ρ under an arbitrary rule ‘ ϕ ’ is then given by the master equation

$$\frac{\delta \rho}{\delta t} = f_{0 \rightarrow 1} - f_{1 \rightarrow 0}, \quad (3.21)$$

where $f_{i \rightarrow j}$ is the average fraction of sites whose value changed from $\sigma = i$ to $\sigma = j$. An explicit form for these fractions is obtained by observing that the probability ‘ P ’ of having the 3-tuple $\vec{\sigma} = \langle \sigma_1 \sigma_2 \sigma_3 \rangle$ appear in a neighborhood is

$$P(\sigma_1, \sigma_2, \sigma_3) = p^{\#_1(\vec{\sigma})} (1-p)^{3-\#_1(\vec{\sigma})}, \quad (3.22)$$

where, as before, $\#_1(\vec{\sigma})$ is the number of times ‘1’ appears in the string $\vec{\sigma}$. Thus,

$$\begin{cases} f_{0 \rightarrow 1} &= \sum_{\{\vec{\sigma} \mid \sigma_2=0\}} \phi(\sigma_1, \sigma_2, \sigma_3) P(\sigma_1, \sigma_2, \sigma_3), \\ f_{1 \rightarrow 0} &= \sum_{\{\vec{\sigma} \mid \sigma_2=1\}} [1 - \phi(\sigma_1, \sigma_2, \sigma_3)] P(\sigma_1, \sigma_2, \sigma_3). \end{cases} \quad (3.23)$$

The equilibrium, or *steady-state*, density $\rho_1(t \rightarrow \infty)$ is achieved when

$$\frac{\delta \rho}{\delta t} = 0. \quad (3.24)$$

For rule **R90**, for example, we find that

$$\begin{cases} f_{0 \rightarrow 1} &= P(0, 0, 1) + P(1, 0, 0) = 2(1-p)^2 p, \\ f_{1 \rightarrow 0} &= P(0, 1, 0) + P(1, 1, 1) = (1-p)^2 p + p^3. \end{cases} \quad (3.25)$$

Thus, $\delta \rho / \delta t = 0 \implies p(1-2p) = 0$, which has solutions $p = 0$ (or the *null* state) and $p = 1/2$. Similarly, for **R18**, we find that $p(1-4p+2p^2) = 0$, with solutions $p = 0$ and $p \approx 0.293$. Both nonzero results appear to be consistent with our earlier observations.

Although differences between mean-field estimates and exact limiting densities are to be expected because of the presence of correlations in actual evolutions, the mean-field approach nonetheless typically comes to within about 10 – 20% of the exact values for all elementary complex rules.

Two point correlations: We have already mentioned several times that evolutions generally induce correlations between cell values at different sites; indeed, the presence of correlations is a telltale signature of self-organization. The average density discussed above, however, is too crude a measure to capture these finer details.

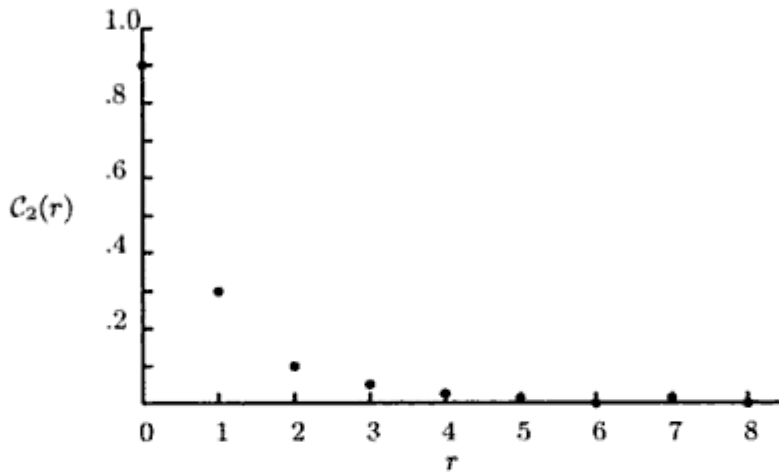


Fig. 3.18 Two point correlation function for large time 't' for elementary $k = 2$, $r = 1$ rule **R22**.

In its place we can use the simplest correlation measure, the two point *correlation function*,

$$C_2(r) = \langle \zeta_i \zeta_{i+r} \rangle - \langle \zeta_i \rangle \langle \zeta_{i+1} \rangle, \quad (3.26)$$

where the average is taken over all possible sites 'i' at a fixed time 't', and

$$\zeta_i = \begin{cases} +1 & \longleftrightarrow \sigma_i = 1, \\ -1 & \longleftrightarrow \sigma_i = 0. \end{cases} \quad (3.27)$$

A completely disordered configuration gives $C_2(r) = 0$ for $r \geq 1$, with $C(0) = \langle \zeta_i^2 \rangle - \langle \zeta_i \rangle^2 = \langle (2\sigma_i - 1)^2 \rangle - \langle 2\sigma_i - 1 \rangle^2 = 4p(1 - p)$. The periodicities frequently evident in complex patterns evolving from initial states with a single nonzero site, give rise to peaks in $C_2(r)$. For the class of additive rules, $C_2(r)$ at time 't' is obtained by convolution of this result with the correlation function for an arbitrary disordered initial state, and thus remains equal to zero for all time. For nonadditive rules, however, there exists the possibility that short-range correlations may be built up from completely disordered initial configurations. The existence of a nonzero correlation length is our first quantitative evidence of the appearance of self-organization. Figure 3.18 shows the form of $C_2(r)$ for rule 22. We see that the correlation appears to fall off exponentially with a correlation length $\ell_c \approx 2$.

Although $\rho(t)$ and $C_2(r)$ do give some insight into the behavior of complex rules, even a casual glance at the earlier space-time patterns reveals a rich diversity of structure that these measures are incapable of capturing.

The most obvious feature is the frequent presence of triangular clearings of various sizes. These occur when a long string of cells all attain the value $\sigma = 1$ so that, if the rule is legal, all sites away from either end of the string revert to $\sigma = 0$ on the next time step. Thereafter, in successive time steps, the newly formed 'clearing' is progressively reduced in length as sites with $\sigma = 1$ steadily migrate in from the sides. What is not readily perceivable, however, is again a kind of universality in the numbers of such clearings.

Defining $\mathcal{T}(n)$ to be the *density of triangular clearings with base length 'n'*, it has been found that, for large 'n' and for patterns generated from disordered initial states, $\mathcal{T}(n)$ behaves as

$$\mathcal{T}(n) \sim \begin{cases} 2^{-n} & \longleftrightarrow \text{additive rules,} \\ (\frac{4}{3})^{-n} & \longleftrightarrow \text{nonadditive rules.} \end{cases} \quad (3.28)$$

The spectrum of triangular clearings is therefore independent both of the particular initial configuration and evolutionary rule.

There are a number of additional local structures and properties that appear even in elementary CA systems. Grassberger [grass84b], for example, has observed that rule **R22** actually harbors very complex long-range effects, similar to a critical phenomenon (see section 3.1.4). Since the majority of these findings require the use of more general and sophisticated correlation measures than we have defined thus far, we will pick up our discussion of them in chapter 4.

3.1.3.2 Global Properties

The preceding section dealt with the statistical properties of the set of cell values in individual configurations. An alternative, and in some sense complementary, approach is to examine the statistical properties of the set of all possible configurations. Such a global view sets the stage for drawing comparisons between the evolution of CA and that of general dynamical systems.

Finite Lattices: Consider a finite CA having $N < \infty$ sites. The total number of possible configurations for this system is 2^N , with each configuration being uniquely specified by a binary string of length N whose digits give the values of each of the sites. For simplicity, we can assume periodic boundary conditions.

Since finite lattices harbor a finite number of possible states, we know that any sequence of configurations starting from an arbitrary initial state *must* become periodic after at most 2^N iterations.

Figure 3.19, for example, shows a few of the cycles that emerge on a size $N = 10$ lattice for a system evolving according to the class **c3** rule **R122**. In practice, and as suggested by this figure, many fewer iterations than the maximum $t_{\max} = 2^N$ are needed before a cyclic state is reached.

If, as is usually the case, the rule is *locally irreversible* – i.e., the rule is such that

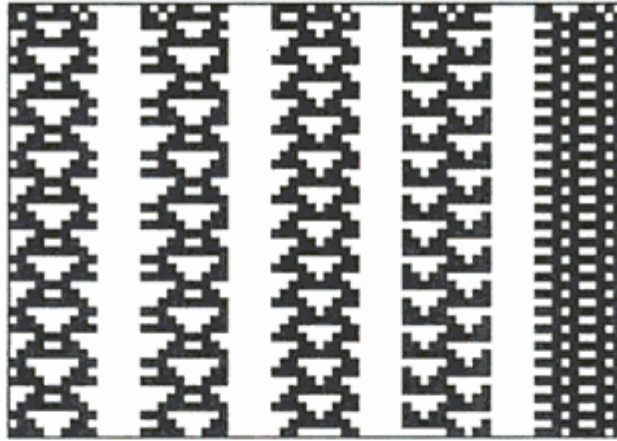


Fig. 3.19 Evolution of typical initial configurations on a size $N=10$ lattice with periodic boundary conditions according to rule 122.

a given local configuration may have more than one local predecessor state – there clearly must exist configurations which can only occur as initial states. On the other hand, local irreversibility does not preclude the overall system from being *globally reversible*. A system is said to be globally reversible if each global configuration has exactly one predecessor and exactly one successor state. Although not immediately obvious, a little thought will demonstrate that this is indeed possible even if the local rule is itself irreversible.

We have just identified three basic kinds of configurations that can conceivably occur in an evolution:

Garden-of-Eden States: which can never be dynamically generated in the course of the evolution and can therefore occur only as initial states. For the trivial *null* rule, for example, in which all local states get mapped to zero, all nonzero states are dynamically unreachable. Under the identity rule, **R204**, on the other hand, all configurations are reachable, making **R204** a trivially *reversible* rule. While a complete characterization of unreachable states for additive rules will be given in chapter 5, we mention here that the fraction of unreachable configurations for irreversible rules *tends to zero* at a rate λ^N , where $\lambda \approx 0.88$ for nonadditive rules.

Cyclic States: which are configurations that appear in cycles and are repeatedly visited over the course of the evolution; they are the *attractor* states of the system in the sense that they comprise the set toward which all evolutions ultimately lead. If *all* states are cyclic then the system is globally reversible.

Transient States: which can arise only in the first $t_T < 2^N$ time steps of an evolution. Since transient states do not lie on cycles, once a transient state is reached from a given initial state, it cannot be revisited later.

Figures 3.20, 3.21 and 3.22 show how the number of cyclic states (N_C), the average cycle length (C_{rmave}) and total fraction of states on cycles (f_C) changes as

a function of lattice size 'N' for a few representative elementary rules (R32 is in the class c1; R108 is in c2; R122 and R150 are both in c3).

Kaneko [kaneko86a] has, in fact, pointed out that, despite being strictly defined only for infinitely large systems, the four generic behavioral classes appear to be well characterized by the number and length of their attractors on finite lattices:[†]

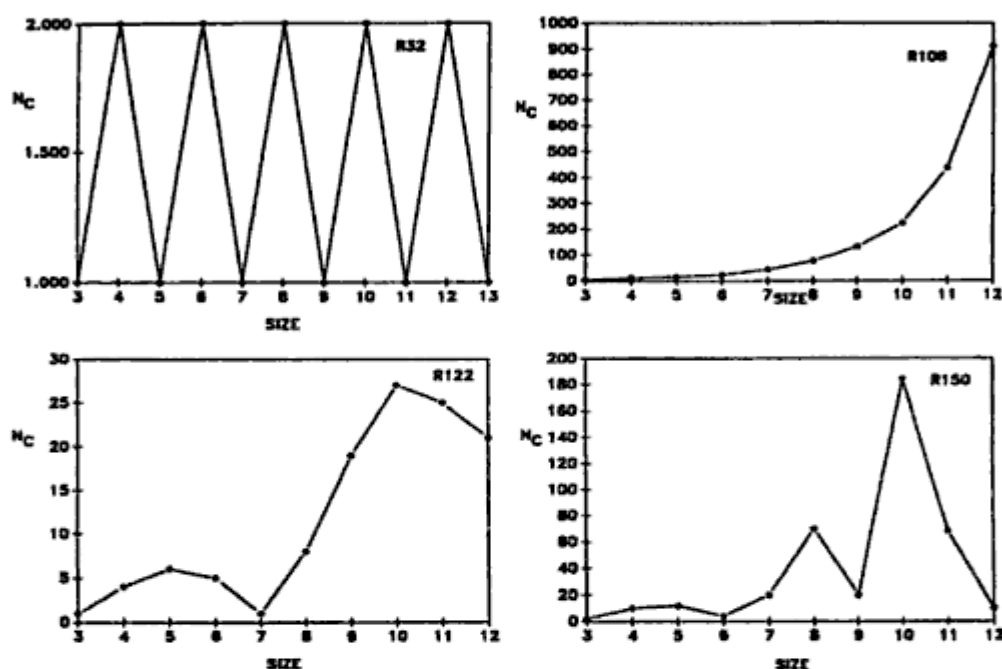


Fig. 3.20 Number of cyclic states as a function of lattice size for a few representative one-dimensional elementary rules; see text.

Class c1: *Small number of attractors with short periods.* The number of attractors typically remains very small ($\approx 1 - 3$), even for large N .

Class c2: *Large number of attractors with short periods.* The number of attractors $N_c \propto \exp(\alpha N)$, $\alpha \approx 0.2 - 0.4$.

Class c3: *Small number of attractors with long periods.* The number of attractors changes irregularly as N increases, and, at least for some rules, appears to depend on some number-theoretic properties of the size and rule. A singular behavior, for example, frequently occurs near $N = 2^k - i$, where $i = 0, 1$ or -1 , depending on the rule.

Class c4: *Large number of attractors with possibly long periods.* Kaneko has found that this class is characterized by an exponentially increasing number of attractors, although the increase is irregular.

[†]A *large number* here means some quantity which is exponential in lattice size ($\mathcal{O}(e^N)$), while a *small number* is anything less than the power of lattice size ($\mathcal{O}(N^a)$); the *period* is large if it is $\mathcal{O}(N)$ and is small if it is bounded by $\mathcal{O}(1)$.

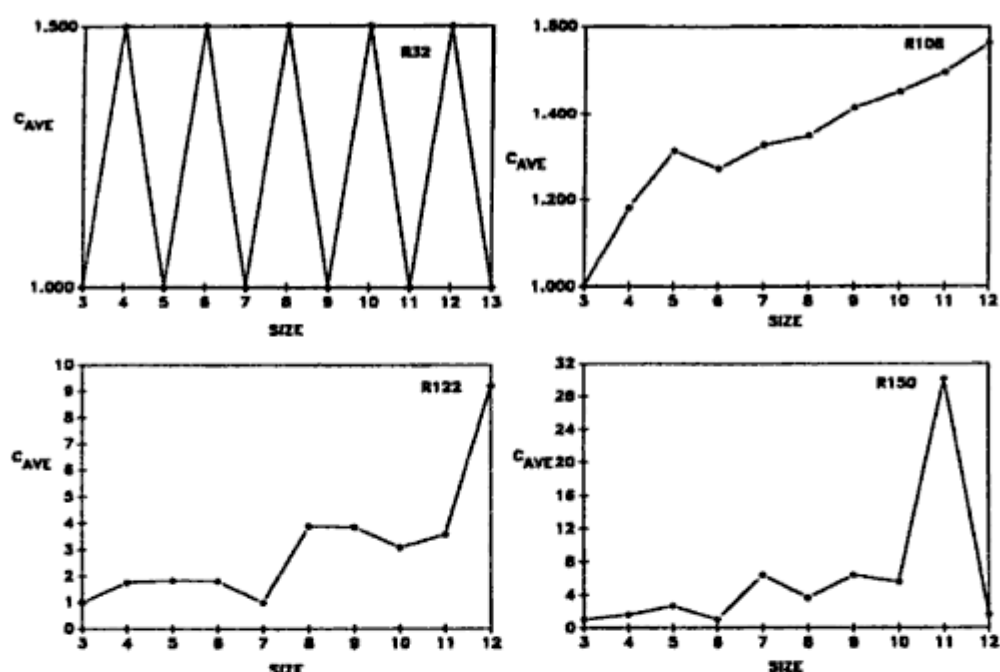


Fig. 3.21 Cycle length as a function of lattice size for a few representative one-dimensional elementary rules; see text.

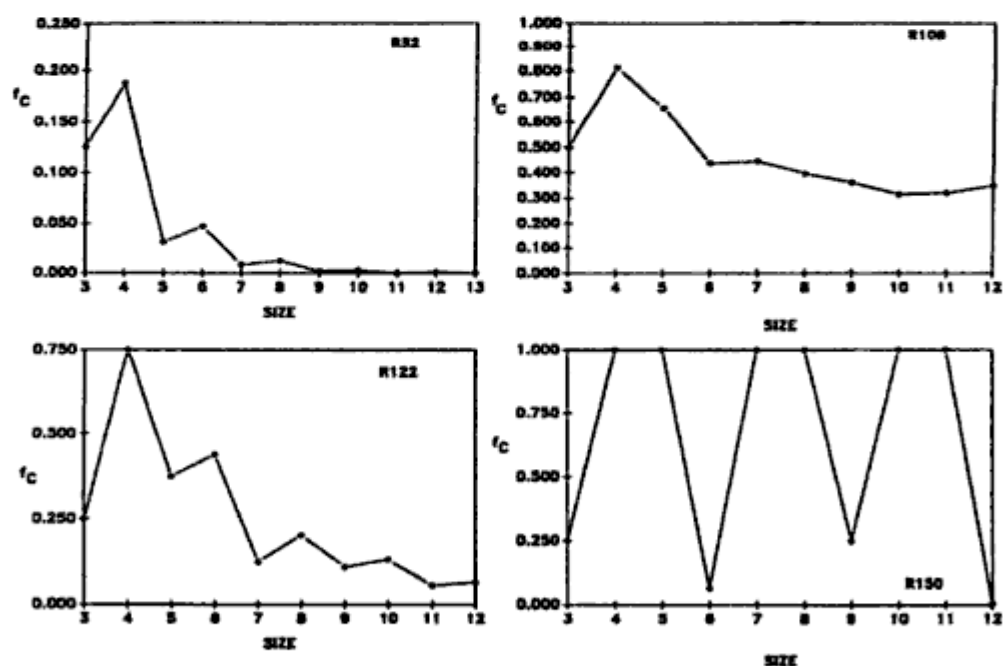


Fig. 3.22 Fraction of states on cycles as a function of lattice size for a few representative one-dimensional elementary rules; see text.

Stability: As was mentioned earlier, an important qualitative characterization of the four behavioral classes is provided by their sensitivity to small changes made to the initial states. A convenient measure for quantifying the difference between evolutions starting from two different binary valued initial states, $\vec{\sigma}^{(1)}$, and $\vec{\sigma}^{(2)}$, is provided by the *Hamming distance*, $H_{\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}}(t)$:

$$H_{\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}}(t) = \sum_{i=1}^N \sigma_i^{(1)}(t) \oplus_2 \sigma_i^{(2)}(t), \quad (3.29)$$

where ' $\oplus_2$ ' is addition *modulo* two.

$H(t)$ thus measures the number of sites at which the two evolutions differ at time ' t '. Since information propagates at a finite speed of r sites per step for a radius- r rule, $H(t)$ is bounded by $H(t) \leq (2rt + 1)$.

Consider two random initial configurations that differ at only one site, so that $H(t=0) = 1$. The *difference plots* shown in figure 3.16 suggest that for class **c1** and **c2** rules, $H(t)$ rapidly approaches some small fixed value. Class **c3** rules, on the other hand, are *unstable* with respect to such small 'perturbations'; $H(t)$ generally grows with time. The rate of growth of $H(t)$ depends on whether the rules are *additive* or *nonadditive*.

For additive rules, which we recall from chapter two are those obeying an additive superposition principle, the difference at time t is equal to the t^{th} step in the evolution of the initial difference. $H(t)$ thus counts the number of 1's appearing in the t^{th} row of the characteristic fractal patterns generated from single seeds (see figure 3.1). For Rule **R90**, for example, it is easy to show that $H(t)$ is given explicitly by $H(t) = 2^{\#_1(t)}$, where $\#_1(t)$ is the number of times the digit '1' appears in the binary representation of the integer ' t '. The average Hamming distance, smoothed out over many iterations, is given approximately by $H(t) = t^{\log_2 3 - 1} \approx t^{0.59}$ [wolf83a] (see figure 3.23).

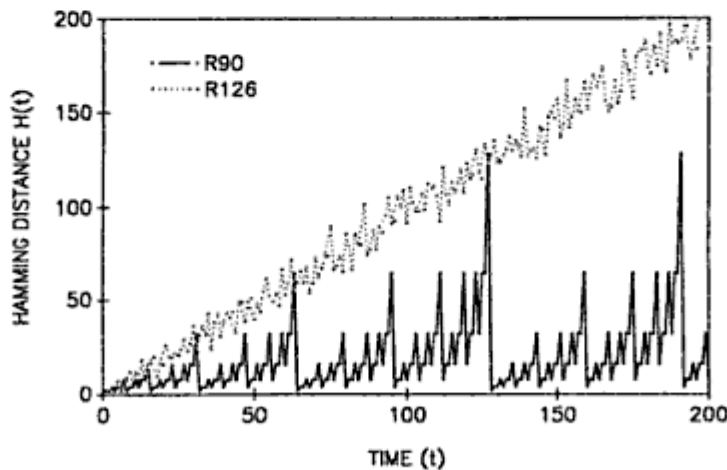


Fig. 3.23 *Hamming distance as a function of time for elementary rule R90; see text.*

For nonadditive rules, $H(t)$ can no longer be obtained by merely looking at the evolution of the initial difference state. A fairly typical nonadditive behavior is that of rule **R126**. We see that, apart from small fluctuations, $H(t)$ tends to steadily increase in a roughly linear fashion. This means that as time increases, the values of particular sites will depend on an ever increasing set of initial sites; *i.e.*, space-time patterns are *sensitively dependent on the initial conditions*. We will pick up this theme in our discussion of *chaos* in continuous systems in chapter 4.

Statistical Ensembles: A statistical ensemble of states can be constructed by assigning the probability for each of the 2^N possible configurations. By an *equiprobable ensemble*, we will mean a (maximally disordered) collection of states such that each configuration appears with equal probability. A self-organizing evolution under a particular rule ϕ modifies the *a-priori* equal probabilities for states of the ensemble to occur.

Figures 3.24 and 3.25, for example, show the probabilities for the 2^{10} possible configurations on an $N = 10$ lattice obtained at time $t = 10$ for evolutions by rules **R126** and **R30** (both in class **c3**), respectively. The figures show that the evolution modifies the probabilities of states from initially being equally likely to distributions in which individual configurations can have widely differing final probabilities. The properties of the more probable states will then tend to dominate the statistical averages over the ensemble.

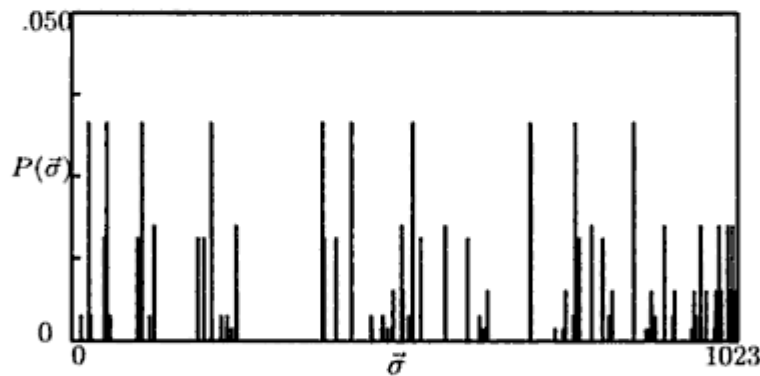


Fig. 3.24 Global configuration probabilities at $t=10$ computed for rule **R126**. The probability for the zero state, $P(\vec{\sigma} = \vec{0}) = .121$, is not shown.

Entropy: Much of the more technical discussion of the dynamical systems approach to CA in chapter 4 will depend on the notions of *information* and *entropy*. We here provide the groundwork for our later analysis by introducing the following two elementary measures:

$$\left\{ \begin{array}{ll} \text{Global Set Entropy:} & S_{\text{set}}(t) = \frac{1}{N} \log_2 \left(\sum_{j=1}^{2^N} \zeta(p_j^t) \right), \\ \text{Global Measure Entropy:} & S_{\text{meas}}(t) = -\frac{1}{N} \sum_{i=1}^{2^N} p_i^t \log_2 p_i^t, \end{array} \right. \quad (3.30)$$

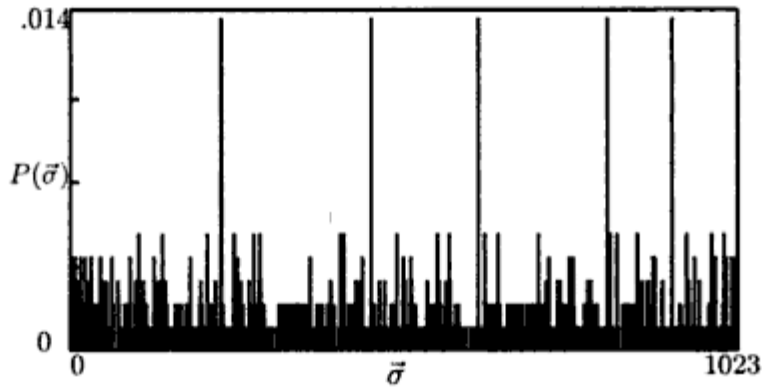


Fig. 3.25 Global configuration probabilities at $t=10$ computed for rule **R30**.

where p_i^t is the probability of the i^{th} state at iteration step ' t ' and $\zeta(p_j) = 1$ for $p_j > 0$ and $\zeta(0) = 0$.

Both measures obviously are related to certain global properties of the state transition graph. $S_{\text{set}}(t)$, for example, is determined by the fraction of possible configurations that can be reached at time ' t ' during the evolution. At large times, $S_{\text{set}}(t \rightarrow \infty)$ is therefore given by the fraction of states that are cyclic. $S_{\text{meas}}(t)$, on the other hand, is a *finer* entropic measure in that it makes use of the individual probabilities of states. Indeed, $S_{\text{meas}}(t)$ can be interpreted as being the *average number of binary bits that are necessary to completely specify a state in a statistical ensemble of all possible states*.

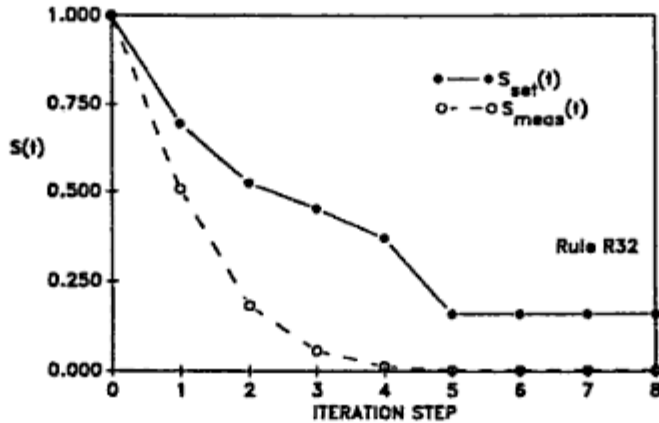


Fig. 3.26 Time evolution of the average entropy for elementary rule **R32**; see text.

The two measures satisfy the relation

$$0 \leq S_{\text{meas}}(t) \leq S_{\text{set}}(t) \leq 1. \quad (3.31)$$

Since entropy is maximum when the system is maximally disordered, $S_{\text{meas}}(t)$ takes its maximal value of *one binary bit per site* for an equiprobable ensemble: $S_{\text{set}}(t \rightarrow \infty) = 1$ only if all states are cyclic. If the system settles onto a unique cyclic

state (which must be the *null* state if the rule is legal), then $S_{\text{meas}}(t \rightarrow \infty) = 0$. $S_{\text{meas}}(t) = S_{\text{set}}(t)$ if and only if all nonzero state probabilities p_j^t are equal.

For reversible systems, evolution almost always leads to an increase in entropy. The evolution of irreversible systems, on the other hand, typically results in a decrease in entropy. Figures 3.26 and 3.27 show the time evolution of the average entropy for elementary rules **R32** (class **c1**) and **R122** (class **c3**) for an ensemble of size $N = 10$ CA starting with an equiprobable ensemble. We see that the entropy decreases with time in both cases, reaching a steady-state value after a transient period. This decrease is a direct reflection of the irreversibility of the given rules.

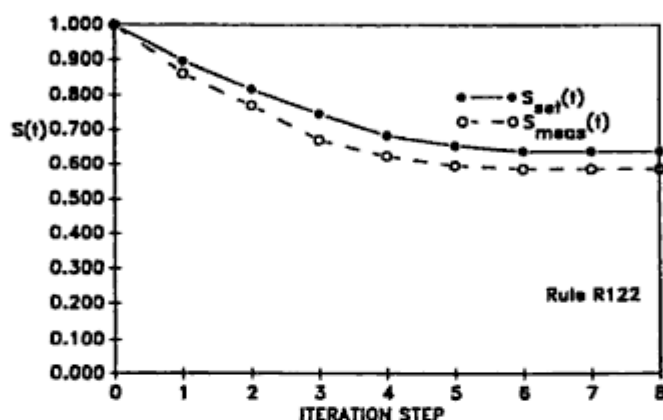


Fig. 3.27 Time evolution of the average entropy for elementary rule **R122**; see text.

Infinite Lattices: Although cyclic behavior is certain to occur under even class **c3** rules for finite systems, it is a rare occurrence for truly infinite systems: *cycles occur only with exceptional initial conditions*. For a finite sized initial seed, for example, the pattern either quickly dies or grows progressively larger with time. Most infinite seeds lead only to complex acyclic patterns. Under the special condition that the initial state is periodic with period ' m ', however, the evolution of the infinite system will be the same as that of the finite CA of size $N = m$; in this case, cycles of length $\ll 2^N$ can occur.

Similarly, if the initial state consists of nothing but infinite repetitions of some invariant block of values, the space-time pattern will again be periodic. Figure 3.28, for example, shows sections of two infinite periodic patterns for elementary class rule **R30**, starting from the states ' $\dots 0101\dots$ ' and ' $\dots 00100110010011\dots$ '.

3.1.4 A Small Sampling of Rules

Perhaps the most conceptually far-reaching lesson to be learned from nonlinear dynamical system theory in general, and the dynamics of CA in particular, is that *complex behavior need not have a complex dynamical origin*. Indeed, one of the principle motivations for studying such deceptively 'simple' systems, is to use their underlying simplicity to gain insight into more general nonlinear phenomena. We have already seen considerable phenomenological evidence that – despite arguably