4

Introduction to dynamical processes: theory and simulation

The present chapter is intended to provide a short introduction to the theory and modeling of equilibrium and non-equilibrium processes on networks and to define the basic modeling approaches and techniques used in the theory of dynamical processes. In particular, we define the master equation formalism and distinguish between equilibrium and non-equilibrium phenomena. Unfortunately, while the master equation allows for important conceptual distinction and categorization, its complete solution is hardly achievable even for very simple dynamical processes. For this reason we introduce the reader to techniques such as mean-field and continuous deterministic approximations, which usually represent viable approaches to understand basic features of the process under study. We also discuss Monte Carlo and agent-based modeling approaches that are generally implemented in large-scale numerical simulation methods.

These different theoretical methods help to define a general framework to demonstrate how the microscopic interactions between the elements of the system lead to cooperative phenomena and emergent properties of the dynamical processes. This strategy, going from microscopic interaction to emergent collective phenomena, has its roots in statistical physics methodology and population dynamics, and is currently viewed as a general paradigm to bridge the gap between the local and the large-scale properties of complex systems. It is important to stress, however, that the following material is a greatly abbreviated presentation of a huge field of research and by necessity just scratches the surface of the statistical theory of dynamical processes. Interested readers who want to dive into the mathematical and formal subtleties of the subject should refer to classic textbooks such as those by Ma (1985), Chandler (1987), Huang (1987), and Balescu (1997).

4.1 A microscopic approach to dynamical phenomena

Two main modeling schemes are adopted when dealing with dynamical processes on networks. In the first one, we identify each node of the network with a single

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individual or element of the system. In the second, we consider dynamical entities such as people, information packets, energy or matter flowing through a network whose nodes identify locations where the dynamical entities transit. In both cases, however, the dynamical description of the system can be achieved by introducing for each node i the notion of a corresponding variable σ_i characterizing its dynamical state. If each node represents a single individual, the variable σ_i may describe a particular attribute of the individual. A typical example that we will study in detail in Chapter 9 is the spread of an epidemic where the variable σ_i indicates if the individual is healthy or infected by a given disease. In the case of dynamical entities moving in a network substrate, the state variable σ_i generally depends on the entities present at that node. Without losing any generality, we can enumerate all possible states $\sigma_i = 1, 2, \ldots, \kappa$ for each node, and the knowledge of the state variable of all nodes in the network therefore defines the microscopic state (microstate) of the whole system. In other words, we can denote a particular configuration of the network at time t by the set $\sigma(t) = (\sigma_1(t), \sigma_2(t), \ldots, \sigma_N(t))$, where the index $i = 1, \ldots, N$ runs over all the nodes of the network of size N.

The dynamical evolution of the system is simply given by the dynamics of the configuration $\sigma(t)$ in the phase space of the system, defined by all possible configurations σ. The dynamical process is described by the transitions $\sigma^a \to \sigma^b$, where the superscripts a and b identify two different configurations of the system. In general, it is impossible to follow the microscopic dynamics of large-scale systems because of the large number of variables and the stochastic nature of most phenomena. For this reason, the basic dynamical description of the system relies on the master equation (ME) approach that we have briefly introduced in the previous chapter in the context of the dynamical evolution of networks. The ME approach focuses on the study of the probability $P(\sigma, t)$ of finding the system at time t in a given configuration σ. This probability has to be normalized, $\sum_\sigma P(\sigma, t) = 1$, and provides a probabilistic description of the system which encodes most relevant information. The so-called ME consists of the evolution equation for $P(\sigma, t)$, which reads (in the continuous time approximation)

$$\partial_t P(\sigma, t) = \sum_{\sigma'} \left[P(\sigma', t) W(\sigma' \to \sigma) - P(\sigma, t) W(\sigma \to \sigma') \right], \tag{4.1}$$

where the sum runs over all possible configurations σ', and the terms $W(\sigma' \to \sigma)$ represent the transition rates from one configuration to the other owing to the microscopic dynamics of the system. The ME is thus made of two terms representing the gain and loss contributions for the probability distribution of the system to be in a given configuration σ. It is important to stress that the terms $W(\sigma' \to \sigma)$ are rates and carry the unit $[\text{time}]^{-1}$ as the ME is a differential equation representing the variation per unit time. The transition rates, in principle, depend on the whole

configurations $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ and $\sigma' = (\sigma'_1, \sigma'_2, \ldots, \sigma'_N)$, but in many cases of interest they can be simplified by considering that the change of state of a node i is determined only by the local interaction with the nodes directly connected to it. In the case where the local dynamics have the same parameters for all nodes, the transition rates can be simplified and read

$$W(\sigma' \to \sigma) = \prod_i w(\sigma'_i \to \sigma_i | \sigma_j). \tag{4.2}$$

The terms on the right-hand side represent the transition rates for the node i from the state σ'_i to the state σ_i, conditional to the state σ_j on the set of nodes j directly connected to it, i.e. of the neighbors $j \in \mathcal{V}(i)$ of i. The previous form decomposes the transition rates for the system into products of single node transition rates that are, in many cases, easier to handle. The network structure enters the dynamics at this point since the transition rate for a given node depends on its neighborhood structure. The network topology will thus have a direct and strong influence on the dynamics, as we will see in the various chapters of this book.

In principle the formal solution of the ME allows the calculation of the expectation values of all quantities of interest in the system. Given any function of the state of the system $A(\sigma)$ it is indeed possible to compute its average value at time t as

$$\langle A(t) \rangle = \sum_\sigma A(\sigma) P(\sigma, t), \tag{4.3}$$

where $\langle \cdots \rangle$ represents the phase space average of the quantity of interest. It is clear that the ME provides only statistical information. Even in the case where the probability distribution in the initial state is a delta function in the phase space with unit probability on a single configuration, $P(\sigma, t = 0) = \delta_{\sigma,\sigma^a}$, the stochastic evolution of the system will spread the probability on different configurations. In this perspective, the phase space average $\langle \cdots \rangle$ can be thought of as an average over different stochastic realizations of the evolution of the same system starting with identical initial conditions. In this context, a case of particular interest is given by systems with a well-defined asymptotic limit $\lim_{t\to\infty} P(\sigma, t) = P_\infty(\sigma)$. The system is then said to be in a stationary state, where the average over the stationary distribution is representative of the system after a typical transient time.

4.2 Equilibrium and non-equilibrium systems

While it is impossible to obtain a solution of the ME in most cases, the ergodic hypothesis and the maximization of entropy axiom allow an explicit form to be obtained for the stationary distribution $P_\infty(\sigma) = P_{eq}(\sigma)$ of equilibrium physical

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systems. Equilibrium statistical mechanics assumes that an isolated system maximizes its entropy and reaches a uniform stationary equilibrium distribution with the same probability of being in any of the fixed energy accessible configurations. In addition, the ergodic hypothesis states that, for isolated systems, the average over the time evolution of any quantity of interest is the same as the average over the stationary equilibrium distribution. In general, however, physical systems are not isolated, but coupled to the external environment which can be considered as a heat bath fixing the equilibrium temperature of the system. By considering that the maximization of entropy applies to the system coupled to the external heat bath and that the energy is globally conserved, it is not difficult to show that the stationary distribution is no longer uniform and that the equilibrium distribution is given by the Boltzmann–Gibbs distribution

$$P_{\mathrm{eq}}(\sigma) = \frac{\exp\left(-H(\sigma)/k_{\mathrm{B}}T\right)}{Z}, \tag{4.4}$$

where T is the temperature, k_{B} is the Boltzmann factor that provides the correct dimensional units, and $H(\sigma)$ is the system's Hamiltonian which expresses the energy associated to each configuration of the system. The partition function Z is the normalization factor obtained by the condition $\sum_{\sigma} P_{\mathrm{eq}}(\sigma) = 1$ and reads $Z = \sum_{\sigma} \exp\left(-H(\sigma)/k_{\mathrm{B}}T\right)$. In other words, in the case of equilibrium physical systems there is no need to solve the complicated ME, and the stationary properties of the system may be obtained by knowing the system's Hamiltonian. As we will see in Chapter 5, the knowledge of the equilibrium distribution does not imply that the system's behavior is trivial. The properties of the system are indeed defined by the trade-off between the probability associated with a certain configuration at a certain energy and the number of configurations (the entropic contribution) close to that energy. The temperature, T, acts as a parameter modulating these two contributions, and the system changes its properties, often abruptly as in the case of phase transition, when the value of T varies. At a mathematical level the changes in the system's properties are associated with the singularities of $P_{\mathrm{eq}}(\sigma)$ whose calculation corresponds to an exact solution for the partition function Z, which is generally not possible.

The equilibrium distribution defines the solution of the ME and it is always possible to find transition rates that drive the system towards the equilibrium distribution by imposing the so-called *detailed balance condition* on the ME

$$P_{\mathrm{eq}}(\sigma)W(\sigma \to \sigma') = P_{\mathrm{eq}}(\sigma')W(\sigma' \to \sigma). \tag{4.5}$$

This relation states that the net probability current between pairs of configurations is zero when $P = P_{\mathrm{eq}}$. We will see in the next sections that this fact will allow

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us to construct the basic dynamical algorithms needed to simulate the microscopic dynamics of equilibrium systems.

The detailed balance is a strong condition that implies that each pair of terms in the ME has a null contribution. This is not the case for systems out of equilibrium, for which the microscopic processes violate the detailed balance and the currents between microstates do not balance. This might simply be the case of a system that has not yet reached the equilibrium stationary state and is still in a transient state. However, a wide range of different systems can be found constantly out of the detailed balance condition. In general, most systems are not isolated but are subject to external currents or external driving forces, the addition of energy and particles, or the presence of dissipation, and are therefore out of equilibrium. This is generally due to the fact that even in the stationary state the transition to a certain subset of configurations may be favored. Furthermore, a large class of non-equilibrium systems is confronted with the presence of absorbing states. These are configurations that can only be reached but not left. In this case we always have a non-zero probability current for some configurations so that the temporal evolution cannot be described by an equilibrium distribution. This is indeed what happens for a large number of spreading and reaction–diffusion systems used to model epidemic processes, as we will see in the following chapters.

It must be clear, however, that the lack of detailed balance does not imply the absence of a stationary state. Indeed, while the detailed balance (4.5) is a sufficient condition to achieve $\partial_t P(\sigma, t) = 0$, it is not necessary and the same result may be obtained through more complicated cancellations among terms of the ME, which can still lead to a stationary state. A typical example is provided in Figure 4.1, where we consider an equilibrium and a non-equilibrium system which can exist in only four different configurations A, B, C, and D. In the equilibrium case we

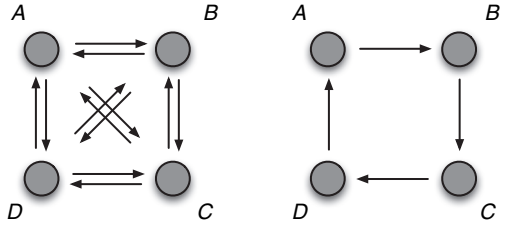

Fig. 4.1. Illustration of the detailed balance and non-equilibrium steady states in the case of different transition rates. The figure sketches two systems with four different microstates A, B, C, and D. On the left, the system obeying the detailed balance has equal transition rates among all pairs of states. On the right, transition rates allow only a specific directionality leading to a non-null probability current. In both cases, however, the system reaches a stationary state distribution function in the phase space with $P(A) = P(B) = P(C) = P(D) = 1/4$.

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have, for all pairs of configurations X and Y, that $W(X \to Y) = W(Y \to X) = 1$, while in the non-equilibrium case the transition rates are $W(A \to B) = W(B \to C) = W(C \to D) = W(D \to A) = 1$ (the other rates being zero). Although the non-equilibrium system does not satisfy the detailed balance condition, both dynamics have the stationary state $P(A) = P(B) = P(C) = P(D) = 1/4$, as can easily be seen from an explicit computation of the ME. In the following we shall see that most of the considered dynamical processes relevant in real-world applications are indeed non-equilibrium phenomena for which it is not possible to provide equilibrium thermodynamic formulations.

4.3 Approximate solutions of the Master Equation

The complete solution of the master equation is rarely achievable even for very simple dynamical processes. For this reason we present suitable approximation schemes that can provide at least an approximate solution for the system behavior.

A first step in the simplification of the ME is the consideration of appropriate projections focusing on specific quantities of interest. For instance, we can inspect quantities such as

$$N_x(t) = \sum_{\sigma} \sum_{i} \delta_{\sigma_i, x} P(\sigma, t), \tag{4.6}$$

where $\delta_{\sigma_i,x}$ is the Kronecker delta symbol, which is 1 if the node i is in the state x and 0 otherwise. The function $N_x(t)$ is simply the average number of nodes in the state x at time t, and we omit for the sake of clarity in the notation the average symbol $\langle \cdots \rangle$, which is, however, implicit in the definition of $N_x(t)$. As we are dealing with average quantities the obtained equations will be deterministic and will not account for the fluctuations inherent to the stochastic process.[1]

The deterministic projection, however, is not sufficient and further approximations are required to obtain a solvable and closed form of the ME. A typical approximation scheme is the so-called homogeneous assumption (HA) or mean-field (MF) theory. This scheme assumes that the system is homogeneous and that no relevant correlation exists between the microstate variables. In other words, all elements i of the system have the same properties and the interaction they feel is an average interaction due to the full system. This is generally encoded in a mass action or mean-field interaction with the other elements of the system. In more mathematical terms, the homogeneous assumption neglects all correlations and considers that the probability for a given element i to be in a given

[1] From the master equation it is possible to obtain stochastic differential equations accounting for the noise present in the system by using the Langevin formulation. Langevin equations are generally solvable in only a few cases.

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state $\sigma_i = x$ is a quantity p_x independent of i. Furthermore, the probability of any system configuration is the product measure (no correlations) of single node probabilities:

$$P(\sigma) = \prod_i p_{\sigma_i}. \tag{4.7}$$

The ME deterministic projection and the mean-field approximation allow writing sets of equations such as

$$\partial_t N_x(t) = F_x(N_1, N_2, \ldots, N_\kappa), \tag{4.8}$$

where $x = 1, 2, \ldots, \kappa$ index the possible states of each individual node. These equations concern average values and are deterministic. The explicit form of the functions F_x depends on the specific interactions among the nodes, the transition rates, and the number of allowed microstates. In the rest of the book we will use the above approximation schemes as a general methodology in order to obtain an approximate analytic description of many systems. In constructing the MF or HA equations we will use general considerations on effective interactions and mass-action laws rather than a precise derivation from the basic ME. This allows a more rapid, versatile and intuitive derivation of the evolution equations of many systems, but it is important to keep in mind that the MF techniques are based on a general and formal approximation scheme. For this reason, we present here an instance of the MF approximation scheme in the case of a simple system and we show in detail how the basic deterministic MF equations are derived. This derivation is not necessary to understand the analytical schemes presented in the rest of the book, but for the sake of completeness we believe that it is important to detail the approximation scheme in at least one case.

Let us consider a very simple system in which each node can be in only two states $\sigma_i = A$ and $\sigma_i = B$. The dynamics of the system are simply described by a reaction process of the type $A + B \to 2B$. More precisely, the transition from A to B is irreversible and occurs with rate β each time a node in the state A is connected to at least one node in the state B. This simple reaction scheme defines the transition rates $w(A \to A|\sigma_j = A) = w(B \to B|\sigma_j = A) = w(B \to B|\sigma_j = B) = 1$, $w(A \to B|\sigma_j = B) = \beta$, where σ_j represents the state of the nodes j connected to i and we considered unitary rates $\sum_{\sigma'} w(\sigma \to \sigma'|\sigma_j) = 1$. In order to define deterministic equations we use the quantities

$$N_A(t) = \sum_\sigma \sum_i \delta_{\sigma_i, A} P(\sigma, t), \tag{4.9}$$

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and

$$N_B(t) = \sum_{\sigma} \sum_{i} \delta_{\sigma_i, B} P(\sigma, t), \tag{4.10}$$

which are the average number of nodes in the state A or B at time t, respectively. By plugging the above projection in the ME we obtain the equation for the average number of nodes in the state B:

$$\begin{aligned} \partial_t N_B(t) &= \sum_{\sigma} \sum_{i} \delta_{\sigma_i, B} \partial_t P(\sigma, t) \\ &= \sum_{i} \sum_{\sigma'} \sum_{\sigma} \Bigg[\delta_{\sigma_i, B} \prod_{k} w(\sigma'_k \to \sigma_k | \sigma'_j) P(\sigma', t) + \\ &\qquad - \delta_{\sigma_i, B} \prod_{k} w(\sigma_k \to \sigma'_k | \sigma_j) P(\sigma, t) \Bigg], \end{aligned} \tag{4.11}$$

which can be readily simplified by noting that the term on the right-hand side can be rewritten using the normalization conditions

$$\sum_{\sigma'} \prod_{k} w(\sigma_k \to \sigma'_k | \sigma_j) = 1, \tag{4.12}$$

$$\sum_{\sigma} \delta_{\sigma_i, B} \prod_{k} w(\sigma'_k \to \sigma_k | \sigma'_j) = w(\sigma'_i \to \sigma_i = B | \sigma'_j), \tag{4.13}$$

finally yielding

$$\partial_t N_B(t) = \sum_{i} \sum_{\sigma'} \left[w(\sigma'_i \to \sigma_i = B | \sigma'_j) P(\sigma', t) \right] - N_B(t). \tag{4.14}$$

So far we have not yet used the MF approximation, which is introduced by stating that the probability for each node to be in the state A or B is $p_A = N_A/N$ and $p_B = N_B/N$, respectively. This implies that all nodes have the same probabilities independent of the states of the other nodes. In addition, neglecting correlations allows us to write $P(\sigma', t) = \prod_i p_{\sigma'_i}$. By using this approximation we have

$$\begin{aligned} &\sum_{\sigma'} w(\sigma'_i \to \sigma_i = B | \sigma'_j) P(\sigma', t) \\ &= \sum_{\sigma'_j} \Bigg[w(\sigma'_i = A \to \sigma_i = B | \sigma'_j) p_A \prod_{j \in \mathcal{V}(i)} p_{\sigma'_j} + \\ &\quad + w(\sigma'_i = B \to \sigma_i = B | \sigma'_j) p_B \prod_{j \in \mathcal{V}(i)} p_{\sigma'_j} \Bigg], \end{aligned} \tag{4.15}$$

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where the sum is now restricted to the nodes j connected to the node i. This expression can be further simplified by noticing that $w(\sigma_i' = B \to \sigma_i = B|\sigma_j') = 1$ whatever the configuration of j and that $w(\sigma_i' = A \to \sigma_i = B|\sigma_j') = \beta$ if at least one of the connected nodes j is in the state B. This will happen with probability $1-(1-p_B)^k$, where k is the number of neighbors of i, which we assume to be the same for all nodes of the network. By substituting the previous expressions in the deterministic equation (4.14) one obtains

$$\partial_t N_B(t) = \sum_i \left(\beta p_A(1-(1-p_B)^k) + p_B\right) - N_B(t), \tag{4.16}$$

and by using the expression for p_B and p_A and summing over all nodes i we obtain

$$\partial_t N_B(t) = \beta N_A(1-(1-N_B/N)^k). \tag{4.17}$$

A final simplification can be obtained in the limit $N_B/N << 1$ that yields the dynamical equation

$$\partial_t N_B(t) = \beta k \frac{N_A N_B}{N}. \tag{4.18}$$

This deterministic equation is easily solved analytically or by numerical integration. The equation for N_A in this case follows trivially from the conservation rule $N_A = N - N_B$. Equation (4.18) is the MF expression for the basic $A + B \to 2B$ process which also describes a wide range of epidemic spreading phenomena without recovery (the so-called SI model, see Chapter 9). The above equation is analogous to a mass action equation in which the per capita force of *transition* is given by the density of particles B times the number of contacts k per unit time. This also shows that in the case of a small probability p_B the MF approximation is equivalent to the homogeneous assumption using mass action laws. The deterministic MF equations can also be used to provide phenomenological Langevin equations in which Poissonian noise is added to the reaction terms. Phenomenological Langevin equations are, however, valid only under a set of precise conditions which in general are only partially satisfied. Finally, it is worth stressing that we have considered here a completely homogeneous network in which all nodes have the same degree k. We will see in the forthcoming chapters how to generalize similar equations to the case of heterogeneous networks.

4.4 Agent-based modeling and numerical simulations

In more complicated models, even the deterministic approach might not lead to solvable equations. In addition, this framework is intrinsically considering a coarse-grained perspective that does not take into account individual heterogeneity or other possible fluctuations. Numerical integration on the computer of the

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obtained equations therefore does not provide a complete picture of the system. In this situation, microscopic computer models, often defined as agent-based models (ABM), can be applied.[2] In these approaches each individual node is assumed to be in one of several possible states. At each time step, the model-specific update procedure that depends on the microscopic dynamics is applied to each node, which as a result changes its state depending on the state of neighboring nodes or other dynamical rules. Notably, the model's stochasticity may be introduced using Monte Carlo simulations in which rates and probabilities are mimicked in the computer with the use of random number generators. The microscopic perspective of this approach is evident in the fact that one can follow the dynamics of each individual element. In addition, the defining dynamics occur at the level of the microscopic interactions among elements, and the statistical regularities and macroscopic properties of the system are studied by looking at aggregate or average quantities. In principle, this kind of approach recreates the system within the computer, providing access to the microscopic dynamics of the system that is in general hindered by the mathematical complexity and the large number of degrees of freedom inherent to large-scale systems. The computer is therefore used as an in-silico laboratory to study complex realities not accessible mathematically or experimentally.

This way of approaching large-scale systems has a long tradition in physics. The physical laws ruling the interactions of molecules and atoms have been used in computer models of fluid dynamics, condensed matter, statistical physics and so on to provide realistic microscopic numerical simulations of systems ranging from material science and engineering to meteorology. Moreover, this tradition is one of the reasons why so many physicists enter other disciplines to exploit numerical and microscopic approaches in contexts outside physics.

In statistical physics the tradition of microscopic numerical simulations has been triggered by the advent of Monte Carlo methods in equilibrium systems. This technique has been introduced to solve the sampling problems in the numerical evaluation of physical observables. In order to provide an average of any physical quantities we must sample the quantity of interest over all the possible configurations σ that the system can assume. Even in the case of a simple system with only two states A and B this corresponds to 2^N configurations, where N is the number of elements in the system. Exhaustive enumeration is feasible only for modest sizes $N \lesssim 100$ and sampling techniques have to be used for large system sizes. On the other hand, each configuration contributes with a factor $P(\sigma)$ and most

[2] In some cases the name individual-based model is a more appropriate characterization in social and economical systems where each agent can be thought of as an individual performing a specific task or pursuing a set of defined tasks.

configurations are virtually inaccessible, so that sampling must take into account this heterogeneity. In the case of equilibrium systems this problem can be tackled by taking advantage of the detailed balance condition stating that

$$\frac{W(\sigma \to \sigma')}{W(\sigma' \to \sigma)} = \frac{\exp(-H(\sigma')/k_{\mathrm{B}}T)}{\exp(-H(\sigma)/k_{\mathrm{B}}T)}. \tag{4.19}$$

Any transition rate or probability at the microscopic level satisfying this relation ensures the convergence to the correct equilibrium distribution and can then be used to generate a microscopic dynamics to sample the configuration space. This relation does not, however, specify the transition rates uniquely as it involves ratios, and a rescaling factor has to be used for both terms. A common choice is the so-called Metropolis algorithm in which the transition probability from a configuration σ to σ' is defined as

$$\begin{aligned} W(\sigma \to \sigma') &= \exp\left(-\frac{H(\sigma') - H(\sigma)}{k_B T}\right) && \text{if } H(\sigma') > H(\sigma) \\ &= 1 && \text{if } H(\sigma') \leq H(\sigma). \end{aligned} \tag{4.20}$$

The Metropolis algorithm can be used to define a microscopic dynamics in which single elements are randomly chosen to change their state. The relative change is therefore accepted or rejected with the above rates (or probability in the case of finite time steps). The physics behind this is very simple. Every microscopic rearrangement that moves the system into a lower energy state is accepted with unit rate, while a move that increases the energy is accepted with a rate progressively smaller (exponentially decaying) according to the Boltzmann factor. It is trivial to see that the above expression satisfies by definition the detailed balance condition. The method can therefore be used in the computer to generate a series of configurations that, in the large time limit, properly samples the phase space. In this framework, the computer generates a Markov chain of states that can be used to correctly sample the phase space and evaluate the average of statistical observables.[3]

While in physical systems energetic considerations provide an intuitive basis to the algorithm, it is clear that in any system obeying the detailed balance condition, an appropriate microscopic dynamics can be defined by starting from the equilibrium distribution. Similar Monte Carlo methods and Markov chains are, for example, used in the modeling of the exponential random graph family presented in Chapter 3. It is important to remark that the dynamics used correctly samples only the equilibrium state and the approach to equilibrium can therefore depend upon the details of implementation, such as the choice of whether to update more

[3] Such a chain is Markovian since every state depends only on the previous one, and not on the full history of the system.

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than one element at a time in choosing the new configuration, and the choice of time scale used. The initial starting configuration can also have an impact on the transient to the equilibrium distribution. We refer the interested reader to the classic books of Newman and Barkema (1999), Binder and Heermann (2002), Krauth (2006) for a thorough survey of Monte Carlo methods.

The success of Monte Carlo methods has paved the way for the use of microscopic computer simulations for the study of large-scale systems and their macroscopic properties. Unfortunately, the lack of detailed balance conditions in the case of non-equilibrium systems requires a different strategy. Indeed, the only way to ensure the study of the correct dynamical evolution and stationary state is the implementation of the actual microscopic dynamics ruling the evolution of the elements of the system. This implies a shift of focus from the static equilibrium perspective to dynamical models where the microscopic interaction is at the center of the system's description. This approach has been exploited in a wide range of non-equilibrium systems and is now customarily used to check the reliability and consistency of analytical results obtained through approximate methods. The microscopic approach has been historically used in other areas including theoretical epidemiology, population ecology, and game theory, often with a different name, such as mechanistic approach or individual-based modeling.

The next chapters will provide numerous examples of the application of such approaches, used in parallel with and as a complementary tool to approximate analytical approaches. For completeness of the present chapter, let us consider the reaction process $A + B \to 2B$ described in the previous section. To this end, we consider an Erdős–Rényi network of N sites, with average degree $\langle k \rangle = 10$. We start from a configuration in which all sites are in state A except for one in state B. The simulation proceeds by updating at each time step the state of all nodes in state A that are in contact with a node in state B. The reaction rate is set to $\beta = 10^{-2}$. It is straightforward to follow the evolution of the number of nodes in state B over time, as shown in Figure 4.2. The different symbols correspond to different stochastic realizations of the dynamics, while the solid line is an average over realizations of the dynamics and of the underlying network. Such simulations give easy access to quantities averaged either for a single run over the nodes or over many realizations of the dynamical process. The extent to which a single realization of the process can deviate from the average behavior can also be inferred from such simulations.

One of the advantages of agent-based numerical simulations is that they allow extremely detailed information to be obtained and, in fact, provide a way to monitor the single state of each agent at any time. Figure 4.3 illustrates such a possibility for the same reaction process $A + B \to 2B$ on a Watts–Strogatz network of $N = 150$

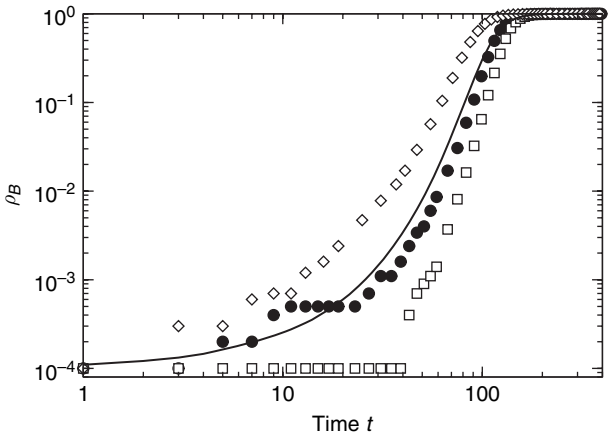

Fig. 4.2. Numerical simulations of the reaction process $A + B \rightarrow 2B$ on an Erdős–Rényi network of size $N = 10^4$ and average degree $\langle k \rangle = 10$, for a reaction rate $\beta = 10^{-2}$. The symbols show the evolution of the density $\rho_B = N_B/N$ of sites in state B for various runs, starting from a single node in state B at time 0, while the full line corresponds to the average of ρ_B over 20 realizations of the network, with 20 runs on each network realization. Especially at short times, the behavior of a single run can deviate substantially from the average evolution.

nodes (see Chapter 2).[4] The network is shown on the left of the figure as a vertical line with shortcuts. Note that periodic boundary conditions are used, i.e. the node at position $N = 150$ and the node at position 1 are considered to be neighbors. Time is shown as the horizontal axis, and the state of each node is coded as white if in state A and black if in state B. The initial state is given by one single node i_0 (here at position 108) in the B state. The first steps correspond to a propagation of the B state to the neighbors of i_0, i.e. to a coarsening phenomenon. When nodes connected to shortcuts change state, they allow new coarsening processes to be nucleated from seeds which are distant on the line. For comparison, we also show in Figure 4.3 the case in which no shortcuts are present on the one-dimensional line: a clear spatial pattern emerges and a single coarsening process is then observed as the B state is passed from each site to its neighbors along the line.

In recent times ABM approaches have become fashionable in a wide range of scientific areas such as economics, urbanscience, ecology, management, and organizational sciences. In some cases, ABMs have been put forward by enthusiasts as alternative approaches destined to revolutionize entire scientific areas and have therefore generated a reaction of mixed skepticism and mistrust from

[4] For the sake of clarity, we use a small network; storing the complete information on the dynamical states of all nodes soon becomes impossible as N grows, but ABMs, in any case, allow control over the precise evolution of any subset of nodes that may have particular relevance in the characterization and understanding of the process dynamics.

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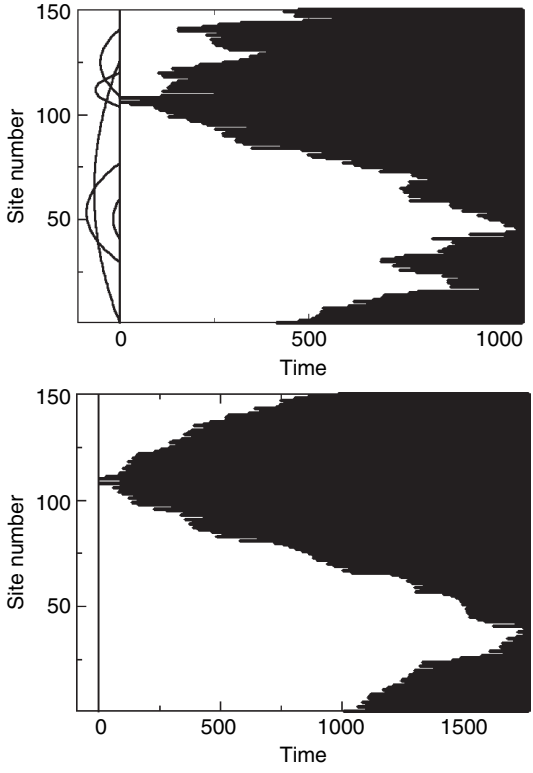

Fig. 4.3. Top: Evolution in time of one realization of the reaction process $A + B \to 2B$ on a small-world network of $N = 150$ sites (rewiring probability $p = 0.02$, average degree $\langle k \rangle = 4$, reaction rate $\beta = 10^{-2}$), with periodic boundary conditions (node 150 and node 1 are neighbors). Each site is shown in white when in state A, and in black when in state B. The dynamics starts with the single site 108 in state B. It first proceeds by coarsening around the initial site, and the long-range links depicted on the left of the figure allow new infection seeds to be nucleated at distant positions: for example, when site 109 changes to state B, it allows the process to reach site 141 directly, before the intermediate sites have changed state. On the bottom figure, we show the same process taking place on a one-dimensional line with no shortcuts. Note that the change of state of node 1 and its neighbors at time $t \approx 1000$ is due to the periodic boundary conditions for which nodes 150 and 1 are neighbors.

many scientists. This is mostly due to works that use a large number of unjustified assumptions, unphysical and/or non-measurable parameters in the definition of the agent-based model. In such cases, the models used are, in general, not falsifiable and propose microscopic rules that can be hardly, if at all, experimentally observed in the real systems.

Indeed, microscopic modeling approaches have the important advantage of fully incorporating stochastic effects and simulating very complicated dynamical

processes. On the other hand, while extremely powerful, ABMs are often not transparent, since it quickly becomes difficult to discriminate the impact of any given modeling assumption or parameter as the number of parameters grows. ABMs in general have very few analytical tools by which they can be studied, and often no backward sensitivity analysis can be performed because of the large number of parameters and dynamical rules incorporated. This calls for a trade-off between the level of details included in the dynamics and the possibility of some understanding of the basic properties of the system beyond the simple computer simulations just described.