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From Newton to Cellular Automata

Franco Bagnoli
Dept. Energy and CSDC
University of Florence
Florence, Italy
and INFN, sec. Firenze
franco.bagnoli@unifi.it

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Abstract

I outline a possible logical path from the formulation of physics of classical mechanics to "abstract" systems like cellular automata. The goal of this article is that of illustrating why physicists often study extremely simplified models, instead of just numerically integrating the fundamental equations of physics. This exposition is obviously only partial and based on my expertise and my interests.

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1 Introduction

Physics investigation is based on building models of reality: in order for a phenomenon to be *understood*, we need to represent it in our minds using a limited amount of symbols. However, it is a common experience that, even using simple "building blocks" one usually obtains systems whose behavior is quite complex. In this case one needs to develop new languages and new *phenomenological* models in order to manage this "complexity".

Computers have changed the way a physical model is studied. Computers may be used to *calculate* the properties of a very complicated model representing a real system, or to investigate *experimentally* what are the essential ingredients of a complex phenomenon. In order to carry out these explorations, several basic models have been developed, which are now used as building blocks for performing simulations and designing algorithms in many fields, from chemistry to engineering, from natural sciences to psychology. Rather than being derived from some fundamental law of physics, these blocks constitute *artificial worlds* still to be completely explored.

In this article we shall first present a pathway from Newton's laws to cellular automata and agent-based simulations, showing (some) computational approaches in classical physics. Then, we shall present some examples of *artificial worlds* in physics.

2 Physics and computers

Some sixty years ago, shortly after the end of Second World War, computers become available to scientists. Computers were used during the last years of the war for performing computations about the atomic bomb [1, 2].

Up to then, the only available tool, except experiments, was paper and pencil. Starting with Newton and Leibnitz, humans discovered that continuous mathematics (*i.e.*, differential and integral calculus) allowed to derive many consequences of the a given hypothesis just by the manipulation of symbols. It seemed natural to express all quantities (*e.g.*, time, space, mass) as continuous variables. Notice however that the idea of a continuous number is not at all "natural": one has to learn how to deal with it, while (small) integer numbers can be used and manipulated (added, subtracted) by illiterate humans and also by many animals. A point which is worth to be stressed is that any computation refers to a model of certain aspects of reality, considered most important, while others are assumed to be not important

Unfortunately most of human-accessible explorations in physics are limited to almost-linear systems, or systems whose effective number of variables is quite small. On the other hand, most of naturally occurring phenomena can be "successfully" modeled only using nonlinear elements. Therefore, most of pre-computer physics is essentially linear physics, although astronomers (like other scientists) used to integrate numerically, by hand, the non-linear equations of gravitation, in order to compute the trajectories of planets. This computation, however, was so cumbersome that no "playing" with trajectories was possible.

While analog computers have been used for integrating differential equations, the much more flexible digital computers are deterministic discrete systems. The way of working of a (serial) computer is that of a very fast automaton, that manipulates data following a program.

In order to use computers as fast calculators, scientists ported and adapted existing numerical algorithms, and developed new ones. This implied the development of techniques able to *approximate* the computations of continuous mathematics using computer algebra. However, numbers in computers are not exactly the same as human numbers, in particular they have finite (and varying) precision.

This intrinsic precision limit has deep consequences in the simulations of nonlinear systems, in particular of chaotic ones. Indeed, chaos was "numerically discovered" by Lorenz [3] after the observation that a simple approximation, a number that was retyped with fewer decimals, caused a macroscopic change in the trajectory under study.

With all their limits, computers can be fruitfully used *just* to speed-up computations that *could* eventually be performed by humans. However, since the increase in velocity is of several order of magnitude, it becomes possible to include more and more details into the basic model of the phenomenon under investigation, well beyond what would be possible with an army of "human computers". The idea of exploiting the *brute power* of fast computers has originated a fruitful line of investigation in *numerical physics* especially in the field of chemistry, biological molecules, structure of matter. The power of computers has allowed for instance to include quantum mechanical effects in the computation of the structure of biomolecules [4], and although these techniques may be targeted as "brute force", the algorithms developed are actually quite sophisticated.

However, a completely different usage of computers is possible: instead of exploiting them for performing computations on models that already proved to approximate the reality, one can use computers as "experimental" apparatus to investigate the patterns of *theoretical* models, generally non-linear. This is what Lorenz did after having found the first examample of chaos in computational physics. He started simplifying his equations in order to enucleate the minimal ingredients of what would be called the *butterfly effect*.

Much earlier than Lorenz, Fermi, Pasta and Ulam (and the programmer Tsingou [5]) used one on the very first available computers to investigate the basis of statistical mechanics: how energy distributes among the oscillation modes of a chain of nonlinear oscillators [6].

Also in this case the model is simplified at its maximum, in order to put into evidence what are the fundamental ingredients of the observed pattern, and also to use all the available power of computers to increase the precision, the duration and the size of the simulation.

This simplification is even more fruitful in the study of systems with many degrees of freedom, that we may denote generically as *extended systems*. We humans are not prepared to manipulate more that a few symbols at once. So, unless there is a way of grouping together many parts (using averages, like for instance when considering the pressure of a gas as an average over extremely many particle collisions), we are in difficulties in *understanding* such systems. They may nevertheless be studied performing "experiments" on computers. Again, the idea is that of simplifying at most the original model, in order to isolate the fundamental ingredients of the observed behavior. It is therefore natural to explore systems whose *physics* is different from the usual one. These *artificial worlds* are preferably formulated in discrete terms, more suitable to be implemented in computers (see Sect. 4).

This line of investigation is of growing interest today: since modern computers can easily simulate thousands or millions of *elementary automata* (often called *agents*), it may be possible to design *artificial worlds* in which *artificial people* behave similarly to real humans. The rules of these worlds are not obtained from the "basic laws" of the real one, since no computer can at present simulate the behavior of all the elements of even a small portion of matter. These rules are designed so to behave similarly to the system under investigation, and to be easily implemented in digital terms. There are two main motivations (or hopes): to be able to understand real complex dynamics by studying simplified models, and to be so lucky to discove r that a finely-tuned model is able to reproduce (or forecast) the behavior of its real counterpart.

This is so promising that many scientists are performing experiments on these artificial world, in order to extract their principal characteristics, to be subsequently analyzed possibly using paper and pencil!

In the following we shall try to elucidate some aspects of the interplay between computer and physics. In Sect. 3, we shall illustrate possible logic pathways (in classical mechanics) leading from Newton's equations to research fields that use computers as investigative tool. In Sect. 4, we shall try to present succinctly some example of "artificial worlds" that are still active research topics in theoretical physics.

3 From Trajectories to Statistics and Back

Let us assume that a working model of the reality can be built using a set of dynamical equations, for instance those of classical mechanics. We shall consider the model of a system formed by many particles, like a solid or a fluid. The state of the resulting system can be represented as a point in a high-dimensional space, since it is given by all coordinates and velocities of all particles. The evolution of the system is a trajectory in such space. Clearly, the visualization and the investigation of such a problem is challenging, even using powerful computers.

Moreover, even if we are able to compute one or many trajectories (in order to have an idea of fluctuations), this does not imply that we have *understood* the problem. Let us consider for instance the meteorology: one is interested in the probability of rain, or in the expected wind velocity, not in forecasting the trajectories of all molecules of air. Similarly in psychology, one is interested in the expected behavior of an individual, not in computing the activity of all neurons in his brain.

Since physics is the oldest discipline that has been "quantified" into equations, it may be illuminating to follow some of the paths followed by researchers to "reduce" the complexity of a high-dimensional problem to something more manageable, or at least simpler to be simulated on a computer.

In particular, we shall see that many approaches consist in "projecting" the original space onto a limited number of dimensions, corresponding to the observables that vary in a slow and smooth way, and assuming that the rest of the dynamics is approximated by "noise"[1]. Since the resulting system is stochastic, one is interested in computing the average values of observables, over the probability distribution of the projected system.

However, the computation of the probability distribution may be hard, and so one seeks to find a way of producing "artificial" trajectories, in the projected space, designed in such a way that their probability distribution is the desired one. So doing, the problem reduces to the computation of the time-averaged values of "slow" observables. For the rest of this section, please make reference to Figure 1

Newton laws. The success of Newton in describing the motion of one body, subjected to a static field force (say: gravitational motion of one planet, oscillation of a body attached to a spring, motion of the pendulum, etc.) clearly proved the validity of his approach, and also the validity of using simple models for dealing with natural phenomena. Indeed, the representation of a body as a point mass, the idea of massless springs and strings, the concept of force fields are all mathematical idealizations of reality.

The natural generalization of this approach is carried out in the XVIII century by Lagrange, Hamilton and many others. It brings to the mathematisation of mechanics and the derivation of *rational mechanics*. The resulting "standard" (or historical) way of modeling physical systems is that of using differential equations, *i.e.*, a continuous description of time, space and other dynamical quantities.

From an abstract point of view, one is faced with two different options: either concentrate on systems described by a few equations (low-dimensional systems), or try to describe systems formed by many components.

Low dimensionality. Historically, the most important problem of Newton's times was that of three bodies interacting via gravitational attraction (the Sun, the Earth and the Moon). By approximating planets with point

[1] The noise can be so small, compared to the macroscopic observables that it can be neglected. In such cases, one has a deterministic, low-dimensional dynamical system, like for instance the usual models for rigid bodies, planets, etc.

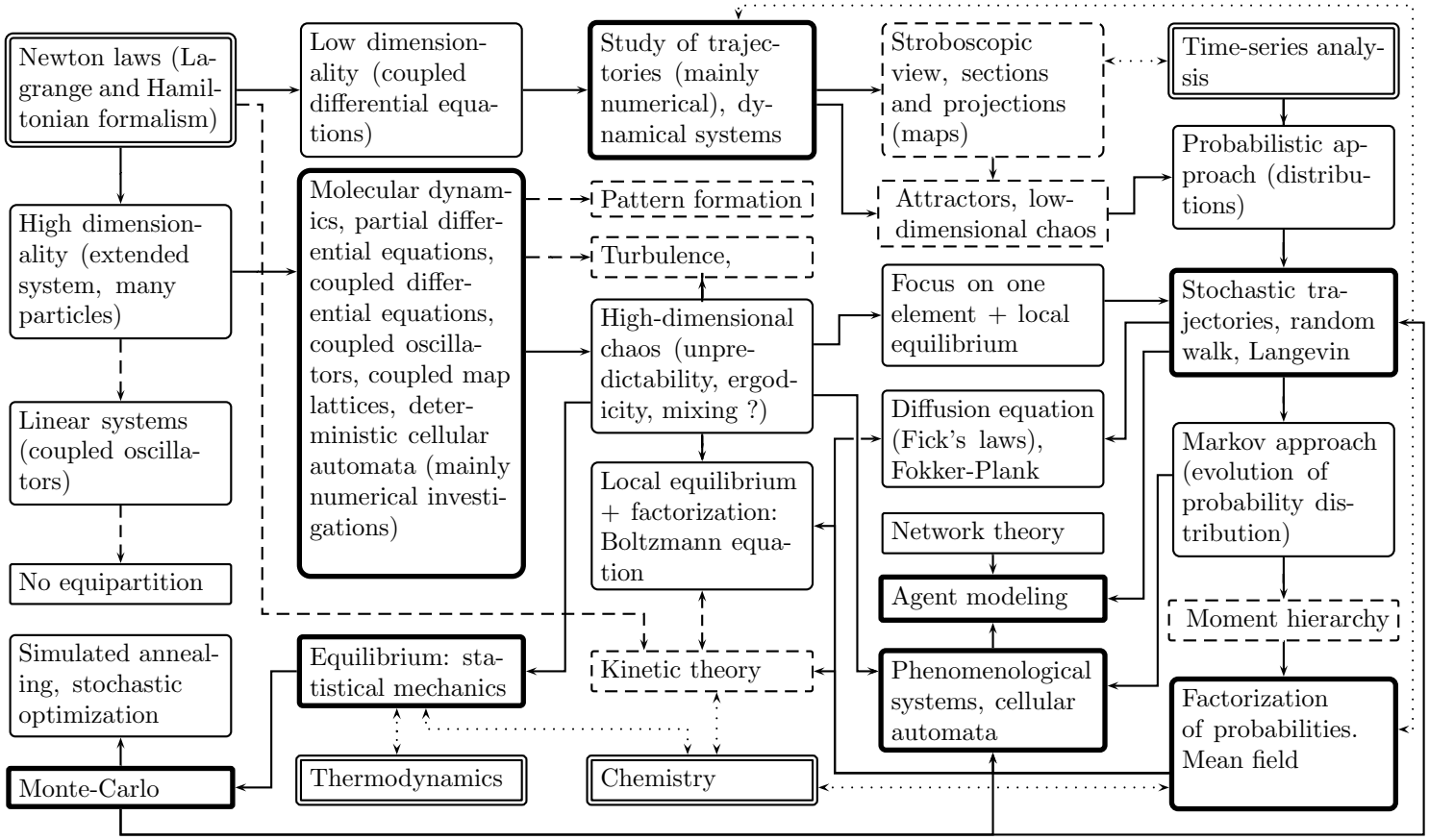

Figure 1: Graphical illustration of the logic path followed in this introduction. Boxes with double frame are "starting points", dashed boxes are topic that are not covered by discussion, boxes with darker frames mark topics that are investigated more in details.

masses, one gets a small number of coupled differential equations. This reduction of dimensionality is an example of a "scale separation": the variables that describe the motion of the planets vary slowly and smoothly in time. Other variables, for instance those that describe the oscillations of a molecule on the surface of a planet, can be approximated by a noise term so small that can be safely neglected. This approximation can also be seen as a "mean field" approach, for which one assumes that variables behave not too differently from their average. Using these techniques, one can develop models of many systems that result in the same mathematical scheme: a few coupled equations. The resulting equations may clearly have a structure quite different from that resulting from Newtonian dynamics (technically, Hamiltonian systems).

However, the reduction of the number of variables does not guarantee the simplicity of the resulting model. The problem of three gravitational bodies cannot be split into smaller pieces, and the computation of an accurate trajectory requires a computer. In general, a *nonlinear* system in a space with three or more dimensions is chaotic. This implies that there it may "react" to a small perturbation of parameters or initial conditions with large variations of its trajectory. This *sensibility* to variation implies the impossibility of predicting its behavior for long times, unless one is content with a probabilistic description.

High dimensionality. In many cases, the "projection" operation results in a system still composed by many parts. For instance, models of nonequilibrium fluids neglect to consider the movement of the individual molecules, but still one has to deal with the values of the pressure, density and velocity in all points. In these cases one is left with a high-dimensional problem. Assuming that the "noise" of the projected dimensions can be neglected, one can either write down a large number of coupled equation (*e.g.*, in modeling the vibration of a crystal), or use a continuous approach and describe the system using partial differential equations (*e.g.*, the model of a fluid).

Linear systems. In general, high and low-dimensional approaches can be systematically developed (with paper and pencil) only in the linear approximation. Let us illustrate this point for the case of coupled differential equation: if the system is linear one can write the equations using matrices and vectors. One can in principle find a (linear) transformation of variables that make the system diagonal, *i.e.*, that reduces the problem to a set of *uncoupled* equations. At this point, one is left with (many) one-dimensional independent problems. Clearly, there are mathematical difficulties, but the path is clear. A similar approach (for instance using Fourier transforms) can be used also for dealing with partial differential equations.

The variables that result from such operations are called normal modes, because they behave independently one from the other (*i.e.*, they correspond to orthogonal or normal directions in the state space). For instance, the linear model of a vibrating string (with fixed ends) predicts that any pattern can be described as a superposition of "modes", which are the standing oscillations with zero, one, two, ... nodes (the harmonics).

However, linear systems behave in a somewhat strange way, from the point of view of thermal physics. Let us consider for instance the system composed by two *uncoupled* oscillators. It is clear that if we excite one oscillator with any amount of energy, it will remain confined to that subsystem. With normal modes, the effect is the same: any amount of energy communicated to a normal mode remains confined to that mode, if the system is completely linear. In other words, the system never forgets its initial condition.

On the contrary, the long-time behavior of "normal" systems does not depend strongly on the initial conditions. One example is the *timbre*, or "sound color" of an object. It is given by the simultaneous oscillations on many frequencies, but in general an object emits its "characteristic" sound regardless of how exactly is perturbed. This would not be true for linear systems.

Since the *distribution* of energy to all available "modes" is one of the assumptions of equilibrium statistical mechanics, which allows us to "understand" the usual behavior of matter, we arrived at an unpleasant situation: linear systems, which are so "easy" to be studied, cannot be used to ground statistical physics on mechanics.

Molecular dynamics. Nowadays, we have computers at our disposal, and therefore we can simulate systems composed by many parts with complex interactions. One is generally interested in computing *macroscopic* quantities. These are defined as *averages* of some function of the microscopic variables (positions, velocities, accelerations, etc.) of the system. A measurement on a system implies an average, over a finite interval of time and over a large number of elementary components (say: atoms, molecules, etc.) of some quantity that depends on the microscopic state of that portion of the body.

Chaos and probabilities. It was realized by Poincaré (with paper and pencil) and Lorenz (with one of the very first computers) that also very few (three) coupled differential equations with nonlinear interactions may give origin to complex (chaotic) behavior. In a chaotic system, a small uncertainty amplifies exponentially in time,

making forecasting difficult. However, chaos may also be simple: the equations describing the trajectory of dice are almost surely chaotic, but in this case the chaos is so strong that the tiniest perturbation or uncertainty in the initial conditions will cause in a very small amount of time a complete variation of the trajectory. Our experience says that the process is well approximated by a probabilistic description. Therefore, chaos is one possible way of introducing probability in dynamics.

Chaotic behavior may be obtained in simpler models, called maps, that evolve in discrete time steps. As May showed [7], a simple map with a quadratic non-linearity (logistic map) may be chaotic. One can also model a system using coupled maps instead of a system of coupled differential equations [8]. And indeed, when a continuous system is simulated on a computer, it is always represented as an array of coupled maps.

Discretization. There is a progression of discretization from partial differential equations, coupled differential equations, coupled map lattices: from systems that are continuous in space, time and in the dynamical variables to systems that are discrete in time and space, and continuous only in the dynamical variables. The further logic step is that of studying completely discrete systems, called *cellular automata*.

Cellular automata show a wide variety of different phenomenologies. They can be considered mathematical tools, or used to model reality. In many cases, the resulting phenomenological models follows probabilistic rules, but it is also possible to use cellular automata as "building blocks". For instance, is possible to simulate the behavior of a hydrodynamical system by means of a completely discrete model, called cellular automata lattice gas (see Sect. 4.2).

Statistics. The investigation of chaotic extended systems proceed generally using a statistical approach. The idea is the following: any system contains a certain degree of non-linearity, that couples otherwise independent normal modes. Therefore, (one hopes that) the initial condition is not too important for the asymptotic regime. If moreover one assumes that the motion is so chaotic that any trajectory spans the available space in a "characteristic" way (again, not depending on the initial conditions), we can use statistics to derive the "characteristic" probability distribution: the probability of finding the system in a given portion of the available space is proportional to the the time that the system spends in that region. See also the paragraph on equilibrium.

Random walks. Another approach is that of focusing on a small part of a system, for instance a single particle. The rest of the system is approximated by "noise". This method was applied, for instance, by Einstein in the development of the simplest theory of Brownian motion, the random walk [9]. In random walks, each steps of the target particle is independent on previous steps, due to collisions with the rest of particles. Collisions, moreover, are supposed to be uncorrelated. A more sophisticated approximation consists in keeping some aspects of motion, for instance the influence of inertia or of external forces, still approximating the rest of the world by noise (which may contain a certain degree of correlation). This is known as the Langevin approach, which includes the random walk as the simplest case. Langevin equations are stochastic differential equations.

The essence of this method relies in the assumption that the behavior of the various parts of the systems is uncorrelated. This assumption is vital also for other types of approximations, that will be illustrated in the following. Notice that in the statistical mechanics approach, this assumption is not required.

In the Langevin formulation, by averaging over many "independent" realizations of the process (which in general is not the same of averaging over many particles that "simultaneously" move, due for instance to excluded volumes) one obtains the evolution equation of the probability of finding a particle in a given portion of space. This is the Kolmogorov integro-differential equation, that in many case can be simplified, giving a differential (Fokker-Plank) equation. The diffusion equation is just the simplest case [10, 11].

It is worth noticing that a similar formulation may be developed for quantum systems: the Feynman path-integral approach is essentially a Langevin formulation, and the Schroedinger equation is the corresponding Fokker-Plank equation.

Random walks and stochastic differential equations find many application in economics, mainly in market simulations. In this cases, one is not interested in the average behavior of the market, but rather in computing non-linear quantities over trajectories (time-series of good values, fluctuations, etc.).

Time-series data analyses. In practice, a model is never derived "ab initio", by projecting the dynamics of all the microscopic components onto a limited number of dimensions, but is constructed heuristically from observations of the behavior of a real system.

It is therefore crucial to investigate how observations are made, *i.e.*, the analysis of a series of a time measurements. In particular, a good exercise is that of simulating a dynamical or stochastic system, analyze the resulting

time-series data of a given observable, and see if one is able to reconstruct from it the relationships or the equations ruling the time evolution.

Let us consider the experimental study of a chaotic, low-dimensional system. The measurements on this system give a time series of values, that we assume discrete (which is actually the case considering experimental errors). Therefore, the output of our experiment is a series of symbols or numbers, a time-series. Let us assume that the system is stationary, *i.e.*, that the sequence is statistically homogeneous in time. If the system is not extremely chaotic, symbols in the sequence are correlated, and one can derive the probability of observing single symbols, couples of symbols, triples of symbols and so on. There is a hierarchy in these probabilities, since the knowledge of the distribution of triples allows the computation of the distribution of couples, and so on.

It can be shown that the knowledge of the probability distribution of the infinite sequence is equivalent to the complete knowledge of the dynamics. However, this would correspond to performing an infinite number of experiments, for all possible initial conditions.

The usual investigation scheme assumes that correlations vanishes beyond a certain distances, which is equivalent to assume that the probability of observing sequences longer than that distance factorize. Therefore, one tries to model the evolution of the system by a probabilistic dynamics of symbols Sect. 4.3. Time-series data analysis can therefore be considered as the main experimental motivation in developing probabilistic discrete models. This can be done heuristically comparing results with observations *a posteriori*, or trying to extract the rules directly from data, like in the Markov approach.

Markov approximation. The Markov approach, either continuous or discrete, also assumes that the memory of the system vanishes after a certain time interval, *i.e.*, that the correlations in time series decay exponentially. In discrete terms, one tries to describe the process under study as an automata, with given transition probabilities. The main problem is: given a sequence of symbols, which is the simplest automata (hidden Markov chains [12]) that can generate that sequence with maximum "predictability", *i.e.*, with transition probabilities that are nearest to zero or one? Again, it is possible to derive a completely deterministic automata, but in general it has a number of nodes equivalent to the length of the time-series, so it is not generalizable and has no predictability. On the contrary, an automata with a very small number of nodes will have typically intermediate transition probabilities, so predictability is again low (essentially equivalent to random extraction). Therefore, the good model is the result of an optimization problem, that can be studied using, for instance, Monte-Carlo techniques.

Mean-field. Finally, from the probabilities one can compute averages of observables, fluctuations and other quantities called "moments" of the distribution. Actually, the knowledge of all moments is equivalent to the knowledge of the whole distribution. Therefore, another approach is that of relating moments at different times or different locations, truncating the recurrences at a certain level. The roughest approximation is that of truncating the relations at the level of averages, which is the mean field approach. It appears so natural that is is often used without realizing the implications of the approximations. For instances, chemical equations are essentially mean-field approximations of a complex phenomena.

Boltzmann equation. Another similar approach is that of dividing an extended system into zones, and assume that the behavior of the system in each zone is well described by a probability distribution. By disregarding correlations with other zones, one obtains the Boltzmann equation, with which many transport phenomena may be studied well beyond elementary kinetic theory. The Boltzmann equation can also be obtained from the truncation of a hierarchy of equations (BBGKY hierarchy) relating multi-particle probability distributions. Therefore, the Boltzmann equations is similar in spirit to a mean-field analysis.

Equilibrium. One of the biggest success of the stochastic approach is of course *equilibrium statistical mechanics*. The main ingredient of this approach is that of minimum information, which, in other words, corresponds to the assumption: *what is not known is not harmful*. By supposing that in equilibrium the probability distribution of the systems maximizes the information entropy (corresponding to a minimum of information on the system) one is capable of deriving the probability distribution itself and therefore the expected values of observables (ensemble averages, see Sect. 4.1). In this way, using an explicit model, one is capable to compute the value of the parameters that appear in thermodynamics. If it were possible to show that the maximum entropy state is actually the state originated by the dynamics of a mechanical (or quantum) system, one could ground thermodynamics on mechanics. This is a long-investigated subject, dating back to Boltzmann, which is however not yet clarified. The main drawback in the derivations is about ergodicity. Roughly speaking, a system is called *ergodic* if the infinite-time average of an observable over a trajectory coincides with its average over a snapshot of infinitely many replicas. For a

system with fixed energy and no other conserved quantities, a sufficient condition is that a generic trajectory passes "near" all points of the accessible phase-space. However, most systems whose behavior is "experimentally" well approximated by statistical mechanics are not ergodic. Moreover, another ingredient, the capability of *forgetting* quickly the information about initial conditions appears to be required, otherwise trajectories are strongly correlated and averages over diferent trajectories cannot be "mixed" together. This capability is strongly connected to the chaoticity or *unpredictability* of extended systems, but unfortunately these ingredients makes analytic approaches quite hard.

An alternative approach, due to Jaynes [13], is much more pragmatic. In essence, it says: let design a model with the ingredients that one thinks are important, and assume that all what is not in the model does not affect its statistical properties. Compute the distribution that maximizes the entropy with the given constraints. Then, compare the results (averages of observables) with experiments (possibly, numerical ones). If they agree, one has captured the essence of the problem, otherwise one have to include some other ingredient and repeat the procedure. Clearly, this approach is much more general than the "dynamical" one, not considering trajectory or making assumptions about the energy, which is simply seen as a constraint. But physicists would be much more satisfied by a "microscopic" derivation of statistical physics.

In spite of this lack of strong basis, the statistical mechanics approach is quite powerful, especially for systems that can be reduced to the case of *almost* independent elements. In this situation, the system (the *partition function*) factorizes, and many computations may be performed by hand. Notice however that this behavior is in strong contrast to that of truly linear systems: the "almost" attribute indicates that actually the elements interact, and therefore share the same "temperature".

Monte-Carlo. The Monte-Carlo technique was invented for computing, with the aid of a computer, thermal averages of observables of physical systems at equilibrium. Since then, this term is often used to denote the technique of computing the average values of observables of a stochastic system by computing the time-average values over "artificial" trajectories.

In equilibrium statistical physics, one is faced by the problem of computing averages of observables over the probability distribution of the system, and since the phase space is very high-dimensional, this is in general not an easy task: one cannot simply draw *random* configurations, because in general they are so different from those "typical" of the given value of the temperature, that their statistical weight is marginal. And one does not want to revert to the original, still-more-highly-dimensional dynamical system, which typically requires powerful computers just to be followed for tiny time intervals.

First of all, one can divide (*separate*) the model into almost independent subsystems, that, due to the small residual interactions (the "almost" independency), are at the same temperature. In the typical example of a gas, the velocity components appear into the formula of energy as additive terms, *i.e.*, they do not interact with themselves or with other variables. Therefore, they can be studied separately giving the *Maxwell distribution* of velocities. The positions of molecules, however, are linked by the potential energy (except in the case of an ideal gas), and so the hard part of the computation is that of generating configurations. Secondly, statistical mechanics guarantees that the asymptotic probability distribution does not depend on the details of dynamics. Therefore, one is free to look for the fastest dynamics still compatible with constraints. The Monte-Carlo computation is just a set of recipes for generating such trajectories. In many problems, this approach allows to reduce the (computational) complexity of the problem of several orders of magnitude, allowing to generate "artificial" trajectories that span statistically significant configuration with small computational effort. In parallel with the generation of the trajectory, one can compute the value of several observables, and perform statistical analysis on them, in particular the computation of time averages and fluctuations.

By extension, the same terms "Monte-Carlo" is used for the technique of generating sequences of states (trajectories) given the transition probabilities, and computing averages of observables on trajectories, instead of on the probability distribution.

One of the most interesting applications of Monte-Carlo simulations concerns stochastic optimization via *simulated annealing*. The idea is that of making an analogy between the status of a system (and its energy) and the coding of a particular procedure (with corresponding cost function). The goal is that of finding the best solution, *i.e.*, the global minimum of the energy. "Easy" system have a smooth energy landscape, funnel shaped, so that usual techniques like gradient descent are successful. However, when the energy landscape is corrugated, there are many local minima where local algorithms tend to be trapped. Methods from statistical mechanics (Monte-Carlo), on the contrary, are targeted to generate trajectories with short correlations, in order to allow the system to quickly explore all available space. By lowering the "temperature", the probability distribution of system obeying statistical mechanics concentrate around minima of energy, and a good Monte-Carlo trajectory should do the same. Therefore,

a sufficiently slow annealing should furnish the desired global minimum.

Critical phenomena. One of the most investigated topics of statistical mechanics concerns phase transitions. This is a fascinating subject: in the vicinity of a continuous phase transitions correlation lengths diverge, and the system behave collectively, in a way which is largely independent of the details of the model. This universal behavior allows the use of extremely simplified models, that therefore can be massively simulated.

The *philosophy* of statistical mechanics may be *exported* to nonequilibrium systems: systems with absorbing states (that correspond to infinitely negative energy), driven systems (live living ones), strongly frustrated systems (that actually never reach equilibrium), etc. In general, one defines these systems in terms of transition probabilities, not in term of energy. Therefore, one cannot invoke a maximum energy principles, and the results are less general. The study is generally performed by a mix of analytic approaches, from Markov chains to stochastic differential equations to *ad-hoc* techniques (conformal invariance, damage spreading, replicas, synchrony etc.).

However, many system exhibit behavior reminiscent of equilibrium systems, and the same language can be used: phase transitions, correlations, susceptibilities,...These characteristics, common to many different models, are sometimes referred as emergent features.

One of the most famous problems in this field is percolation: the formations of giant clusters in systems described by a local stochastic aggregation dynamics. This "basic" model has been used to describe an incredibly large range of phenomena [14].

Equilibrium and nonequilibrium phase transitions occur for a well-defined value of a control parameter. However, in nature one often observes phenomena whose characteristic resemble that of a system near a phase transition, a critical dynamics, without any *fine-tuned* parameter. For such system the term self-organized criticality has been coined [15], and they are subject of active researches.

Networks. A recent "extension" of statistical physics is the theory of networks. Networks in physics are often regular, like the contacts in a crystal, or only slightly randomized. Characteristics of these networks are the fixed (or slightly dispersed around the mean) number of connections per node, the high probability of having connected neighbors (number of "triangles"), the large time needed to cross the network. The opposite of a regular network is a random graph, which, for the same number of connections, exhibit low number of triangles, short crossing time. The statistical and dynamical properties of systems whose connection are regular or random are generally quite different.

Watts and Strogatz [16] argued that *social networks* are never completely regular. They showed that the simple random rewiring of a small number of links in a regular network may induce the small world effect: local properties, like the number of triangles, are not affected, but large-distance ones, like the crossing time, quickly became similar to that of random graphs. Also the statistical and dynamical properties of models defined over a rewired networks are generally similar to those correlated to random graphs.

After this finding, many social networks were studied, and they revealed a yet different structure: instead of having a well-defined connectivity, many of them present a few highly-connected "hubs", and a lot of poorly-connected "leafs". The distribution of connectivity of often distributed as a power-law (or similar [17]), without a well-defined mean connectivity (scale-free networks [18]). Many of phenomenological models are presently re-examined in order to investigate their behavior if defined over such networks. Moreover, scale-free networks cannot be "laid down", they need to be "grown" following a procedure (similar in this to fractals). It is natural therefore to include such a procedure in the model, design therefore models that not only evolve "over" the networks, but also evolve "the" network [19].

Agents. Many of the described tools are used is the so-called agent-based models. The idea is that of exploiting the powerful capabilities of present computers to simulate directly a large number of *agents* that interact among them. Traditional investigations of *complex systems*, like crowds, flocks, traffic, urban models, and so on, have been performed using *homogeneous* representation: partial differential equations (*i.e.*, mean-field), Markov equations, cellular automata, etc. In such an approach, it is supposed that each agent type is present in many identical copies, and therefore they are simulated as "macrovariables" (cellular automata), or aggregated like independent random walkers in the diffusion equation. But live elements (cells, organisms) do not behave in such a way: they are often individually unique, carry information about their own past history, and so on. With computers, we are now in the position of simulating large assemblies of individuals, possibly geographically located (say, humans in an urban simulation).

One of the advantages of such approach is that of offering the possibility of measuring quantities that are inaccessible to experimentalists, and also to experiment with different scenarios. The disadvantages are the proliferation

of parameters, that are often beyond experimental confirmation.

4 Artificial worlds

A somewhat alternative approach to that of "traditional" computational physics is that of studying an artificial model, build with little or no direct connection with reality, trying to include only those aspect that are considered relevant. The goal is to be able to find the *simplest* system still able to exhibit the relevant features of the phenomena under investigation. For instance, this is the spirit with which the Ising model was build.

4.1 Ising

The Ising (better: Lenz-Ising) model is probably one of the most known models in statistical physics. Its history [20] is particularly illuminating in this context, even if it happened well before the advent of computers in physics.

Let us first illustrate schematically the model. It is defined on a lattice, that can be in one, two or more dimensions, or even on a disordered graph. We shall locate a cell with an index $\boldsymbol{i}$, corresponding to the set of spatial coordinates for a regular lattice or a label for a graph. The dynamical variable $x_{\boldsymbol{i}}$ for each cell is just a binary digit, traditionally named "spin" that takes the values ± 1. We shall indicate the whole configuration as $\boldsymbol{x}$. Therefore, a lattice with N cells has 2^N distinct configurations. Each configuration $\boldsymbol{x}$ has an associated energy

$$E(\boldsymbol{x}) = -\sum_{\boldsymbol{i}} (H + h_{\boldsymbol{i}}) x_{\boldsymbol{i}},$$

where H represents the external magnetic field and $h_{\boldsymbol{i}}$ is a local magnetic field, generated by neighboring spins,

$$h_{\boldsymbol{i}} = \sum_{\boldsymbol{j}} J_{\boldsymbol{ij}} x_{\boldsymbol{i}}.$$

The coupling $J_{\boldsymbol{ij}}$ for the original Lenz-Ising model is

$$J_{\boldsymbol{ij}} = \begin{cases} J & \text{if } \boldsymbol{i} \text{ and } \boldsymbol{j} \text{ are first neighbors,} \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

The spins belonging to the neighborhood of cell $\boldsymbol{i}$ ($J_{\boldsymbol{ij}} > 0$) are indicated as $\boldsymbol{X}_{\boldsymbol{i}}$.

The maximum-entropy principle [13] gives the probability distribution

$$P(\boldsymbol{x}) = \frac{1}{Z} \exp\left(-\frac{E(\boldsymbol{x})}{T}\right)$$

from which averages can be computed. The parameter T is the temperature, and Z, the "partition function" is the normalization factor of the distribution.

The quantity $E(\boldsymbol{x})$ can be though as a "landscape", with low-energy configurations corresponding to valley and high-energy ones to peaks. The distribution $P(\boldsymbol{x})$ can be interpreted as the density of a gas, each "particle" corresponding to a possible realization (a replica) of the system. This *gas* concentrates in the valleys for low temperatures, and diffuses if the temperature is increased. The temperature is related to the average level of the gas.

In the absence of the local field ($J = 0$), the energy is minimized if each $x_{\boldsymbol{i}}$ is *aligned* (same sign) with H. This ordering is counteracted by thermal noise. In this case it is quite easy to obtain the average magnetization per spin (order parameter)

$$\langle x \rangle = \tanh\left(\frac{H}{T}\right),$$

which is a plausible behavior for a paramagnet. A ferromagnet however present hysteresis, *i.e.*, it may maintain for long times (metastability) a pre-existing magnetization opposed to the external magnetic field.

With coupling turned on ($J > 0$), it may happen that the local field is strong enough to "resist" H, *i.e.*, a compact patch of spins oriented against H may be stable, even if the energy could be lowered by flipping all them, because the flip of a single spin would rise the energy (actually, this flip may happen, but is statistically re-absorbed in short times). The fate of the patch is governed by boundaries. A spin on a boundary of a patch feels a weaker local field, since some of its neighbors are oriented in the opposite. Straight boundaries in two or more dimensions

separate spins that "know" the phase they belong to, since most of their neighbors are in that phase, the spins on the edges may flip more freely. Stripes that span the whole lattice are rather stable objects, and may *resist* an opposite external field since spins that occasionally flip are surrounded by spins belonging to the opposite phase, and therefore feel a strong local field that pushes them towards the phase opposed to the external field.

In one dimensions with finite-range coupling, a single spin flip is able to create a "stripe" (perpendicularly to the the lattice dimension), and therefore can destabilize the ordered phase. This is the main reason for the absence of phase transitions in one dimension, unless the coupling extends on very large distances or some coupling is infinite (see the part on directed percolation, Sect. 4.3).

This model was proposed in the early 1920s by Lenz to Ising for his PhD dissertation as a simple model of a ferromagnet. Ising studied it in one dimension, found that it shows no phase transition and concluded (erroneously) that the same happened in higher dimensions. Most of contemporaries rejected the model since it was not based on Heisenberg's quantum mechanical model of ferromagnetic interactions. It was only in the forties that it started gaining popularity as a model of cooperative phenomena, a prototype of order-disorder transitions. Finally, in 1940, Onsager [21] provided the exact solution of the two-dimensional Lenz-Ising model in zero external field. It was the first (and for many year the only) model exhibiting a non-trivial second-order transition whose behavior could be exactly computed.

Second-order transition have interested physicists for almost all the past century. In the vicinity of such transitions, the elements (say, spins) of the system are correlated up to very large distances. For instance, in the Lenz-Ising model (with coupling and more than one dimension), the high-temperature phase is disordered, and the low-temperature phase is almost completely ordered. In both these phases the connected two-points correlation function

$$G_c(r) = \langle x_{\boldsymbol{i}} x_{\boldsymbol{i}+\boldsymbol{r}} \rangle - \langle x_{\boldsymbol{i}} \rangle^2$$

decreases exponentially, $G_c(r) \simeq \exp(-r/\xi)$, with $r = |\boldsymbol{r}|$. The length ξ is a measure of the typical size of patch of spins pointing in the same direction.

Near the critical temperature T_c, the correlation length ξ diverges like $\xi(T - T_c) \simeq (T - T_c)^{-\nu}$ ($\nu = 1$ for $d = 2$ and $\nu \simeq 0.627$ for $d = 3$, where d is the dimensionality of the system). In such case the correlation function is described by a power law

$$G_c(r) \simeq \frac{1}{r^{d-2+\eta}},$$

with $\eta = 1/4$ for $d = 1$ and $\eta \simeq 0.024$ for $d = 3$. This phase transition is an example of a *critical phenomenon* [22], ν and η are examples of *critical exponents*.

The divergence of the correlation length indicates that there is no characteristic scale (ξ) and therefore fluctuations of all sizes appear. In this case, the details of the interactions are not so important, so that many different models behave in the same way, for what concerns for instance the critical exponents. Therefore, models can be grouped into *universality classes*, whose details are essentially given by "robust" characteristics like the dimensionality of space and of the order parameter, the symmetries, etc.

The power-law behavior of the correlation function also indicates that if we perform a *rescaling* of the system, it would appear the same or, conversely, that one is unable to estimate the *distance* of a pattern by comparing the "typical size" of particulars. This scale invariance if typical of many natural phenomena, from clouds (whose height and size are hard to be estimated), trees and other plant elements, lungs, brain, etc.

Many examples of power laws and collective behavior can be found in natural sciences [23]. Differently from what happens in the Lenz-Ising model, in these cases there is no parameter (like the temperature) that has to be fine-tuned, so one speaks of *self-organized criticality* [15].

Since the Lenz-Ising model is so simple, exhibits a critical phase and can be exactly solved (in some case), it has become the playground for a variety of modifications and applications to various fields. Clearly, most of modifications do no allow analytical treatment and have to be investigated numerically. The Monte-Carlo method allows to add a temporal dimension to a statistical model [24], *i.e.*, to transform stochastic integrals into averages over fictitious trajectories. Needless to say, the Ising-Lenz model is the standard test for every Monte-Carlo beginner, and most of techniques for accelerating the convergence of averages has been developed with this model in mind [25].

Near a second-order phase transitions, a physical system exhibits *critical slowing down*, *i.e.*, it reacts to external perturbations with an extremely slow dynamics, with a convergence time that increases with the system size. One can extend the definition of the correlation function including the time dimension: in the critical phase also the temporal correlation length diverges (as a power law). This happens also for the Lenz-Ising model using the the Monte-Carlo dynamics, unless very special techniques are used [25]. Therefore, the dynamical version of the Lenz-Ising model can be used also to investigate relaxational dynamics and how this is influenced by the characteristics of the energy landscape. In particular, if the coupling $J_{\boldsymbol{ij}}$ changes sign randomly for every couple of sites (or the

field H has random sign for each site), the energy landscape becomes extremely rugged. When spins flip in order to align to the local field, they may invert the field felt by neighboring ones. This *frustration* effect is believed to be the basic mechanism of the large viscosity and memory effects of *glassy* substances [26, 27].

The rough energy landscape of glassy systems is also challenging for optimization methods, like *simulated annealing* [28] and its "improved" cousin, *simulated tempering* [29]. Again, the Lenz-Ising model is the natural playground for these algorithm.

The dynamical Lenz-Ising model can be formulated such that each spin is updated in parallel [30] (with the precaution of dividing cells into sublattices, in order to keep the neighborhood of each cell fixed during updates). In this way, it is essentially a probabilistic cellular automata, as illustrated in Sect. 4.3.

4.2 Cellular Automata

In the same period in which traditional computation was developed, in the early fifties, John Von Neumann was interested in the logic basis of life and in particular in self-reproduction, and since the analysis of a self-reproduction automata following the rules of real physics was too difficult, he designed a playground (a cellular automaton) with just enough "physical rules" in order to make its analysis possible. It was however just a theoretical exercise, the automaton was so huge that up to now it has not yet completely implemented [31].

The idea of cellular automata is quite simple: take a lattice (or a graph) and put on each cell an automaton (all automata are equal). Each automaton exhibit its "state" (which is one out of a small number) and is programmed so to react (change state) according to the state of neighbors, and its present one (the *evolution rule*). All automata update their state synchronously.

Cellular automata share many similarities with the parallel version of the Lenz-Ising model. Differently from that, their dynamics is not derived from an energy, but is defined in terms of the transition rules. These rules may be deterministic or probabilistic. In the first case (illustrated in this section), cellular automata are *fully discrete, extended dynamical systems*. Probabilistic cellular automata are illustrated in Sect. 4.3. The temporal evolution of deterministic cellular automata can be computed *exactly* (regardless of any approximation) on a standard computer.

Let us illustrate the simplest case, *elementary cellular automata*, in Wolfram's jargon [32]. The lattice is here one dimensional, so to identify an automaton it is sufficient to give one coordinate, say i, with $i = 1, \ldots, N$. The state of the automaton on cell i at time t is represented by a single variable, $x_i(t)$ that can take only two values, "dead/live", or "inactive/active" or 0/1. The time is also discrete, so $t = 1, 2, \ldots$.

The parallel evolution of each automaton is given by the rule

$$x_i(t+1) = f(x_{i-1}(t), x_i(t), x_{i+1}(t)).$$

Since $x_i = 0, 1$, there are only eight possible combinations of the triple $\{x_{i-1}(t), x_i(t), x_{i+1}(t)\}$, from $\{0, 0, 0\}$ to $\{1, 1, 1\}$. For each of them, $f(x_{i-1}(t), x_i(t), x_{i+1}(t))$ is either zero or one, so the function f can be simply coded as a vector of eight bits, each position labeled by a different configuration of inputs. Therefore, there are only $2^8 = 256$ different elementary cellular automata, that have been studied carefully (see for instance Ref. [32]).

In spite of their simplicity, elementary cellular automata exhibit a large variety of behaviors. In the language of dynamical systems they can be "visually" classified [32] as fixed points (class-1), limit cycles (class-2) and "chaotic" oscillations (class-3). A fourth class, "complex" CA, emerges with larger neighborhood or in higher dimensions. A classical example is the *Game of Life* [33]. This two-dimensional cellular automaton is based on a simple rule. A cell may be either empty (0) or "alive" (1). A living cell survives if, among its 8 narest neighbors, there are two or three alive cells, otherwise it dies and disappears. Generation is implemented through a rule for empty cells: they may become "alive" if surrounded by exactly three living cells. In spite of the simplicity of the rule, this automaton generates complex and long-living patterns, some of them illustrated in Figure 2.

Complex CA have large transients, during which interesting structures emerge, after which they relax to class-1 automata. It has been conjectured that they are able of computation, *i.e.*, that one can "design" an universal computer using these CA as building blocks, as has been proved to be possible with the Game of Life. Another hypothesis, again confirmed by the Game of Life, is that these automata are "near the edge" of self-organizing complexity. One can slightly "randomize" the Game of Life, allowing sometimes an exception to the rule. Let us introduce a parameter p, that measures this randomness, with the assumption that $p = 0$ is the true "life". Well, it was shown [35] that the resulting model exhibits a second-order phase transition for a value of p very near zero.

Deterministic cellular automata have been investigated as prototypes of discrete dynamical systems, in particular for what concerns the definition of chaos. Visually, one is tempted to use this word also to denote the irregular behavior of "class 3" rules. However, the usual definition of chaos involves the sensitivity to an infinitesimally small perturbation: following the time dynamics of two initially close configurations one can observe an amplification

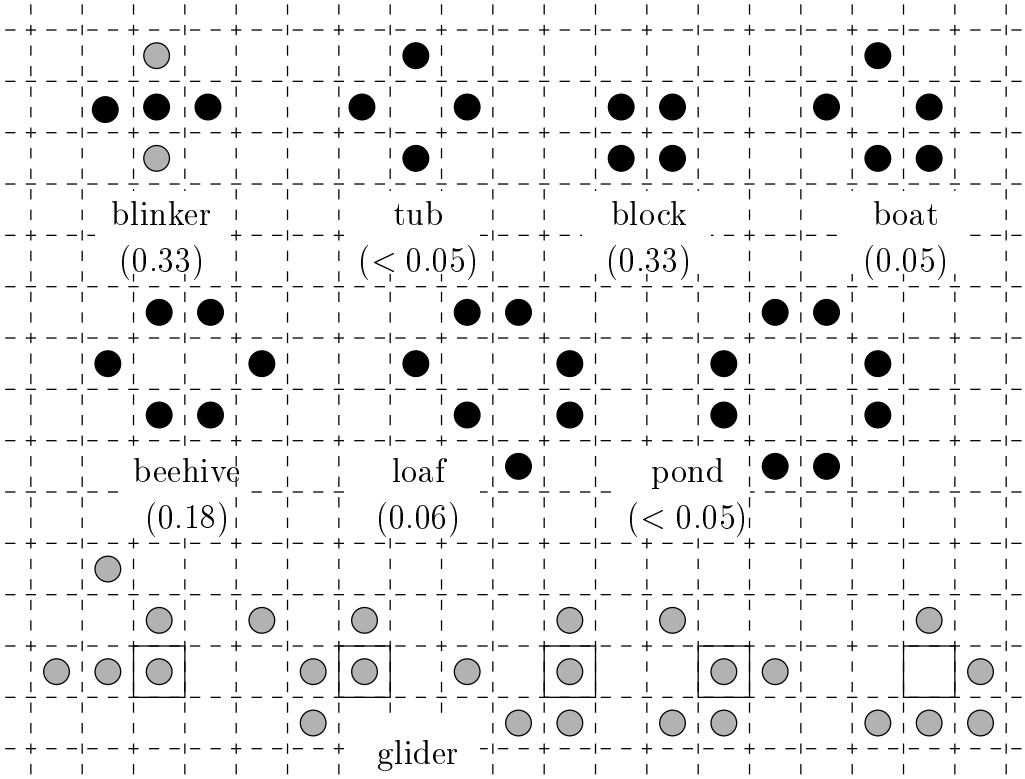

Figure 2: Some of the most common "animals" in the game of life, with the probability of encountering them in an asymptotic configuration [34].

of their distance. If the initial distance (δ_0) is infinitesimal, then the distance grows exponentially for some time ($\delta(t) \simeq \delta_0 \exp(\lambda t)$), after which it tends to saturate (since the trajectories are generally bounded inside an attractor, or due to the dimensions of the accessible space. The exponent λ depends on the initial configuration, and if this behavior is observed for different portions of the trajectory, it fluctuates: a trajectory spends some time in regions of high chaoticity, after which may pass through "quiet" zones. If one "renormalizes" periodically this distance, considering one system as the "master" and the other as a measuring device, one can accumulate good statistics, and define a Lyapunov exponent λ, that gives indications about the chaoticity of the trajectory, through a limiting procedure.

The accuracy of computation poses some problems. Since in a computer numbers are always approximate, one cannot follow "one" trajectory. The small approximations accumulates exponentially, and the computer time series actually *jumps* among neighboring trajectories. Since the Lyapunov exponent is generally not so sensible to a change of precision in computation, one can assume that the chaotic regions are rather compact and uniform, so that in general one associate a Lyapunov exponent to a system, not to an individual trajectory. Nevertheless, this definition cannot apply to completely discrete systems like cellular automata.

However, chaoticity is related to unpredictability. As first observed by Lorenz, and following the definition of Lyapunov exponent, the precision of an observation over a chaotic system is related to the average time for which predictions are possible. Like in weather forecasts, in order to increase the time span of a prediction one has to increase the precision of the initial measurement. In extended system, this also implies to extend the measurements over a larger area. One can also consider a "synchronization" approach. Take two replicas of a systems and let them evolve starting from different initial configurations. With a frequency and a strength that depends on a parameter q, one of these replica is "pushed" towards the other one, so to reduce their distance. Suppose that $q = 0$ is the case of no push and $q = 1$ is the case of extremal push, for which the two systems synchronize in a very short time. There should be a critical value q_c that separates these two behaviors (actually, the scenario may be more complex, with many phases [36]). In the vicinity of q_c the distance between the two replicas is small, and the distance δ grows in exponential way. The critical value q_c is such that the exponential growth exactly compensates the shrinking factor, and is therefore related to the Lyapunov exponent λ.

Finite-size cellular automata always follow periodic trajectories. Let us consider for instance a Boolean automata, of N cells. The number of possible different states is 2^N and due to determinism, once that a state has been visited twice the automata has entered a limit cycle (or a fixed point). One may have limit cycles with large basins of transient configurations (configurations that do not belong to the cycle). Many scenarios are possible. The set of different configurations may be divided in many basins, of small size (small transient) and small period, like in class 1 and 2 automata. Or one may have large basins, with long transients that lead to short cycles, like in class-4 automata. Finally, one may have one or very few large basins, with long cycles that includes most of configurations belonging to the basin (small transients). This is the case of class-3 automata. For them, the typical period of a limit cycle grows exponentially (like the total number of configurations) with the system size, so that for moderately large system it is almost impossible to observe a whole cycle in a finite time. Another common characteristic of class-3 automata is that the configurations quickly decorrelates (in the sense of the correlation function) along a trajectory. If one takes into consideration as starting points two configurations that are the same except for a local difference, one observes that this difference amplifies and diffuses in class-3 automata, shrinks or remains limited in class-1 and class-2, and have an erratic transient behavior in class-4, followed by the fate of class-1 and 2. Therefore, if one considers the possibility of not knowing exactly the initial configuration of an automata, unpredictability grows with time also for such discrete systems. Actually, also (partially) continuous systems like coupled maps may exhibit this kind of behavior [36, 37, 38, 39]. Along this line, it is possible to define an equivalent of the Lyapunov exponents for CA [40]. The synchronization procedure can be applied also to cellular automata, and it correlates well with the Lyapunov exponents [41].

An "industrial" application of cellular automata is their use for modeling gases. The *hydrodynamical equations*, like the Navier-Stokes ones, simply reflect the conservation of mass, momentum and energy (*i.e.*, rotational, translational and time invariance) for the microscopic collision rules among particles. Since the modeling of a gas via molecular dynamics is rather cumbersome, some years ago it was proposed [42, 43] to simplify drastically the microscopic dynamics using particles that may travel only along certain directions with some discrete velocities and jumping in discrete time only among nodes of a lattice. Indeed, a cellular automaton. It has been shown that their macroscopic dynamics is described by usual hydrodynamics laws (with certain odd feature due to the underlining lattice and finiteness of velocities) [44, 45].

The hope was that these Lattice Gas Cellular Automata (LGCA) could be simulated so efficiently in hardware to make possible the investigation of turbulence, or, in other words, that they could constitute the Ising model of hydrodynamics. While they are indeed useful to investigate certain properties of gases (for instance, chemical

reactions [46], or the relationship between chaoticity and equilibrium [47]), they resulted too noisy and too viscous to be useful for the investigation of turbulence. Viscosity is related to the transport of momentum in a direction perpendicular to the momentum itself. If the collision rule does not "spread" quickly the particles, the viscosity is height. In LGCA there are many limitations to collisions, so that in order to lower viscosity one has to consider averages over large patches, thus lowering the efficiency of the method.

However, LGCA inspired a very interesting approximation. Let us consider a large assembly of replicas of the same system, each one starting from a different initial configuration, all compatible with the same macroscopic initial conditions. The macroscopic behavior after a certain time would be the *average* over the status of all these replicas. If one assumes a form of local equilibrium, *i.e.*, applies the mean-field approximation for a given site, one may try to obtain the dynamics of the *average* distribution of particles, which in principle is the same of "exchanging" particles that happen to stay on the same node among replicas.

It is possible to express the dynamics of the average distribution in a simple form: it is the Lattice Boltzmann Equation (LBE) [45, 48, 49]. The method retains many properties of LGCA like the possibility of considering irregular and varying boundaries, and may be simulated in a very efficient way with parallel machines [48]. Differently from LGCA, there are numerical stability problems to be overcome.

Nowadays, the word *cellular automata* has enlarged its meaning, including any system whose elements do not move (in opposition to "agent-based modeling"). Therefore, we now have cellular automata on non-regular lattices, non-homogeneous, with probabilistic dynamics (see Sect. 4.3), etc. (see for instance Ref.[50]). They are therefore considered more as a "philosophy" of modeling rather than a single tool. In some sense, cellular automata (and agent-based) modeling is opposed to the spirit of describing a phenomena using differential equations (or partial differential equations). One of the reasons is that the language of "automata" is simpler and requires less training than that of differential equations. Another reason is that at the very end, any "reasonable" problem has to be investigated using computers, and while the implementation of cellular automata is straightforward (even if careful planning may speed-up dramatically the simulation), the computation of partially differential equations is an art in itself.

4.3 Probabilistic Cellular Automata

In deterministic automata, given a local configuration, the future state of a cell is univocally determined. But let us consider the case of measuring experimentally some pattern and trying to analyze it in terms of cellular automata. In time-series analysis, it is common to perform averages over spatial patches and temporal intervals and to discretize the resulting value. For instance, this is the natural result of using a camera to record the temporal evolution of an extended system, for instance the turbulent and linear regions of a fluid. The resulting pattern symbolically represents the dynamics of the original system, and if it is possible to extract a "rule" out of this pattern, it would be extremely interesting for the construction of a model. In general, however, one observes that sometimes a local configuration is followed by a symbol, and sometime the same local configuration is followed by another one. One should conclude that the neighborhood (the local configuration) does not univocally determines the following symbol.

One can extend the "range" of the rule, adding more neighbors farther in space and time [12]. By doing so, the "conflicts" generally reduce, but at the price of increasing the complexity of the rule. At the extremum, one could have an automaton with infinite "memory" in time and space, that perfectly reproduces the observed patterns but with almost none predictive power (since it is extremely unlucky that the same *huge* local configuration is encountered again.

So, one may prefer to limit the neighborhood to some finite extension, and accept that the rule sometimes "outputs" a symbol and sometimes another one. One defines a local transition probability $\tau(x_{\boldsymbol{i}}(t+1)|\boldsymbol{X}_{\boldsymbol{i}}(t))$ of obtaining a certain symbol $x_{\boldsymbol{i}}$ at time $t+1$ given a local configuration $\boldsymbol{X}_{\boldsymbol{i}}$ at time t. Deterministic cellular automata correspond to the case $\tau = 0, 1$. The parallel version of the Lenz-Ising model can be re-interpreted as a probabilistic cellular automaton.

Starting from the local transition probabilities, one can build up the transition probability $T(\boldsymbol{x}|\boldsymbol{y})$ of obtaining a configuration $\boldsymbol{x}$ given a configuration $\boldsymbol{y}$ ($T(x|y)$ is the product of the local transition probabilities τ, for each site [51]). One can read the configurations $\boldsymbol{x}$ and $\boldsymbol{y}$ as indexes, so that T can be considered as a matrix. The normalization of probability corresponds to the constraint $\sum_{\boldsymbol{x}} T(\boldsymbol{x}|\boldsymbol{y}) = 1$, $\forall \boldsymbol{y}$.

Denoting with $P(\boldsymbol{x}, t)$ the probability of observing a given configuration $\boldsymbol{x}$ at time t, and with $\boldsymbol{P}(t)$ the whole distribution at time t, we have for the evolution of the distribution

$$\boldsymbol{P}(t+1) = T\boldsymbol{P}(t),$$

with the usual rules for the product of matrices and vectors. Therefore, the transition matrix T defines a Markov process, and the asymptotic state of the system is given by the eigenvalues of T. The largest eigenvalue is always 1, due to the normalization of the probability distribution, and the corresponding eigenvector is the asymptotic distribution. The theory of Markov processes says that if T is irreducible, *i.e.*, it cannot be rewritten (renumbering rows and columns) as blocks of noninteracting subspaces, like

$$T = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix},$$

then the second eigenvalue is strictly less than one and the asymptotic state is unique. In this case the second eigenvalue determines the convergence time to the asymptotic state. For finite matrices, if all elements are greater than zero (and therefore strictly less than one), the matrix T is irreducible. However, in the limit of infinite size, the largest eigenvalue may become degenerate, and therefore there are more than one asymptotic state. This is the equivalent of a phase transition for Markov processes.

For the parallel Lenz-Ising model, the elements of the matrix T are given by the product of local transition rules of the Monte-Carlo dynamics. They depend on the choice of the algorithm, but essentially have the form of exponentials of the difference in energy, divided by the temperature. Although a definitive proof is still missing, it is plausible that matrices with all elements different from zero correspond to some equilibrium model, whose transition rules can be derived from an energy function [52].

Since probabilistic cellular automata are defined in terms of the transition probabilities, one is free to investigate models that go beyond equilibrium. For instance, if some transition probability takes the value zero or one, in the language of equilibrium system this would correspond to some coupling (like the J of the Lenz-Ising model) that become infinite. This case is not so uncommon in modeling. The inverse of a transition probability correspond to the average waiting time for the transition to occur in a continuous-time model (one may think to chemical reactions). Some transitions may have a waiting time so long with respect to the observation interval, to be practically irreversible. Therefore, probabilistic cellular automata (alongside other approaches like for instance annihilating random walks) allow the exploration of out-of-equilibrium phenomena.

One such phenomena is directed percolation, *i.e.*, a percolation process with a special direction (time) along which links can only be crossed one-way [53]. Let think for instance to the spreading of an infection in a one-dimensional lattice, with immediate recovery (SIS model). An ill individual can infect one of both of his two neighbors but returns to the susceptible state after one step. The paths of infection (see Figure 3) can wander in the space directions, but are directed in the time directions.

The parallel version of a directed percolation process can be mapped onto probabilistic cellular automata. The simplest case, in one spatial dimension and with just two neighbors, is called the Domany-Kinzel model [54]. It is even more general than the usual directed percolation, allowing "non-linear" interactions among sites in the neighborhood (*e.g.*, two wet sites may have less probability of percolating than one alone).

These processes are interesting because there is a *absorbing state* [55, 56], which is the dry state for the wetting phenomenon and the healthy state for the spreading of epidemics. Once the system has entered this absorbing state, it cannot exit, since the spontaneous appearing of a wet site or of a ill individual is forbidden. For finite systems, the theory of Markov chains says that the system will "encounter", sooner or later, this state, that therefore corresponds to the unique asymptotic state. For infinitely extended systems, a phase transition can occur, for which wet sites percolate for all "times", the epidemics become endemic, and so on.

Again these are examples of *critical phenomena*, with exponents different from the equilibrium case.

4.4 Cellular Automata and Agent-Based Simulations

Cellular automata can be useful in modeling phenomena that can be described in lattice terms. However, many phenomena requires "moving particles". Examples may be chemical reactions, ecological simulations, social models. When particles are required to obey hydrodynamics constraints, *i.e.*, to collide conserving mass, momentum and energy, one can use lattice gas cellular automata or the lattice Boltzmann equation. However, in general one is interested in modeling just a macroscopic scale, assuming that what happens at lower level is just "noise". According with the complexity (and "intelligence") assigned to particles, one can develop models based on the concept of walkers, that move more or less randomly. From the simulation point of view, walkers are not very different from the graphs succinctly described above. In this case the identifier $\boldsymbol{i}$ is just a label, that allows to access walker's data, among which there are the coordinates of the walker (that may be continuous), its status and so on.

In order to let walker interact, one is interested in finding efficiently all walkers that are nearer than a given distance from the one under investigation. This is the same problem one is faced with when developing codes for

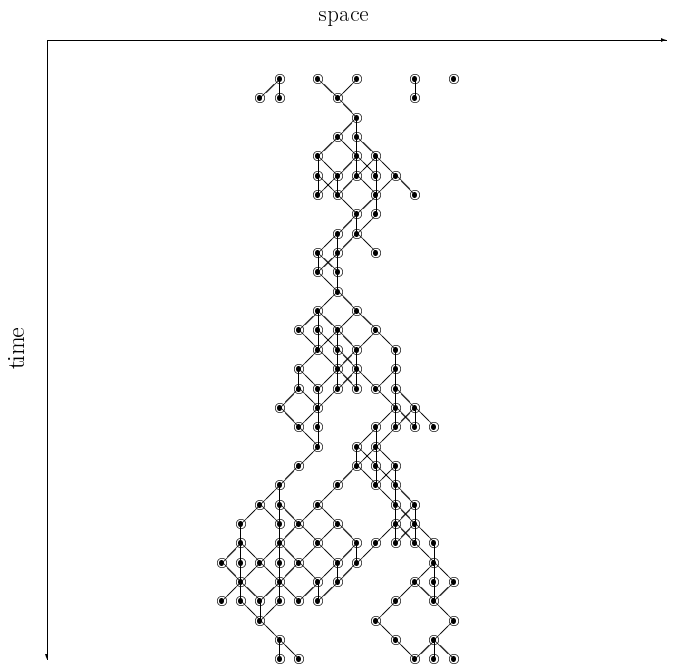

Figure 3: An example of a directed percolation cluster.

molecular dynamics simulations [57]: scanning all walkers in order to compute their mutual distance is a procedure that grows quadratically with the number of walkers. One "trick" is that of dividing the space in cells, *i.e.*, to define an associated lattice. Each cell contains a list of all walkers that are locate inside it. In this way, one can directly access all walkers that are in the same or neighboring cells of the one under investigation.

Moreover, one can exploit the presence of the lattice to implement on it a "cellular automaton", that may interact with walkers, in order to simulate the evolution of "fields". Just for example, the simulation of a herd of herbivore that move according to the exhaustion of the grass, and the parallel growing of the vegetation can be modeled associating the "grass" to a cellular automaton, and the herbivores to walkers. This simulation scheme is quite flexible, allowing to implement random and deterministic displacements of moving objects or agents, continuous or discrete evolution of "cellular objects" and their interactions. Many simulation tools tools and games are based on this scheme [58, 59, 60], and they generally allow the contemporary visualization of a graphical representation of the state of the system. They are valuable didactic tool, and may be used to "experiment" with these artificial worlds. As often the case, the flexibility is paid in terms of efficiency and speed of simulation.

5 Future Directions

Complex systems, like for instance human societies, cannot be simulated starting from "physical laws". This is sometimes considered a weakness of the whole idea of studying such systems from a quantitative point of view. We have tried to show that actually even the "hardest" discipline, physics, always deals with models, that have finally to be simulated on computers making various assumptions and approximations. Theoretical physics is accustomed since a long time to "extreme simplifications" of models, hoping to enucleate the "fundamental ingredients" of a complex behavior. This approach have proved to be quite rewarding for our understanding of nature.

In recent years, physics have been seen studying many fields not traditionally associated to physics: molecular biology, ethology, evolution theory, neurosciences, psychology, sociology, linguistics, and so on. Actually, the word "physics" may refer either to the classical subjects of study (mainly atomic and subatomic phenomena, structure of matter, cosmological and astronomical topics), or to the "spirit" of the investigation, that may apply to almost any discipline. This spirit is essentially that of building simplified quantitative models, composed by many elements, and study them with theoretical instruments (most of times, applying some form of mean-field treatment) and with computer simulations.

This approach has been fruitful in chemistry and molecular biology and nowadays many physical journals have

sections devoted to "multidisciplinary studies". The interesting thing is that not only have physicists brought some "mathematics" into fields that are traditionally more "qualitative" (which often corresponds to "linear" modeling, plus noise), but physicists have also discovered many interesting questions to be investigated, and new models to be studied. One example is given by the current investigations about the structure of social networks, that were "discovered" by physicists in the nontraditional field of social studies.

Another contribution of physicists to this "new way" of performing investigations, is the use of networked computers. Since a long time, physicists have used computers for performing computations, storing data and diffusing information using the Internet. Actually, the concept of what is now the World Wide Web was born at CERN, as a method for sharing information among laboratories [61]. The high-energy physics experiments require a lot of simulations and data processing, and physicists (among others) developed protocols to distribute this load on a grid of networked computers. Nowadays, an European project aims to "open" grid computing to other sciences [62].

It is expected that this combination of quantitative modeling and grid computing will stimulate innovative studies in many fields. Here is a small sparse list of possible candidates:

- Theory of evolution, especially for what concerns evolutionary medicine.
- Social epidemiology, coevolution of diseases and human populations, interplay between sociology and epidemics.
- Molecular biology and drug design, again driven by medical applications.
- Psychology and neural sciences, it is expected that the "black box" of traditional psychology and psychiatry will be replaced by explicit models based on brain studies.
- Industrial and material design.
- Earth sciences, especially meteorology, vulcanology, seismology.
- Archaeology: simulation of ancient societies, reconstruction of historical and pre-historical climates.

However, the final success of this approach is related to the availability of high-quality experimental data that allow to discriminate among the almost infinite number of models that can be built.

6 Glossary

Nonlinear system: A system composed by parts whose combined effects are different from the sum of the effects of each part.

Extended system: A system composed by many parts connected by a network of interactions that may be regular (lattice) or irregular (graph).

Graph, lattice, tree: A graph is set of nodes connected by links, oriented or not. If the graph is translationally invariant (it looks the same when changing nodes), it is called a (regular) lattice. A disordered lattice is a lattice with a fraction of removed links or nodes. An ordered set of nodes connected by links is called a path. A closed path not passing on the same links is a loop. A cluster is a set of connected nodes. A graph can be composed by one cluster (a connected graph) or more than one (a disconnected graph). A tree is a connected graph without loops.

Percolation: The appearance of a "giant component" (a cluster that contains essentially all nodes or links) in a graph or a lattice, after adding or removing nodes or links. Below the percolation threshold the graph is partitioned into disconnected clusters, none of which contains a substantial fraction of nodes or links, in the limit of infinite number of nodes/links.

State of a system: A complete characterization of a system at a given time, assigning or measuring the positions, velocities and other dynamical variables of all the elements (sometimes called a configuration). For completely discrete systems (cellular automata) of finite size, the state of the system is just a set of integer numbers, and therefore the state space is numerable.

Trajectory: A sequence of states of a system, labeled with the time, *i.e.*, a path in the state space.

Probability distribution: The probability of finding a system in a given state, for all the possible states.

Mean field: An approximate technique for computing the value of the observables of an extended system, neglecting correlations among parts. If necessary, the dynamics is first approximated by a stochastic process. In its simpler version, the probability of a state of the system is approximated by the product of the probability of each component, neglecting correlations. Since the state of two components that depend on a common "ancestor" (that interact with a common node) is in general not uncorrelated, and this situation corresponds to an interaction graph with loops, the simplest mean field approximation consists in replacing the graph or the lattice of interactions with a tree.

Monte-Carlo: A method for producing stochastic trajectories in the state space designed in such a way that the time-averaged probability distribution is the desired one.

Critical phenomenon: A condition for which an extended system is correlated over extremely long distances.

References

[1] N. Metropolis, J. Hewlett, and Gian-Carlo Rota, editors. *A History of Computing in the Twentieth Century*. Academic Press, New York, 1980.

[2] H. Harlow and N. Metropolis. Computing & computers - weapons simulation leads to the computer era. *Los Alamos Science*, 4(7):132, Winter-Spring 1983.

[3] History of chaos: Lorenz. `http://library.thinkquest.org/3120/old_htdocs.1/text/fraz1.txt`.

[4] R. Car and M. Parrinello. Unified approach for molecular dynamics and density-functional theory. *Phys. Rev. Lett.*, 55(22):2471–2474, Nov 1985.

[5] T. Daxois, M. Peyrard, and S. Ruffo. The Fermi-Pasta-Ulam 'numerical experiment': History and pedagogical perspectives. *Eur. J. Phys*, 26:S3–S11, 2005.

[6] E. Fermi, J. Pasta, and S. Ulam. Los alamos report la-1940. In E. Segré, editor, *Collected papers of Enrico Fermi*. University of Cicago press, Chicago, IL, 1955.

[7] R. May. Simple mathematical models with very complicated dynamics. *Nature*, 261:459–467, jun 1976.

[8] K. Kaneko. Spatiotemporal intermittency in coupled map lattices. *Progr. Theor. Phys.*, 74(5):1033–1044, 1985.

[9] M. Haw. Einstein's random walk. *Physics World*, 18:19–22, Jan 2005.

[10] N. G. Van Kampen. *Stochastic Processes in Physics and Chemistry*. North-Holland, Amsterdam, nov 1992.

[11] C. W. Gardiner. *Handbook of Stochastic Methods for Physics, Chemistry, and the Natural Sciences*, volume 13 of *Springer series in synergetics*. Springer, Berlin, 1994.

[12] L. R. Rabiner. A tutorial on hidden markov models and selected applications in speech recognition. *Proceedings of the IEEE*, 77(2):257–286, feb 1989.

[13] E. T. Jaynes. Information theory and statistical mechanics. *Phys. Rev.*, 106(4):620–630, 1957.

[14] D. Stauffer and A. Aharony. *Introduction To Percolation Theory*. Taylor & Francis, London, 1994.

[15] P. Bak, C. Tang, and K. Weisenfeld. Self-organizing criticality: An explanation of $1/f$ noise. *Phys. Rev. A*, 38:364–374, 1987.

[16] D. J. Watts and S. H. Strogatz. Collective dynamics of 'small-world' networks. *Nature*, 393:440–441, 1998.

[17] M. E. Newman. Power laws, pareto distributions and zipf's law. *Contemporary Physics*, 46:323–351, 2005.

[18] R. Albert and A.-L. Barabasi. Statistical mechanics of complex networks. *Rev. Mod. Phys.*, 74:47–97, jan 2002.

[19] S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, and D.-U. Hwang. Complex networks: Structure and dynamics. *Phys. Rep.*, 424(4–5):175–308, feb 2006.

[20] M. Niss. History of the Lenz-Ising model 1920–1950: From ferromagnetic to cooperative phenomena. *Archive for History of Exact Sciences*, 59(3):267–318, March 2005.

[21] L. Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65:117–149, 1944.

[22] J.J. Binney, N. J. Dowrick, A. J. Fisher, and M. E. J. Newman. *The Theory of Critical Phenomena*. Oxford Science Publications. Clarendon Press, Oxford, 1993.

[23] D. Sornette. *Critical Phenomena in Natural Sciences*. Springer Series in Synergetics. Springer, Berlin, 2006.

[24] K. Kawasaki. Kinetics of Ising model. In C. M. Domb and M. S. Green, editors, *Phase Transitions and Critical Phenomena*, volume 2, page 443. Academic Press, New York, 1972.

[25] R. H. Swendsen and J.-S. Wang. Nonuniversal critical dynamics in Monte Carlo simulations. *Phys. Rev. Lett.*, 58(2):86–88, January 1987.

[26] M. Mezard, G. Parisi, and M.-A. Virasoro. *Spin Glass Theory and Beyond*, volume 9 of *World Scientific Lecture Notes in Physics*. World Scientific, Singapore, 1987.

[27] Viktor Dotsenko. *An Introduction to the Theory of Spin Glasses and Neural Networks*. World Scientific, Singapore, 1994.

[28] S. Kirkpatrick, C. D. Gelatt Jr., and M. P. Vecchi. Optimization by simulated annealing. *Science*, 220:671–680, 1983.

[29] E. Marinari and G. Parisi. Simulated tempering: A new Monte Carlo scheme. *Europhys. Lett.*, 19:451–458, 1992.

[30] G. T. Barkema and T. MacFarland. Parallel simulation of the ising model. *Phys. Rev. E*, 50(2):1623–1628, Aug 1994.

[31] Von Neumann universal constructor. `http://en.wikipedia.org/wiki/Von_Neumann_Universal_Constructor`.

[32] S. Wolfram. Statistical mechanics of cellular automata. *Rev. Mod. Phys.*, 55:601–644, jul 1983.

[33] E. Berlekamp, J. H. Conway, and R. K. Guy. *What is Life?*, volume 2: Games in Particular, chapter 25. Academic Press, London, jul 1982.

[34] F. Bagnoli, R. Rechtman, and S. Ruffo. Some facts of life. *Physica A*, 171:249, 1994.

[35] J. Nordfalk and P. Alstrøm. Phase transitions near the "game of life". *Phys. Rev. E*, 54(2):R1025–R1028, Aug 1996.

[36] F. Bagnoli and F. Cecconi. Synchronization of non-chaotic dynamical systems. *Phys. Lett. A*, 282(1–2):9–17, apr 2001.

[37] J. P. Crutchfield and K. Kaneko. Are attractors relevant to turbulence? *Phys. Rev. Lett.*, 60(26):2715–2718, Jun 1988.

[38] A. Politi, R. Livi, G.-L. Oppo, and R. Kapral. Unpredictable behaviour of stable systems. *Europhys. Lett.*, 22(8):571–576, jun 1993.

[39] F. Cecconi, R. Livi, and A. Politi. Fuzzy transition region in a one-dimensional coupled-stable-map lattice. *Phys. Rev. E*, 57(3):2703–2712, Mar 1998.

[40] F. Bagnoli, R. Rechtman, and S. Ruffo. Damage spreading and Lyapunov exponents in cellular automata. *Phys. Lett. A*, 172:34, 1992.

[41] F. Bagnoli and R. Rechtman. Synchronization and maximum Lyapunov exponents of cellular automata. *Phys. Rev. E*, 59(2):R1307–R1310, Feb 1999.

[42] J. Hardy, Y. Pomeau, and O. de Pazzis. Time evolution of a two-dimensional classical lattice system. *Phys. Rev. Lett.*, 31(5):276–279, Jul 1973.

[43] U. Frisch, B. Hasslacher, and Y. Pomeau. Lattice-gas automata for the navier-stokes equation. *Phys. Rev. Lett.*, 56(14):1505–1508, Apr 1986.

[44] D. H. Rothman and S. Zaleski. *Lattice-Gas Cellular Automata*. Monographs and Texts in Statistical Physics. Collection Alea-Saclay, Paris, dec 2004.

[45] D. A. Wolf-Gladrow. *Lattice-Gas Cellular Automata and Lattice Boltzmann Models : An Introduction*, volume 1725 of *Lecture Notes in Mathematics*. Springer, Berlin, 2004.

[46] A. Lawniczak, D. Dab, R. Kapral, and J.-P. Boon. Reactive lattice gas automata. *Physica D*, 47(1-2):132–158, 1991.

[47] F. Bagnoli and R. Rechtman. Entropy and chaos in a discrete hydrodynamical system. arXiv:cond-mat/0702074, 2007.

[48] S. Succi. *The Lattice Boltzmann Equation For Fluid Dynamics and Beyond*. Numerical Mathematics and Scientific Computation. Oxford University Press, Oxford UK, 2001.

[49] B. Chopard, P. Luthi, A. Masselot, and A. Dupuis. Cellular automata and lattice Boltzmann techniques: An approach to model and simulate complex systems. *Advances in Complex System*, 5(2), 2002.

[50] S. El Yacouby, B. Chopard, and S. Bandini, editors. *Cellular Automata*, volume 4173 of *Lecture Notes in Computer Science LNCS*. Springer, Berlin, 2006.

[51] F. Bagnoli. Cellular automata. In F. Bagnoli and S. Ruffo, editors, *Dynamical Modeling in Biotechnologies*, page 1. World Scientific, Singapore, Dec 2000.

[52] A. Georges and P. le Doussal. From equilibrium spin models to probabilistic cellular automata. *J. Stat. Phys.*, 54(3–4):1011–1064, feb 1989.

[53] S. R. Broadbent and J. M. Hammersley. Percolation processes I. Crystals and mazes. *Proc. Camb. Philos. Soc.*, 53:629–641, 1957.

[54] E. Domany and W. Kinzel. Equivalence of cellular automata to ising models and directed percolation. *Phys. Rev. Lett.*, 53(4):311–314, Jul 1984.

[55] H. Hinrichsen. Stochastic lattice models with several absorbing states. *Phys. Rev. E*, 55(1):219–226, Jan 1997.

[56] F. Bagnoli, N. Boccara, and R. Rechtman. Nature of phase transitions in a probabilistic cellular automaton with two absorbing states. *Phys. Rev. E*, 63(4):046116, Mar 2001.

[57] D. C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, Cambridge UK, 2004.

[58] U. Wilensky. Netlogo, 1999. `http://ccl.northwestern.edu/netlogo/`. Center for Connected Learning and Computer-Based Modeling, Northwestern University. Evanston, IL.

[59] repast - recursive porus agent simulation toolkit. `http://repast.sourceforge.net/`.

[60] W. Wright. Simcity, 1989. `http://www.maxis.com/`.

[61] R. Cailliau. A short history of the web. `http://www.netvalley.com/archives/mirrors/robert_cailliau_speech.htm`.

[62] Enabling grids for e-science. `http://www.eu-egee.org/`.