Pattern Formation in Cellular Automaton Models –
Characterisation, Examples and Analysis

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**Cellular automata** (von Neumann 1966) are fully discrete dynamical systems. Space is represented by a regular lattice while time proceeds in finite steps. Each cell of the lattice is assigned a state, chosen from a finite set of ‘values’. The states of the cells are updated synchronously according to a local interaction rule, whereby each cell obeys the same rule. A basic problem in cellular automaton modelling is the so-called **inverse problem.** It concerns the search for local rules which reproduce a given phenomenon, e.g. spatial pattern formation. On the other hand, the **forward problem** is to connect given spatially localised dynamic rules and the corresponding ‘global’ space–time dynamic patterns (Gutowitz 1990c). The subject of this thesis is to investigate both problems with regard to space–time processes, in particular movement, single–component growth and many–component interactions. Rules, which characterise such processes are designed and explored. It turns out, that combinations of interaction and movement processes allow an analytic treatment of the cellular automaton by means of approximation models.
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1 Introduction

1.1 Modelling approaches for spatially extended dynamical systems

Models are tools for dealing with reality (Bossel 1994). They are ‘caricatures’ of the real system\(^1\) and built with a particular purpose in mind. In other words, models exist to answer questions. For example, by capturing the consequences of a small number of key processes, while leaving out many details, simple models might be designed just to gain a better understanding of reality (Gurney and Nisbet 1989). Here, not only the investigation of a ‘final model’ is important but also the process of modelling, because it forces the modeller to a detailed system analysis. Other objectives may be to try out changes in the assumptions\(^2\), to test different scenarios, to demonstrate that certain ideas should or cannot be realised or to give predictions for the future. Models presented in this thesis are not aimed to reproduce or to predict concrete field situations, but to obtain an understanding of the relatively simple mechanisms they are meant to represent. This kind of models are called strategic (Gurney and Nisbet 1989). Especially formal models\(^3\) for dynamical systems, where the set of assumptions about reality is expressed in mathematical (mathematical model) or a computer (simulation model) language, have turned out to be very useful. Note that not all mathematical models are open to mathematical analysis but that all of them can be simulated on a computer. When an analytic solution is available, it provides a complete characterisation of the system dynamics. However, in many cases analytic solutions tend to be impossible to derive or to involve formulas which are too complex. On the other hand many simulation models can not be described in a mathematical framework in a way that they become accessible to an analytical mathematical analysis\(^4\). These models have to be investigated by means of statistics of many simulation runs. Here, we concentrate on mathematical model approaches. The choice of a model approach depends on the characteristics of the dynamical system

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\(^1\)Loosely stated, a ‘system’ is defined as a set of elements which are interrelated and related to a precisely defined environment (Bossel 1994).

\(^2\)Especially, in order to find out which assumptions are essential.

\(^3\)In contrast to physical models, e.g. scale models (maps, miniaturised realistic representations of a house or a car), and pure semantic models, which are mainly used in psychology and social sciences.

\(^4\)For example agent-based models and models in the framework of artificial life research (Langton 1989)
itself and on the aspects of the dynamical system which have to be emphasised according to the model purpose (Hastings 1994). Therefore, interdisciplinary work is important because those who are experts on the structure of the real system have to work together with those who are experts on the structure of the mathematical modelling approaches. One possibility to classify approaches to modelling spatially extended dynamical systems is to distinguish between continuous and discrete state, time and space variables. A classification of different approaches along this line is shown in Tab. 1.1.

<table>
<thead>
<tr>
<th>model approach</th>
<th>state variable</th>
<th>time variable</th>
<th>space variable</th>
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<tbody>
<tr>
<td>coupled differential equations</td>
<td>continuous</td>
<td>continuous</td>
<td>discrete</td>
</tr>
<tr>
<td>partial differential equations</td>
<td>continuous</td>
<td>continuous</td>
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<tr>
<td>deterministic / stochastic</td>
<td>continuous</td>
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<td>coupled map lattices</td>
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<td>lattice Boltzmann models</td>
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<td>interacting particle systems</td>
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<td>cellular automata</td>
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<tr>
<td>lattice–gas cellular automata</td>
<td>discrete</td>
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Table 1.1: Various approaches for mathematical modelling.

The answer to the question if a process is state–, time– or space– ‘discrete’ or ‘continuous’ is very important, because the particular choice may influence the results significantly. For example, while the time–continuous logistic ordinary differential equation describes a simple growth process, the time–discrete logistic map leads to ‘complex’ dynamical behaviour, including chaotic motion (Kaplan and Glass 1995). In order to give appropriate answers the scales of all involved processes and their relation to each other have to be analysed. For instance, a variable (e.g. temperature) can be regarded as constant if the chosen time–scale is short, but if it is large the dynamics of the variable might become important.

**Coupled differential equations**

An example for this approach is Turing’s cellular model (Turing 1952), whose purpose is to explore how spatial structures (forms, patterns) can emerge from a homogeneous situation (see also Sec. 5.1). Space is divided into discrete compartments \( r = 1, \ldots, L \) (spatially homogeneous cells) in which different components \( \sigma = 1, \ldots, \varsigma \) are dynamically governed by ordinary differential equations. The component variables \( a_\sigma(r, t) \in \mathbb{R} \) usually represent macroscopic quantities, e.g. densities. Spatial interactions are modelled by discrete
coupling of components of different cells. In particular, Turing suggested the following nearest neighbour coupling of a ring of cells for a two-component one-dimensional system:

\[
\begin{align*}
\frac{\partial a_1(r,t)}{\partial t} &= F_1(a_1(r,t),a_2(r,t)) + D_1 \left( a_1(r-1,t) - 2a_1(r,t) + a_1(r+1,t) \right), \\
\frac{\partial a_2(r,t)}{\partial t} &= F_2(a_1(r,t),a_2(r,t)) + D_2 \left( a_2(r-1,t) - 2a_2(r,t) + a_2(r+1,t) \right),
\end{align*}
\]

with continuous time \( t \in \mathbb{R} \) and \( D_\sigma \in \mathbb{R} \), which expresses the rate of exchange of species \( \sigma \) at cell \( r \) and the neighbouring cells (‘diffusive coupling’).

An advantage of coupled differential equations is the possible adaptation of the transport scheme (coupling) to particular system demands, e.g. to extended local neighbourhood relations. Furthermore, e.g., in ecology, truly ‘patchy environmental situations’ as species on oceanic islands or forest patches can be adequately described using the coupled differential equation ansatz (Levin 1986).

**Partial differential equations (PDEs)**

**Deterministic PDEs** The classical approach to model spatially extended dynamical systems are partial differential equations, which model space as a continuum\(^5\), \( x \in \mathbb{R}^d \), where \( d \) is the space dimension. In the simplest version movement is assumed to be passive diffusion (see also Chapter 3). Then, a two-component one-dimensional system is described by

\[
\begin{align*}
\frac{\partial a_1(x,t)}{\partial t} &= F_1(a_1(x,t),a_2(x,t)) + D_1 \frac{\partial^2 a_1(x,t)}{\partial x^2}, \\
\frac{\partial a_2(x,t)}{\partial t} &= F_2(a_1(x,t),a_2(x,t)) + D_2 \frac{\partial^2 a_2(x,t)}{\partial x^2},
\end{align*}
\]

where \( t \in \mathbb{R} \) and \( D_\sigma \in \mathbb{R} \) are ‘diffusion coefficients’. A vast literature deals with a framework based on ‘reaction–diffusion’ models\(^6\) (reviewed in Okubo (1980)). They describe interaction processes and demographic dynamics, commonly called reaction, which are combined with movement processes.

**Stochastic PDEs** The so-called *Langevin approach* defines a stochastic partial differential equation which results from a microscopic stochastic description of the system. Random moving particles \( i = 1, \ldots, N \) are characterised by their space–position \( x_i(t) \in \mathbb{R}^d \), where \( d \) is the spatial dimension. Furthermore, the random particle movement might be influenced by an external field \( s(x,t) \). Hence, the state of the system is determined by the vector \( \mathbf{x}(t) = \left( x_i(t) \right)_{i=1}^N \), and the time evolution of the position of each particle is

\(^5\)Note that this implies an infinite amount of information about the state values in any arbitrarily small space–time volume.

\(^6\)Although movement is not generally of purely diffuse nature, such systems are also referred to as reaction–diffusion systems.
assumed to be described by a Langevin equation of the type

\[
\frac{dx_i}{dt} = v_i, \quad \frac{dv_i}{dt} = -\gamma v_i + \nabla s(t, x_i) + \sqrt{2\epsilon \gamma \xi_i(t)},
\]

where \( \gamma \) is a friction constant, \( \nabla s(t, x_i) \) is the gradient of the external field, and \( \xi_i(t) \) is Gaussian white noise with intensity \( \epsilon \), which reflects individual variations of state changes. A typical example of this approach in biology is the active random walk of many particles, e.g. cells, which leads to pattern formation. For example, chemotactic cell aggregation has been studied using this ansatz (e.g. Stevens and Schweitzer 1997; see also Chap. 6, p. 143).

**Coupled map lattices**

If both, space \( (r) \) and time \( (k) \), are considered as subdivided into units, one refers to coupled map lattices or **time- and space-dependent difference equations**\(^7\). An example for a one-dimensional two-component system is

\[
\begin{align*}
a_1(r, k + 1) &= F_1(a_1(r, k), a_2(r, k)) \\
&\quad + D_1(a_1(r - 1, k) - 2a_1(r, k) + a_1(r + 1, k)), \\
a_2(r, k + 1) &= F_2(a_1(r, k), a_2(r, k)) \\
&\quad + D_2(a_2(r - 1, k) - 2a_2(r, k) + a_2(r + 1, k)).
\end{align*}
\]

This model approach was introduced in order to study spatio-temporal chaos, which is important in the study of turbulence (Kaneko 1993). Coupled map lattices are also used as a tool for numerical studies of partial differential equations. **Lattice Boltzmann models** are a particular case of coupled map lattices. They can be derived from a microscopic description (lattice–gas cellular automaton) of (physical) systems\(^8\), which are composed of many ‘particles’ (e.g. fluid dynamics, McNamara and Zanetti 1988). Then, the state variables \( a_n(r, k) \in [0, 1] \) are defined by averaging over an ensemble of independent copies of the lattice–gas cellular automaton, i.e. they represent the probability of the presence of a particle at a cell \( r \) at time \( k \). When spontaneous fluctuations and many–particle correlations can be ignored this approach offers an effective simulation tool in order to obtain the macroscopic behaviour of the system and provides a ‘natural interpretation’ of the numerical scheme (Chopard and Droz 1998).

**Interacting particle systems**

Interacting particle systems model directly interactions between finitely or infinitely many particles (e.g. individuals, molecules). They are stochastic models consisting of a collection of spatial locations called sites and a finite set of states. Each site can be in one particular state at each time \( t \in \mathbb{R} \). The temporal evolution is described by specifying a rate at which each site changes

\(^7\)for finite–difference equations

\(^8\)for further details see Sec. 2.3.1
Modelling approaches

its state. The rate depends upon the states of a finite number of neighbouring sites. In the absence of interaction, each site would evolve according to independent finite or countable state Markov chains (Liggett 1985). When an event occurs at a constant rate $\alpha$ then the time intervals between successive occurrences are exponentially distributed (Poisson distribution) with expectation $\alpha$ (Durrett 1993). The ensemble of states of all lattice sites defines a configuration or a microstate of the system$^9$.

**Cellular automata**

The extreme level of discreteness is reached by cellular automaton modelling (Wolfram 1983). Cellular automata can be viewed as discrete–time interacting particle systems. In the 1950’s John von Neumann (1903–1957) and Stanislaw Ulam (1909–1984) proposed the concept of cellular automata with the specific purpose to determine the kind of logical organisation that is sufficient for an automaton$^{10}$ to be self–reproducing (von Neumann 1966). The following definition of a cellular system is quoted from Burks (1970) and is based on a manuscript which von Neumann had left incomplete$^{11}$:

“The notion of a cellular automaton is built up in the following way. We begin with a cellular space, which consists of an infinite $n$–dimensional Euclidean space together with a neighborhood relation defined on this space. The neighborhood relation gives, for each cell, a finite list of cells which are its neighbors. The time basis of the system is synchronous, with $t = 0, 1, 2, 3, \ldots$ . A cellular automaton system (or “cellular system,” for short) is specified by giving a finite list of states for each cell, a distinguished state (called the “blank state”), and a rule which gives the state of a cell at time $t + 1$ as a function of its own state and the states of its neighbors at time $t$. We will call the list of states for a cell together with the rule governing the state transition of a cell a transition function.”

Note that we give a more formal definition of cellular automata in Sec. 2.1. Von Neumann’s specific self–reproductive cellular system is based on a (very large) two–dimensional square lattice and 29 possible states. The neighbourhood of each cell consists of the cell itself and the four nearest neighbours. The very complex transition function is deterministic (Burks 1970).

In physics, discrete velocity models, e.g., of fluids or gases, have been developed independently from cellular automaton theory (Gutowitz 1990a). However, these types of models, now called lattice–gas cellular automata$^{12}$ (LGCA),

---

$^9$A good introduction into this modelling field can be found in Durrett (1999).

$^{10}$An automaton is a robot which gives specific responses to specific inputs.

$^{11}$manuscript title: 'The Theory of Automata: Construction, Reproduction, Homogeneity'

$^{12}$Note that there is still a controversial discussion whether lattice–gases should be viewed as cellular automata. For example, Hénon (1989) states that “Lattice gases differ in essence from cellular automata. A confusion of the two fields distorts our thinking, hides the special properties of lattice gases, and makes it harder to develop a good intuition. Lattice gases deserve a name of their own.” Contrary, according to Wolf-Gladrow (2000), traditional lattice–gases are referred to as lattice–gas cellular automata.
fit into the framework of cellular automata. The system is composed of ide-
alised particles. Each particle has associated a velocity taken from a finite set
of velocities, which indicate direction and distance that the particle will move
in one time step. At each node (cell) of the lattice at most one particle with
a particular velocity is allowed (exclusion principle). The transition rule of
LGCA is split into two parts: The first part corresponds to a transition rule for
cellular automata. It assigns new values to each node (cell) of the lattice based
on the values of the cells in a local neighbourhood. For example, particles can
change their velocity due to collisions with other particles at the same node. In
the second part, called propagation step, each particle is moved according to
its velocity. For a formal description of LGCA models see Sec. 2.1. The special
construction of the LGCA state space allows to describe synchronous move-
ment of many particles as, e.g., the independent random walk in the framework
of cellular automata (see Chap. 3).

Cellular automaton models are well suited for computer implementation due to
their discrete nature. They are computationally efficient, because no round–off
errors arise in the evaluation of the dynamics. Furthermore, cellular automaton
models are inherently numerically stable, whether additional rules are added to
or removed from the set of local rules. Therefore, it is straightforward to model
phenomena, e.g. complex boundary conditions, that are difficult to include
in more traditional approaches as partial differential equations. Moreover,
the derivation of local rules from a ‘microscopic level of description’ offers
an intuitive approach to represent the knowledge of the experts about the
structure of the real system. This might lead to more transparency of the
model. Since, in principle, there are no limitations to the design of local
rules, the cellular automaton approach has applications in many fields. On the
other hand, this ‘freedom’ makes it difficult to choose the appropriate rules.
There will always a trade–off between realism and tractability of the model
(Gutowitz 1990c). A few applications of physical, biological, chemical and
socio–economical systems are outlined in the next section.

1.2 Applications of cellular
automaton models

In principle, motivations for cellular automaton models are (I) the substantial
interest in the dynamics of cellular automata per se and (II) the interest in a
fundamental description of natural systems,

(I) Because cellular automata are discrete dynamical systems with simple con-
struction but complex self–organising behaviour, they are particularly suitable
for investigations under aspects of logical– and/or construction–universality
and ~complexity (von Neumann 1966). The probably most widely known and
1.2 Applications of cellular automaton models

studied cellular automaton model is the ‘game of life’, introduced in 1970 by the British mathematician John Horton Conway (Gardner 1970). It is a two–dimensional abstract ‘toy system’, with an analogy to the death and birth of stylized organisms. In each time step, the value of each cell which can be either ‘alive’ or ‘dead’ is updated according to the following rules which govern survival, birth and death: A ‘living’ cell surrounded by less than two or more than three ‘living’ cells amongst its eight nearest neighbours dies of isolation or overcrowdedness. On the other hand, a ‘dead’ cell will come to ‘life’ when it has exact three ‘living’ cells amongst its eight nearest neighbours. These rules lead to an amazingly complex behaviour. If the automaton is started with a random configuration of ‘living’ and ‘dead’ cells, eventually many different little stationary, moving or oscillating ‘objects’ emerge. Figure 1.1 shows the evolution of three objects called ‘glider’ (moving object), ‘blinker’ (oscillating object) and ‘boat’ (stationary object). The ‘glider’ moves down each

![Figure 1.1: Evolution of the ‘game of life’ automaton; black cells represent ‘living’ cells whereas ‘dead’ cells are white. Parameters: two–dimensional lattice with 11 x 11 cells, k = 0, ..., 15 time steps.](image)

time step along the diagonal from the top right to the top left in the lattice while permanently changing its shape. Every four time steps it appears in the same form (self–replicated). The ‘blinker’ changes every time step between a horizontal and a vertical orientation. When the ‘glider’ meets the ‘blinker’ (k = 8) both objects merge and evolve to a new stationary object, which is called ‘boat’. Many more such structures have been identified and studied in the ‘game of life’ (e.g. Gardner 1983, Berlekamp et al. 1985, Poundstone 1985). Because of the interesting structural features of the ‘game of life’ model, it has strongly motivated the study of so–called ‘artificial life’ systems (see e.g. Langton 1989). Furthermore, it was surprising that it could be proved that these simple rules lead to the capability of computational universality, i.e. any
A describable function of any other machine can be emulated by the defined set of rules (Poundstone 1985).

Another milestone in studying computational–theoretical aspects of cellular automata was the work by the British physicist Stephen Wolfram (1983). He studied in great detail a large family of simple one-dimensional cellular automaton rules and developed a comprehensive qualitative classification of their dynamics\textsuperscript{13}.

(II) Cellular automata of the second category can be viewed either as approximations of partial differential equations or as models of elementary interactions in nature (cf. Fig. 1.2).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure1.2}
\caption{Cellular automaton modelling dependent on the observation perspective; $\implies$ indicates discretisation while $\sim$ indicates averaging connections.}
\end{figure}

In the first case (i), the local cellular automaton rules are derived directly and systematically from given partial differential equations, using suitable deterministic or probabilistic rounding to enforce a discretisation of the variables (see e.g. Weimar 1997). This ‘top–down’ approach is based on a ‘macroscopic level’ of description, and not without difficulties. Since typically partial differential equations have to be solved numerically, special attention has to be put on numerical instabilities and on the conservation of certain quantities.

\textsuperscript{13}A collection of Wolfram’s papers from the period 1982 to 1986 can be found in Wolfram (1994).
1.2 Applications of cellular automaton models

The starting point in case (ii), the ‘bottom-up’ approach, is a ‘discrete microscopic point of view’. Cellular automata provide a very intuitive and powerful approach to capture the essential aspects of complex phenomena. Although these models are numerically stable and easily implemented on a computer, a major problem is to detect and avoid artificial behaviour.

During the last fifteen years the application of cellular automata in modelling the dynamics of complex physical, biological, chemical and socio-economic systems has become more and more popular. In order to illustrate the variety of cellular automaton applications or closely related models, we now describe some examples\(^{14}\).

Physical systems A well-known model used for understanding phase transitions in physical systems is the Ising model (Ising 1925), which was originally introduced for the study of ferromagnetic materials. Vichniac (1984) proposed a cellular automaton for this model. Each cell of a two-dimensional square lattice hosts a spin, which is the magnetic dipole associated to an atom. Spins are either ‘up’ or ‘down’. They can change their state (flip) if this does not cause any energy change locally. This is the case if the number of its nearest neighbours with spin ‘up’ is the same as the number of neighbours with spin ‘down’. Since the decision to flip is based on the assumption that the neighbours are not changing, even and odd sublattices are updated separately. Although in the real system spins can point into any direction and interact with more than just the nearest neighbours, with the simplified automaton description certain experimentally observed phenomena can be reproduced. For example, with this model it is easy to verify that if one kind of spin–state dominates the initial configuration, then a macroscopic magnetisation builds up as time goes on.

Other well-known applications of cellular automaton modelling in physics are lattice–gas cellular automata (LGCA) as models for fluids and gases. These models consist of fictitious particles, each with the same mass, moving and colliding in a two-dimensional lattice. Interestingly, although the particle dynamics has nothing in common with real molecular dynamics, the macroscopic flow mimics real fluids or gases. The first model of this kind was introduced by Hardy, de Pazzis, and Pomeau (1976) (HPP) who defined collision rules for particles living on a two-dimensional square lattice. At each time steps particles at a node experience a collision, in which the particle velocities are rearranged under the constraint of mass and momentum conservation. Subsequently, all particles ‘stream’ to the node in the direction of their velocity vector. Later on Frisch, Hasslacher, and Pomeau (1986) (FHP) proposed an extended model

which is based on a hexagonal lattice\textsuperscript{15}. They were able to show formally that on an appropriate macroscopic scale their model corresponds to the standard Navier–Stokes equations for fluid flow. Thereby, the extension to a hexagonal lattice was essential in order to obtain an isotropic fluid flow. Later, LGCA have been developed as models of flows in porous media, immiscible flows or microemulsions. However, not any fluid can be appropriately modelled with a LGCA. Lattice–gas fluids possess a relatively high viscosity, which is intrinsic to the model and is not an adjustable parameter (Chopard and Droz 1998). The viscosity of the discrete fluid primarily depends on the particle collision probability, which is determined by the collision rules: the smaller the particle collision probability is, the higher is the viscosity and hence the smaller is the Reynolds number\textsuperscript{16} of the fluid. Therefore, flows with relatively high Reynolds numbers cannot be adequately simulated with the LGCA approach. It turned out that the corresponding lattice–Boltzmann models (see p. 4), which are based on the neglect of any correlations, constitute a promising approach to modelling flows with higher Reynolds numbers (McNamara and Zanetti 1988). The Boolean dynamics of LGCA particle collisions is replaced by bulk particle behaviour (mean occupation numbers)\textsuperscript{17}.

**Biological systems**

Cellular automaton models have been applied to various biological problems, in particular developmental biology, neurobiology, immunology or population biology. As an example, we consider a cellular automaton–like **predator–prey model** (Wilson et al. 1993). Cells in a two-dimensional square lattice can be empty or occupied by a prey and/or a predator individual. The rules capture essential aspects of localised prey and predator reproduction, interaction and movement. Potential problems which can be analysed in this framework are the influence of individual mobility on the spatial distribution of individuals living in a homogeneous environment, the effect of an age–structured predator population or an age–structured predator mobility on spatial pattern formation (McCauley et al. 1993, McCauley et al. 1996).

Another biological application of cellular automata is **swarm dynamics**. A two–dimensional LGCA was introduced by Deutsch (1996)\textsuperscript{18} in order to model aligned motion of ‘oriented particles’ (e.g. birds, ants or myxobacteria). Every time step before particles move a fixed distance along their directions, they might change their orientations according to the orientation field in some neighbourhood. Simulations of this simple rule exhibit various spatial orientation

\textsuperscript{15}This model was almost simultaneously proposed also by (Wolfram 1986).

\textsuperscript{16}The Reynolds number is a dimensionless quantity which is the ratio of the characteristic spatial scale times velocity to viscosity of the flow. It is important in analysing any type of flow with a substantial velocity gradient. Turbulence is associated with high Reynolds numbers.

\textsuperscript{17}Rothman and Zaleski (1997), Chopard and Droz (1998) and Wolf-Gladrow (2000) are very recommendable references to this topic.

\textsuperscript{18}see also Bussemaker et al. (1997) and Deutsch (1999)
1.2 Applications of cellular automaton models

patterns, which can be characterised by means of microscopic and macroscopic variables as averaged density, mean velocity, local condensation and directionality. Deutsch (1999) extended the model by allowing the particles to rest. The change in the particle orientation is additionally influenced by the number of resting particles in the neighbourhood. With this supplement the model exhibits phase transitions between random dispersal, collective motion and (stationary) aggregation depending on a parameter shift of swarming and aggregation sensitivity, respectively.

Chemical systems  A model for the catalytic oxidation of carbon monoxides was proposed by Gerhardt and Schuster (1989). The surface oxidation of CO$_2$ is catalysed by palladium crystallites\(^{19}\) in a proper carrier\(^2^{20}\). The authors assume that each palladium crystallite first agglomerates oxygen (inactive phase) which is subsequently released after a certain threshold is reached (active phase). Furthermore, active crystallites catalyse the production of CO$_2$, which is enhanced by high temperatures. This process also releases heat which ‘diffuses’ locally. The cellular automaton model of this process is viewed as a two–dimensional lattice of palladium crystallites (cell–‘catalytic units’). The local rules defining the transition from active to inactive states of the cells are a variation of a general infection process. The temporal and spatial patterns produced by this automaton, e.g. circular waves, spiral waves, fractal–like oscillations or quasi–stationary patterns with only small fluctuations, have the same characteristics as the patterns observed in the real chemical catalytic system. Especially the formation of circular and spiral waves is surprisingly similar to pattern formation in excitable media\(^{21}\).

A collection of LGCA models for reactive systems can be found in Boon et al. (1996). Molecules of different species are represented as idealised particles which perform an independent random walk on a two–dimensional lattice\(^2^{22}\). The creation and destruction of particles at a lattice–node is governed by reaction probabilities which are derived from the reaction scheme in a systematic way. The authors illustrate this method by considering applications to bistable (Schlögl rate eqn.) and excitable (Selkov rate eqns.) media, oscillatory behaviour (Maginn rate eqns.) in reactive systems, chemical chaos (Willamowski–Rössler rate eqns.) and pattern formation triggered by Turing bifurcations (Selkov and Maginn rate eqns.). The study of this kind of models focuses on nucleation processes, the early stages of pattern formation, and a quantitative study of the role of fluctuations.

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\(^{19}\)This is a precious metal.

\(^{20}\)which is a zeolite matrix. Zeolites are minerals with a very porous structure which are found in nature or can be synthesized.

\(^{21}\)for a definition of excitable media see Sec. 5.2.

\(^{22}\)for a detailed description of the random walk of particles in LGCA see Sec. 3.4.
**Socio-economic systems** A cellular automaton–like model for opinion formation processes with a ‘strong leader’ was proposed by Kacperski and Holyst (1996, 1999). Individuals modelled as cells in a two–dimensional lattice–disc (social space) are assumed to share one of two opposite opinions on a certain subject. The geometric distance in the lattice models the social ‘immediacy’. Furthermore, initially each individual is characterised by a parameter which describes the strength of his/her influence on other individuals (spatial inhomogeneity). The individual located in the center of the lattice is defined as the ‘leader’, i.e. his/her ‘strength parameter’ is much larger than that of all others. Every individual is exerted to the ‘social impact’⁵³ which might lead to a change of his/her opinion. The ‘social impact’ depends on the strength to maintain a current opinion, on an additional external impact (i.e. by mass–media or government policy) and on the opinions and influences of the other individuals which are weighted by a decreasing function of the distance. Investigations are devoted to the formation and stability of clusters of individuals sharing the same opinion, and to the effects of competition between the ‘strong leader’ and the external impact, which influences the group homogeneously.

The traffic model introduced by Nagel and Schreckenberg (1992) is the probably simplest cellular automaton model capable of capturing basic qualitative features of realistic one–lane traffic flow. The cells of the one–dimensional cellular automaton represent parts of a road, which can be empty or occupied by just one car. The state of a car is characterised by a discrete velocity. The next state of each cell is determined according to the following sequence of rules: Each car which has a velocity less than the maximum velocity increases its velocity by one. Then, in order to avoid ‘accidents’, each car for which the number of empty cells in front of it is less than its velocity–number breaks, i.e. the car reduces its velocity to the number of free cells in front of it. Next, each car breaks at random, i.e. it reduces its velocity by one, so as to take into account psychological effects or road conditions. Finally, the cars move (all simultaneously) according to their new velocities, i.e. the position of each car is shifted by its velocity. Many variations of this basic model have been considered (e.g. Schadschneider and Schreckenberg 1997, Barlovic et al. 1998, Simon and Gutowitz 1998, Chowdhury et al. 2000). Furthermore, due to the computational efficiency of cellular automaton traffic flow models they are suitable to simulate large–scale road networks in multiple real time, which is a basic requirement for a ‘traffic forecast’. Based on the Nagel–Schreckenberg–model and in combination with real traffic data an online–simulation of downtown Duisburg (Germany) has been carried out (Esser 1997).

Most of the cellular automaton examples that we have sketched in this subsection are based on particle–particle interactions with and without particle conservation laws and on local particle movement. In general, the term ‘particle’ is not restricted to atomic or molecular scales. Often, a detailed analysis of

---

⁵³The theory of ‘social impact’ (Latané 1981) claims that the impact on an individual by a group of people is a certain function of their strength, immediacy, and number.
the automaton dynamics solely relies on computer simulations. In this thesis, we systematically investigate cellular automaton rules for random particle motion and particle interactions. We demonstrate, that particular combinations of local particle interactions and motion allow an analytic treatment of the cellular automaton by means of approximation models.

1.3 Outline of the thesis

In the previous sections an overview of modelling approaches for spatially extended dynamical systems was presented. In particular, cellular automata can be interpreted as discrete models of spatially extended systems, discrete in state, time and space. Examples of cellular automaton applications have been presented. Especially, lattice–gas cellular automata as a particular cellular automaton type, turn out to be a successful tool for studying particle interaction and movement. Cells (nodes) in lattice–gas cellular automata are divided into channels, in each of which at most one ‘particle’ resides. Particles can move from one channel at a node to the corresponding channel at a neighbouring node.

Formal definitions of deterministic, probabilistic and lattice–gas cellular automata are presented in the second chapter, which also introduces an analytical method, the so-called mean-field approximation. With this approximation, which neglects any temporal and spatial correlations between cell states, any cellular automaton model can be transformed into a deterministic model with continuous state space. In the case of deterministic and probabilistic cellular automata the approximated model is typically a system of time–discrete difference equations, while it is a system of time- and space-dependent difference equations (or coupled map lattice) in the case of lattice–gas cellular automata. In the latter case the mean–field equations are called lattice–Boltzmann equations. In order to get insight into the spatio–temporal pattern formation of these ‘approximate models’ we outline the general method of linear stability analysis.

Chapter 3 is devoted to processes of particle motion, which are motivated by classical stochastic models for the random walk of many particles. Using appropriate spatio–temporal scalings this microscopic random walk process leads to the macroscopic process of diffusion. Afterwards, we illustrate the difficulties in modelling motion in the framework of probabilistic cellular automata. Problems arise due to the finiteness of the set of states and from the synchronous dynamics. We present two classical approaches to overcome these difficulties by extending the cellular automaton concept. Furthermore, we present a lattice–gas cellular automaton which realises a synchronous random walk of many particles. We show that the lattice–Boltzmann equations of this model correspond to difference equations for the classical random walk.
A further emphasis is put on the detection of artificial lattice–gas cellular automaton dynamics, i.e. checkerboard patterns. We show that this behaviour can be avoided by introducing zero–velocity channels at each node.

As an example of simple one–component interaction processes, spatio–temporal growth processes are described and analysed in the following chapter (Chap. 4). Motivated by classical non–spatial growth models introduced by Malthus, Verhulst and Gompertz, several (probabilistic) cellular automaton rules are studied with respect to their (very different) temporal dynamics (in terms of the relative growth rate of the global component–density). We show that these models can not be adequately described by mean–field approximation, because of the rapid increase of spatio–temporal correlations in the cellular automaton. But we demonstrate further, that combined growth and motion processes can be captured by a mean–field approximation, because of the ‘particle–mixing’ and hence correlation destroying effect of the motion process. It is demonstrated that lattice–gas cellular automata offer a suitable tool for modelling growth and motion processes and for analysing them by means of the corresponding lattice–Boltzmann model.

Chapter 5 is the main part of this thesis. We introduce and study two types of many–component interactions in lattice–gas cellular automaton models. Both models are combined with a random walk process, which is independent for each component. The rules for the first two–component model are designed to capture essential aspects of activator–inhibitor interactions and to be ‘as simple as possible’. Activator–inhibitor interactions combined with diffusion are traditionally studied by means of partial differential equations. For these models it is well known that the combination of an autocatalytic activator component, which diffuses much slower than a self–repressing inhibitor component, leads to macroscopic spatial pattern formation (Turing 1952). Typical spatial patterns, called ‘Turing patterns’, are stationary, periodic structures, which are characterised by an intrinsic wave length. Taking the theoretical background from continuous systems, we study the pattern formation process of our lattice–gas cellular automaton in one– and two–dimensional lattices. The lattice–gas cellular automaton exhibits diffusion–induced pattern formation for appropriate reaction– and motion–parameter values. It turns out that the evolution of the lattice–gas cellular automaton is very well captured by the linear–stability analysis of the lattice–Boltzmann equations. Especially in the one–dimensional case theoretical predictions of the wave length of typical striped patterns are very precise. Furthermore, with these theoretical considerations artificial pattern formation, such as checkerboard patterns or patterns with very small wave lengths, are explained. We also characterise the influence of the inherent stochasticity of the lattice–gas cellular automaton, and of the dependence of the pattern formation process on initial conditions. Starting from the ‘mesoscopic’ lattice–Boltzmann description of the activator–inhibitor model macroscopic partial differential equations are derived. The macroscopic model is also capable of pattern formation as it is shown in the analysis and by
numerical simulation. Furthermore, we are able to derive a scaling relation of the macroscopic and mesoscopic levels of description. Two-dimensional patterns, generated by the lattice–gas cellular automaton defined on a square or hexagonal lattice, are stripes and spots. With the help of linear stability analysis of the lattice–Boltzmann equations, we can explain the strong anisotropies of patterns emerging on a square lattice, and the relation of model parameters and pattern type (spots or stripes).

In the same chapter, qualitatively different (moving) patterns are investigated with a model which is based on a three–component interaction, and whose rules are designed to mimick excitable dynamics. Excitable dynamics is characterised as follows: starting at a stable equilibrium a stimulus above a certain threshold generates a burst of activity followed by a refractory period. Spatial patterns produced by this dynamics are spiral waves and target patterns (ring waves). These patterns are also observed in simulations of the lattice–gas cellular automaton. A linear stability analysis of the corresponding lattice–Boltzmann equations indicates the existence of travelling waves isotropically rotating in the medium with a fixed spatial period.

The closing Chap. 6 comprises a discussion of the presented models and an outlook for future research.
2 Deterministic, probabilistic and lattice–gas cellular automata

2.1 General definitions

In the 1950’s John von Neumann and Stanislaw Ulam proposed the concept of cellular automata. In recent years, their very restrictive definition has been extended to many different applications. In general, a cellular automaton is specified by the definition of

- a regular lattice of cells (nodes, sites) and boundary conditions,
- a finite – typically small – set of states of the cells,
- a set of cells which defines the interaction neighbourhood, and
- a local rule which determines the dynamics of the states of the cells.

In this section we give a characterisation of cellular automaton models, especially of the classical (v. Neumann) deterministic cellular automaton, the probabilistic cellular automaton and the lattice–gas cellular automaton (LGCA). Together with the definitions, we also present as examples of deterministic and probabilistic cellular automata a simple model for the ‘diffusion of innovations’ introduced by Bocca and Fulk (1998). Here, the term innovation is used in a general sense, meaning also news, rumors, new products, etc.

2.1.1 Lattice geometry and boundary conditions

We start with a definition of a ‘cellular space’ (regular lattice) in which the automaton is defined. A regular lattice $\mathcal{L} \subseteq \mathbb{R}^d$ consists of a set of cells, labelled by its positions $r \in \mathcal{L}$, which homogeneously covers (a portion of) a $d$-dimensional Euclidean space. In this work, we focus on models with one or two dimensions. If LGCA are concerned, the cells are commonly called nodes while
they are referred to as sites in stochastic process models. The arrangement of the cells is specified by the shape of the nearest neighbour connections. For any spatial coordinate \( r \in \mathcal{L} \), the nearest lattice neighbourhood \( \mathcal{N}_b(r) \) is a finite list of neighbouring cells and is defined as

\[
\mathcal{N}_b(r) := \{ r + c_i : c_i \in \mathcal{N}_b, i = 1, \ldots, b \}
\]

where \( b \) is the coordination number, i.e. the number of nearest neighbours on the lattice. With \( \mathcal{N}_b \) we denote the nearest neighbourhood template with elements \( c_i, i = 1, \ldots, b \). The template depends on the topology of the lattice under consideration.

A one-dimensional \((d = 1)\) regular lattice consists of an array of cells, in which each cell is connected to its right and left neighbour \((b = 2)\). Then, for example,

\[
\mathcal{L} = \mathbb{Z} = \{ r : r \in \mathbb{Z} \}, \\
\mathcal{N}_2 = \{ 1, -1 \}.
\]

In two dimensions \((d = 2)\), the only regular lattices are triangular \((b = 3)\), square \((b = 4)\) or hexagonal \((b = 6)\), such as shown in Fig. 2.1 (Ames 1977). For \( b = 4 \) the lattice is defined as

\[
\mathcal{L} = \mathbb{Z}^2 = \{ r : r = (r_1, r_2), r_j \in \mathbb{Z}, j = 1, 2 \}, \\
\mathcal{N}_4 = \{ (1,0), (0,1), (-1,0), (0,-1) \}.
\]

![Figure 2.1](image)

Figure 2.1: Cells and nodes (dots) in two-dimensional lattices; the grey area indicates the shape of a cell which is a triangle, a square or a hexagon.

The number of cells in each space direction \( i \) is denoted by \( L_i, i = 1, \ldots, d, \) and the total number of cells by

\[
|\mathcal{L}| = L_1 \cdots L_d.
\]

Cellular automata are usually explored by computer experiments in which the lattice has to be considered as finite. In finite lattices it is necessary to impose
2.1 General definitions

![boundary conditions](image)

Figure 2.2: Boundaries in a one-dimensional lattice; cells \( r \in \mathcal{L} = \{0, \ldots, 9\}, |\mathcal{L}| = 10 \), represent the lattice of a cellular automaton. The single cells at the left and right of the dashed lines define the corresponding left and right nearest neighbour cells for the boundary cells \( r = 0 \) and \( r = 9 \), respectively. Grey cells are cells with a prescribed fixed value.

**boundary conditions** which define the set of nearest neighbours for cells at the boundary of the lattice.

A lattice can be periodically extended, i.e. opposite bounds of the lattice are glued together (Fig. 2.2a). In one dimension this leads to a ring and in two dimensions to a torus. These so-called **periodic** boundary conditions are often used for the approximation of a simulation on an infinite lattice. Note that they can introduce artificial spatial periodicities into the system. In order to define a boundary condition which is comparable with a zero-flux (Neumann) boundary condition used in continuous diffusion models, the lattice is **reflected** at the boundary (see Fig. 2.2b). To model boundary conditions corresponding to Dirichlet boundary conditions related to PDEs, cells at the boundary have nearest neighbours with a prescribed **fixed** value (see Fig. 2.2c) (Schönfisch 1993). Of course, all types of boundary conditions can be combined with each other.

If interaction processes of more than one component (species) are to be examined it can be useful, especially for LGCA, to take into consideration separate lattices for each component. From now on, in the first place we give the formal description of one-component systems. Subsequently, for LGCA we note very briefly the extension to multi-component systems. The component dependence of any variable will be expressed by adding the subscript \( \sigma \), \( \sigma = 1, \ldots, \varsigma \), i.e. the lattice for component \( \sigma \) is \( \mathcal{L}_\sigma \). We will assume that all \( \mathcal{L}_\sigma \) are labelled identically and consist of the same number of cells. Then, solely for simplicity of notation, we identify all lattices and denote them by \( \mathcal{L} \).
2.1.2 States

To each cell $r \in \mathcal{L}$ we assign a state value $s(r) \in \mathcal{E}$ which is taken from the (usually ‘small’) finite set of elementary states $\mathcal{E}$, i.e.

$$s : \mathcal{L} \rightarrow \mathcal{E}.$$  

The elements of $\mathcal{E}$ can be numbers, symbols or other objects. A simple example is shown in Fig. 2.3.

A global configuration of the automaton is given by a vector $s$ determined by the knowledge of the state values of all cells on the lattice (Fig. 2.3), i.e.

$$s := (s(r_1), \ldots, s(r_{|\mathcal{L}|})) = (s(r_i))_{r_i \in \mathcal{L}}.$$  

This vector takes its values in the state space $\mathcal{S} = \mathcal{E}^{|\mathcal{L}|}$.

Here and in the sequel we use the notation $y^T = (y_i)_i$ to indicate the entire vector as opposed to a single component $y_i$. This is especially useful when multiply-indexed objects occur.\footnote{The vector $y^T$ specifies the transpose of the vector $y$.}

A local configuration is a vector $s_M$ consisting of state values of cells in an ordered subset $\mathcal{M}$ of the lattice $\mathcal{L}$ (Fig. 2.3), i.e.

$$s_M := (s(r_1), \ldots, s(r_{|\mathcal{M}|})) = (s(r_i))_{r_i \in \mathcal{M}}, \quad \mathcal{M} \subset \mathcal{L}.$$  

If $s \in \mathcal{S}$ is a global configuration, then $s|_{\mathcal{M}} = s_M \in \mathcal{S}|_{\mathcal{M}}$. $s_{\mathcal{N}(r)}$ is considered to be the local configuration according to the interaction neighbourhood $\mathcal{N}(r) \subseteq \mathcal{L}$ (defined in Subsec. 2.1.3, p. 22) of a focal cell $r$ and $\mathcal{S}_{\mathcal{N}(r)} := \mathcal{S}|_{\mathcal{N}(r)}$.

Example: For the model of ‘diffusion of innovations’, each cell of a one-dimensional (periodic) lattice $\mathcal{L}$ is occupied by an individual (social space). Each individual can be either neutral or an adopter, i.e. $s(r) \in \mathcal{E} = \{\text{neutral, adopter}\}$. It is convenient to label these elementary states by numbers: if node $r$ is occupied by an adopter: $s(r) = 1$ and if it is occupied by a neutral individual: $s(r) = 0$, i.e. $\mathcal{E} = \{0, 1\}$. A possible lattice configuration is illustrated in Fig. 2.3.

States in lattice–gas cellular automata

In LGCA (velocity) channels, $(r, c_i), \ c_i \in \mathcal{N}_b, \ i = 1, \ldots, b$, are associated with each node $r$ of the lattice. In addition, a variable number $\beta \in \mathbb{N}_0$ of rest channels (zero–velocity channels), $(r, c_i), \ b < i \leq \beta$, with $c_i = \{0\}^b$ may be
2.1 General definitions

\[
\begin{array}{cccccccccc}
& 9 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\
\end{array}
\]

\[E = \{0,1\}, \quad L = \{0, \ldots, 9\}, L = 10, \quad S = \{0,1\}^{10} \quad M = \{2,3,4\}\]

\[s(3) = 0, \quad s = (0,0,1,0,0,0,1,0,1,1), \quad s_M = (1,0,0)\]

Figure 2.3: Example of a one-dimensional global \((s)\) and local \((s_M)\) lattice configuration.

introduced. Furthermore, an **exclusion principle** is imposed. It demands that not more than one particle can be at the same node within the same channel. As a consequence, each node \(r\) can host up to \(\tilde{b} = b + \beta\) particles, which are distributed in different channels \((r,c_i)\) with at most one particle per channel. Therefore, state \(s(r) \in E\) is given by the **node configuration** \(\eta(r)\) with

\[s(r) = \eta(r) = (\eta_1(r), \ldots, \eta_b(r))\,.
\]

\(\eta_i(r), i = 1, \ldots, \tilde{b},\) are Boolean variables that indicate the presence \((\eta_i(r) = 1)\) or absence \((\eta_i(r) = 0)\) of a particle in the respective channel \((r,c_i)\). The **total number of particles** present at a node \(r\) will be denoted by

\[n(r) := \sum_{i=1}^{\tilde{b}} \eta_i(r)\,.
\]

Hence, the set of elementary states \(E\) is defined as

\[E = \{0, 1\}^{\tilde{b}}\,.
\]

The **local configuration** \(s_{N(r)}\) is given by

\[s_{N(r)} = \eta_{N(r)} = (\eta_{r_i})_{r_i \in N(r)}\,.
\]

Figure 2.4 gives an example of the representation of a node in a two-dimensional lattice with \(b = 4\) and \(\beta = 1\), i.e., \(\tilde{b} = 5\).

In multi-component LGCA, \(\zeta\) different types \((\sigma)\) of particles reside on separate lattices \((L_\sigma)\) and the exclusion principle is applied independently to each lattice. The state variable is given by

\[s(r) = \eta(r) = (\eta_\sigma(r))_{\sigma=1}^\zeta = (\eta_\sigma 1(r), \ldots, \eta_\sigma \tilde{b}(r))_{\sigma=1}^\zeta \in E = \{0, 1\}^{\tilde{b} \zeta}\,.
\]
Since we can define an interaction neighbourhood $\mathcal{N}_b^l(r) \subseteq \mathcal{L}_\sigma$ for each component $\sigma$, the local configuration $s_{\mathcal{N}(r)}$ is given by

$$s_{\mathcal{N}(r)} = \eta_{\mathcal{N}(r)} = \left( (\eta_\sigma(r))_{r \in \mathcal{N}_b^l(r)} \right)_{\sigma=1}^c.$$  

2.1.3 Neighbourhood of interaction

An interaction neighbourhood $\mathcal{N}_b^l(r)$ specifies a set of lattice–cells which influence the state at cell $r$. Following the cellular automaton definition of John von Neumann, its size and topology do not depend on the lattice cell, and it does not change in time. Therefore, the interaction neighbourhood is defined as an ordered set

$$\mathcal{N}_b^l(r) = \{ r + c_i : c_i \in \mathcal{N}_b^l \} \subseteq \mathcal{L},$$

where $\mathcal{N}_b^l$ is an interaction neighbourhood template which can be chosen in several ways. Note that this definition implies translation invariance of the interaction neighbourhood. Furthermore, for cells at the lattice–boundaries the interaction neighbourhood has to be additionally specified if non–periodic boundary conditions are imposed. In the case of periodic boundary conditions, we always assume that the sum $r + c_i$ is taken modulo some appropriate value such that $r + c_i \in \mathcal{L}$, $\forall c_i \in \mathcal{N}_b^l$. Famous examples of a two–dimensional square lattice are the von Neumann neighbourhood (Burks 1970, cf. Fig. 2.5(a))

$$\mathcal{N}_4^l = \{(0,0), (1,0), (0,1), (-1,0), (0,-1)\} = \mathcal{N}_4 \cup \{(0,0)\},$$

and the Moore neighbourhood (Moore 1962, cf. Fig. 2.5(b))

$$\mathcal{N}_4^l = \{(0,0), (1,0), (1,1), (0,1), (-1,1), (-1,0), (-1,-1), (0,-1), (1,-1)\}.$$
In some applications (i.e. Gerhardt and Schuster 1989, Wolfram 1994, Young 1984), extended neighbourhoods are considered. They are defined as either **R–radial** (Fig. 2.5(c))

\[ \mathcal{N}_I^j = \{ r = (r_1, r_2) : r_j \in \{ -R, \ldots, R \} \land |r_1 - r_2| \leq R, \; j = 1, 2 \} , \]

or **R–axial** (Fig. 2.5(d))

\[ \mathcal{N}_I^j = \{ r = (r_1, r_2) : r_j \in \{ -R, \ldots, R \}, \; j = 1, 2 \} . \]

(a) von Neumann neighbourhood  
(b) Moore neighbourhood

(c) 2–radial neighbourhood  
(d) 2–axial neighbourhood

Figure 2.5: Examples of interaction neighbourhoods (grey and black cells) for the black cell in a two-dimensional square lattice.

In most applications the interaction neighbourhood template is chosen to be symmetrical, but also asymmetrical schemes are possible. Furthermore, the cell \( r \) itself does not necessarily have to be included in the neighbourhood of interaction, i.e. \( r \not\in \mathcal{N}_I^j(r) \). In this case we will refer to an **outer** interaction neighbourhood. Moreover, in an extreme case, the interaction neighbourhood contains only one element – the cell \( r \) itself, i.e. \( \mathcal{N}_0^j = \{ r \} \). Then, each cell is independent of other cells.

## 2.2 System dynamics

The local dynamics of the automaton is determined by a **local transition rule** \( \mathcal{R} \), which specifies the new state of a focal cell as a function of its interaction
neighbourhood configuration, i.e.

\[ R : \mathcal{E}^\nu \to \mathcal{E}, \quad \text{where} \quad \nu := |\mathcal{N}_b^r|. \]

The rule is **spatially homogeneous**, i.e. it does not depend explicitly on the cell position \( r \). However, the rule can be extended to include spatial and/or temporal inhomogeneities. A typical example of spatial inhomogeneity is a cellular automaton with fixed boundary conditions (cf. p. 19). Similarly, time-dependent rules can be introduced, for example, by alternating two rules at even and odd time steps, as used for the formulation of cellular automata for the problem of directed percolation or the model for Ising spin dynamics (Chopard and Droz 1998). In Subsec. 3.3.1 we present a time- and space-dependent local transition rule which was designed to model a simultaneous random walk of many particles in the framework of probabilistic cellular automata. However, in general, the transition rule is assumed to be **spatially homogeneous**.

In deterministic cellular automata the local rule is **deterministic**, i.e. the local transition rule yields a unique next state for each cell. Therefore, given fixed initial conditions the future is foreseeable and uniquely determined, i.e. the automaton has a unique history.

**Example:** In the model of ‘diffusion of innovations’ the local rule is defined as follows: Once an individual becomes an adopter, it remains an adopter; a neutral individual will remain neutral if all neighbours are neutral; an individual adopts, if, at least, one of his/her neighbours is an adopter.

In **probabilistic** cellular automata the local transition rule specifies a time- and cell-independent probability distribution of next states for each possible neighbourhood configuration. It is defined by

\[
R(s_{N(r)}) = \begin{cases} 
    z^1 \text{ with probability } W(s_{N(r)} \to z^1) \\
    \vdots \\
    z^\varepsilon \text{ with probability } W(s_{N(r)} \to z^\varepsilon),
\end{cases}
\]

where \( z^i \in \mathcal{E} := \{z^1, \ldots, z^\varepsilon\} \) and \( W(s_{N(r)} \to z^j) \) is a time-independent transition probability specifying the probability to reach an elementary state \( z^j \) given the neighbourhood configuration \( s_{N(r)} \). This transition probability has to satisfy the following conditions

\[
W : \mathcal{E}^\nu \to [0,1] \quad \text{and} \quad \sum_{j=1}^\varepsilon W(s_{N(r)} \to z^j) = 1.
\]

Note that any deterministic local rule can be viewed as a special case of a probabilistic rule with

\[
W(s_{N(r)} \to z^j) = 1 \quad \text{and} \quad W(s_{N(r)} \to z^l) = 0 \quad \forall l \neq j.
\]
2.2 System dynamics

**Example:** A probabilistic version of the local rule for the ‘diffusion of innovations’ can be defined as follows: Once an individual becomes an adopter, it remains an adopter; a neutral individual will remain neutral if all neighbours are neutral; an individual becomes an adopter with a certain probability depending on the number of adopters in its interaction neighbourhood, where opinions of all neighbours have equal weight.

Assuming synchronous updating of the cellular automaton, the local rule is applied simultaneously to each cell of the lattice. Then, the global dynamics is specified by a global function \( \mathcal{R}_g : \mathcal{S} \rightarrow \mathcal{S} \) such that for each global configuration \( s \in \hat{\mathcal{S}} \)

\[
\mathcal{R}_g(s)(r) = \mathcal{R}(s_{N(r)}), \quad \forall r \in \mathcal{L}.
\]

Accordingly, global dynamics is exclusively defined by the local rule \( \mathcal{R} \). At subsequent discrete time steps \( k \in \mathbb{N}_0 \), the global configuration is given by \( s(k) \in \mathcal{S} \), the local configuration of cell \( r \) by \( s_{N(r)}(k) \in \hat{\mathcal{S}}_{N(r)} \), and the state of cell \( r \) by \( s(r, k) \in \mathcal{E} \). For each initial \( (k = 0) \) global configuration \( s(0) \in \mathcal{S} \), the temporal development of the system is determined by

\[
s(k + 1) = \mathcal{R}_g(s(k)),
\]

where the dynamics of a state \( s(r, k) \) follows

\[
s(r, k + 1) = \mathcal{R}(s_{N(r)}(k)). \tag{2.1}
\]

**Example:** In mathematical terms the local rule for the model of ‘diffusion of innovations’ is defined by

\[
\mathcal{R}(s_{N(r)}) = \begin{cases} 
0 & \text{with probability } W(s_{N(r)} \rightarrow 0), \\
1 & \text{with probability } W(s_{N(r)} \rightarrow 1),
\end{cases}
\]

where the deterministic model is defined by

\[
W(s_{N(r)} \rightarrow 0) = (1 - s(r)) \prod_{\hat{r} \in \mathcal{N}_f(r)} (1 - s(\hat{r})) \in \{0, 1\},
\]

\[
W(s_{N(r)} \rightarrow 1) = 1 - W(s_{N(r)} \rightarrow 0) \in \{0, 1\},
\]

and the probabilistic model is defined by

\[
W(s_{N(r)} \rightarrow 0) = (1 - s(r)) (1 - d_a(r)) \in [0, 1]
\]

\[
W(s_{N(r)} \rightarrow 1) = 1 - W(s_{N(r)} \rightarrow 0) \in [0, 1],
\]
with the density of adopters

\[ d_a(r) := \frac{1}{\nu - 1} \sum_{\bar{r} \in \mathcal{N}_2(r)} s(\bar{r}), \quad \nu = |\mathcal{N}_2| > 1. \]

Figure 2.6 shows an example of the action of the deterministic local rule in one time step.

\[
\begin{array}{cccccccccc}
  r & : & 9 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 0 \\
  k : & & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\
  k+1 : & & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\
\end{array}
\]

\[ s(3, k) = 0, \quad s(3, k + 1) = \mathcal{R}(s_{\mathcal{N}(3)}(k)) = \mathcal{R}((1, 0, 0)) = 1 \]

Figure 2.6: Example for the action of a deterministic local rule ('diffusion of innovations') in a one-dimensional lattice with 10 nodes and periodic boundary conditions. The interaction neighbourhood template is given by \( \mathcal{N}_2 = \{-1, 0, 1\} \) and the set of elementary states is \( \mathcal{E} = \{0, 1\} \).

As the number of possible configurations is finite for a finite lattice, any initial condition must eventually map to a temporally periodic cycle in a deterministic cellular automaton. However, the period can become uninterestingly large. For example, if \( |\mathcal{E}| = 2 \) and \( |\mathcal{L}| = 1000 \), a global configuration will be repeated certainly after at most \( 2^{1000} \approx 10^{300} \) time steps.

In extensions of cellular automaton models, asynchronous updating is allowed. This can be achieved, for instance, by applying the local rule at each cell only with a certain probability. In Schönisch and de Roos (1999), several different asynchronous updating algorithms are presented and analysed. In many applications involving particle interaction and movement a subdivided local rule is used: the first part (interaction) is applied synchronously while the second part (movement) changes the values of pairs of cells sequentially. In Subsec. 3.3.2 we present a more detailed algorithm for the process of asynchronous random particle walk.

In the following, a **cellular automaton** is defined by a regular lattice \( \mathcal{L} \), an interaction neighbourhood template \( \mathcal{N}_b \), the finite set of elementary states \( \mathcal{E} \), and the local space- and time-independent transition rule \( \mathcal{R} \) which is applied synchronously. In a **deterministic cellular automaton** the local rule is deterministic while a **probabilistic cellular automaton** is characterised by a probabilistic local rule.
2.2 System dynamics

Dynamics in lattice–gas cellular automata

The dynamics of a LGCA arises from repetitive applications of superpositions of local interaction and propagation (migration) steps applied simultaneously at all lattice nodes at each discrete time step. The definitions of these steps have to satisfy the exclusion principle, i.e. two or more particles of a given species are not allowed to occupy the same channel.

According to a model–specific interaction rule \( \mathcal{R}_i \), particles can change channels (i.e. due to collisions, see Fig. 2.7) and/or are created or destroyed. This rule can be deterministic or stochastic. The dynamics of a state \( s(r,k) = \eta(r,k) \in \{0,1\}^b \) in a LGCA is determined by the dynamics of the occupation numbers \( \eta_i(r,k) \) for each \( i \in \{1, \ldots, \hat{b}\} \) at node \( r \) and time \( k \). Therefore, the pre–interaction state \( \eta_i(r,k) \) is replaced by the post–interaction state \( \eta_i^\dagger(r,k) \) determined by

\[
\eta_i^\dagger(r,k) = \mathcal{R}_i^\dagger(\mathbf{s}_{N_i}(k)), \quad \mathcal{R}_i^\dagger = (\mathcal{R}_i^\dagger)_{i=1}^\hat{b} .
\] (2.2)

![Diagram](image)

\( \eta(r,k) = (1,0,1,0,0) \) \( \eta_i^\dagger(r,k) = (0,1,0,1,0) \)

Figure 2.7: Example for a collision of particles on a two–dimensional square lattice node \( r \); here, the interaction neighbourhood is taken to be \( \mathcal{N}_i(r) = \{r\} \) and therefore \( \mathbf{s}_{N_i}(k) = \eta(r,k) \). Grey shaded circles denote the presence of a particle in that channel. No confusion should arise by the arrows indicating the channel directions.

In the deterministic propagation or streaming step \( \mathcal{P} \), all particles are moved simultaneously to neighbours in the direction of their velocity, i.e. a particle residing in channel \( (r,c_i) \) at time \( k \) is moved to another channel \( (r + m c_i, c_i) \) during one time step (Fig. 2.8). Here, \( m \in \mathbb{N} \) determines the speed and \( m c_i \) the velocity of movement. Because all particles residing at velocity channels move the same number \( m \) of lattice units the exclusion principle is maintained. Particles occupying rest channels do not move since they have "zero velocity". In terms of occupation numbers, the state of channel \( (r + m c_i, c_i) \) after propagation is given by

\[
\eta_i^\dagger(r + m c_i, k + 1) = \eta_i(r,k), \quad c_i \in \mathcal{N}_b .
\] (2.3)

Hence, if only the propagation step is applied then particles occupying velocity channels would simply move along straight lines.
Combining interactive dynamics with propagation, Eqns. (2.2) and (2.3) imply that

$$\eta_i(r + mc_i, k + 1) = \eta_i(r, k).$$

(2.4)

This can be rewritten as the microdynamical difference–equations

$$\eta_i(r + mc_i, k + 1) - \eta_i(r, k) = \mathcal{C}_i(s_{N(\sigma)}(k)) \quad i = 1, \ldots, \hat{b},$$

(2.5)

where the change in the occupation numbers due to interaction is given by

$$\mathcal{C}_i(s_{N(\sigma)}(k)) = \begin{cases} 
1 & \text{creation of a particle in channel } (r, c_i), \\
0 & \text{no change in channel } (r, c_i), \\
-1 & \text{annihilation of a particle in channel } (r, c_i). 
\end{cases}$$

In a multi–component system with $\sigma = 1, \ldots, \varsigma$ components, Eqn. (2.5) becomes

$$\eta_{\sigma,i}(r + m\sigma c_i, k + 1) - \eta_{\sigma,i}(r, k) = \mathcal{C}_{\sigma,i}(s_{N(\sigma)}(k)) \quad i = 1, \ldots, \hat{b},$$

(2.6)

with speeds $m_\sigma \in \mathbb{N}$ for each component $\sigma = 1, \ldots, \varsigma$. Here, the change in the occupation numbers due to interaction is given by

$$\mathcal{C}_{\sigma,i}(s_{N(\sigma)}(k)) = \begin{cases} 
1 & \text{creation of a particle } X_\sigma \text{ in channel } (r, c_i)_\sigma, \\
0 & \text{no change in channel } (r, c_i)_\sigma, \\
-1 & \text{annihilation of a particle } X_\sigma \text{ in channel } (r, c_i)_\sigma, 
\end{cases}$$

where $(r, c_i)_\sigma$ specifies the $i$th channel associated with node $r$ of the lattice $\mathcal{L}_\sigma$.
2.3 Analytical methods

Despite the simple construction of cellular automata, they are capable of complex behaviour. For most cellular automaton models the only general method to determine the qualitative dynamic properties of the system is to 'run simulations' on a computer for various initial global configurations (Jackson 1991). Then, statistical dynamical systems methods can be applied. For example, a measure for the strength of sensitive dependence on initial conditions of dynamical systems is the 'Lyapunov exponent' (Kaplan and Glass 1995). A possible comparable concept for deterministic cellular automata is the Hamming distance which is simply the number of cells that are in different states at two successive time steps (Bagnoli et al., 1992, Wolfram 1994). Local irreversibility is an important feature of many cellular automata, which means that different initial global configurations may eventually evolve to the same final configuration. This behaviour allows that certain global configurations may occur with larger probability than others which is an important feature of systems which are capable of 'self-organising behaviour' (Hurley 1990). As a measure for the irreversible behaviour of a cellular automaton, Wolfram (1994) applied the concept of information-theoretical (Shannon) entropy. Entropy decreases with time for irreversible systems, while it must increase for reversible systems. Geometrical aspects of self-similar spatial patterns generated by cellular automata evolution can be investigated, e.g., by the Hausdorff-Basicovitch or fractal dimension of the pattern. In this work we focus on a characterisation of cellular automaton configurations by a mean-field approximation, which is based on averaged densities or expectation values of the elementary states.

In the previous section (2.2) we provided a description of cellular automaton models in terms of microdynamical discrete variables (Eqns. (2.1) and (2.5)), discrete in space and time. Our aim in this section is to derive difference equations which remain discrete in time (and in space) but have continuous state variables. Then, in order to gain more insight into the automaton dynamics, standard analytical techniques can be applied to these equations. Such a description will typically be statistical, not specifying an exact configuration, but merely the probabilities for the appearance of different configurations.

Recall from the definition of a probabilistic local rule (cf. p. 24) that any deterministic cellular automaton can be viewed as a probabilistic rule. Then, instead of specifying the configuration $s(k) \in S$, we analyse the probability distribution of each configuration at each time step. At each time $k \in \mathbb{N}_0$ let $\xi_k \in S$ be a random variable which assigns a lattice configuration as a stochastic realisation of the process $\{\xi_k\}_{k \in \mathbb{N}_0}$ defined in the state space $S$. In

---

2Here, the entropy for a deterministic cellular automaton is defined as $\sum_i p_i \log_2 p_i$, where $p_i$ are the probabilities for each of the finite set of $2^{2L}$ possible global configurations.

3Note that Wolfram (1983) defines entropy with a different sign compared to the classical definition.
the following, given an arbitrary distribution of initial states $\xi_0, s \in \mathcal{S}$,

$$P(\xi_k(r_1), \ldots, \xi_k(r_m) = s(r_1), \ldots, s(r_m)) =: P_k(s(r_1), \ldots, s(r_m))$$

$r_i \in \mathcal{M}$, $m = |\mathcal{M}| \subseteq \mathcal{L}$

specifies the probability of observing configuration $s_M \in \mathcal{S}|_M$ at time $k$. Furthermore, $W(s_A \to s_B)$ specifies the time–independent transition probability to reach a configuration $s_B = s|_B$ given the configuration $s_A = s|_A$ for any $A, B \subseteq \mathcal{L}$.

By construction of the cellular automaton, the stochastic process $\{\xi_k\}_{k \in \mathbb{N}_0}$ is Markovian, i.e. there is no memory effect. It is fully characterised by its transition probability matrix with elements $P(\xi_{k+1} = s | \xi_k = \tilde{s})$ defining the probability to find the system in a state $s$ at time $k + 1$, when the state at the previous time $k$ was $\tilde{s}$. Using the fact that the local cellular automaton rule (cf. p. 24) is applied to each site simultaneously and that it specifies the next state of a single site as a function of the interaction neighbourhood configuration, we get

$$P(\xi_{k+1} = s | \xi_k = \tilde{s}) = \prod_{r \in \mathcal{L}} P(\xi_{k+1}(r) = s(r) | \xi_k(r_1) = \tilde{s}(r_1), \ldots, \xi_k(r_\nu) = \tilde{s}(r_\nu)),$$

and since the local rule is time–independent

$$= \prod_{r \in \mathcal{L}} W(\tilde{s}_{N(r)} \to s(r)) =: W(\tilde{s} \to s)$$

for $s, \tilde{s} \in \mathcal{S}$, $r_i \in N_k(r)$, $i = 1, \ldots, \nu$. Hence, the stochastic process $\{\xi_k\}_{k \in \mathbb{N}_0}$ is a stationary Markov chain (Gardiner 1983) and the time evolution of the probability distribution is given by the Chapman–Kolmogorov equation or Master equation (i.e. Gardiner 1983) which becomes with Eqn. (2.7)

$$P_{k+1}(s) = \sum_{\tilde{s} \in \mathcal{S}} P_k(\tilde{s}) W(\tilde{s} \to s)$$

$$= \sum_{\tilde{s} \in \mathcal{S}} P_k(\tilde{s}) \prod_{r \in \mathcal{L}} W(\tilde{s}_{N(r)} \to s(r)).$$

Furthermore, using Eqn. (2.8) the probability for a site state to be in a specific elementary state is given by

$$P(\xi_{k+1}(r) = z_j) = \sum_{s \in \mathcal{S}, s(r) = z'_j} P_{k+1}(s)$$

$$= \sum_{s \in \mathcal{S}, s(r) = z'_j} \sum_{\tilde{s} \in \mathcal{S}} P_k(\tilde{s}) \prod_{r \in \mathcal{L}} W(\tilde{s}_{N(r)} \to s(r))$$
\[ \sum_{\tilde{s} \in \tilde{S}_{N(r)}} P_k(\tilde{s}(r_1), \ldots, \tilde{s}(r_{\nu})) W(\tilde{s}_{N(r)} \rightarrow z^j) \]

for \( r_i \in \mathcal{N}^j_b(r), i = 1, \ldots, \nu \).

Although it is straightforward to write down Eqns. (2.8) and (2.9), which keep track of all information concerning the state of the system, the complete analytical solution is not possible in most cases. Therefore, in order to analytically studying a cellular automaton some approximation is necessary.

### 2.3.1 Cellular automaton mean-field equations

The simplest approximation is known as the **mean-field theory** (Schulman and Seiden 1978, Wolfram 1983). It is based on the assumption that at any time the states of sites are not correlated with the states of other sites in the lattice. Although this assumption is generally not valid, a simple formula for an estimate of the limit density of each possible state of a cell can be derived from Eqn. (2.9). Thus, the states of all sites in the lattice are assumed to be independent at all times and therefore the probability of a local configuration \( s_M \) is the product of the probabilities of the states of the sites in \( \mathcal{M} \), i.e.

\[ P(s_M) = P(s(r_1), \ldots, s(r_{|\mathcal{M}|})) = \prod_{r_i \in \mathcal{M}} P(s(r_i)), \tag{2.10} \]

with \( \mathcal{M} \subseteq \mathcal{L} \).

For each \( k \in \mathbb{N}_0 \), let \( x_k^j \) be a Boolean random variable which equals 1, if the random variable \( \xi_k(r) \) is in the elementary state \( z^j \in \mathcal{E} := \{z^1, \ldots, z^\varepsilon\} \). For \( j = 1, \ldots, \varepsilon \) it is defined as

\[ x_k^j(r) := \delta_{\xi_k(r), z^j} \in \{0, 1\}, \]

where \( \delta_{u,v} \) is the Kronecker delta. Then, using Eqns. (2.9) and (2.10), the temporal evolution of the expected value \( E(x_k^j(r)) \) is given by

\[ E(x_{k+1}^j(r)) = P(\xi_{k+1}(r) = z^j) \]

\[ = \sum_{\tilde{s} \in \tilde{S}_{N(r)}} P_k(\tilde{s}(r_1), \ldots, \tilde{s}(r_{\nu})) W(\tilde{s}_{N(r)} \rightarrow z^j) \]

\[ = \sum_{\tilde{s} \in \tilde{S}_{N(r)}} W(\tilde{s}_{N(r)} \rightarrow z^j) \prod_{r_i \in \mathcal{N}^j_b(r)} P_k(\tilde{s}(r_i)), \]

with \( r_i \in \mathcal{N}^j_b(r), i = 1, \ldots, \nu \). According to the spatial homogeneity of the local transition rule (cf. p. 24), the transition probabilities \( W(\tilde{s}_{N(r)} \rightarrow z^j) \) are translation invariant, that is they depend only on the site states which
define the interaction neighbourhood but not on their location \( r \). Hence, an equivalent representation of Eqn. (2.11) is

\[
E(x_k^j(r)) = \sum_{(z_1, \ldots, z_{\nu}) \in \mathcal{E}^\nu} W((z_1, \ldots, z_{\nu}) \rightarrow z^j) \prod_{i=1}^{\nu} \sum_{l=1}^{|\mathcal{E}|} \delta_{z_i,l} E(x_k^l(r_i)),
\]

with \( \nu = |\mathcal{N}_0^j| \). Furthermore, spatially averaged values \( x_j(k) \in [0, 1] \), which for each \( j \) denote the expected density of an elementary state \( z^j \) on the lattice at time \( k \), are defined by

\[
x_j(k) := \frac{1}{|\mathcal{E}|} \sum_{r \in \mathcal{E}} E(x_k^j(r)) = E(x_k^j(r')) \in [0, 1] \quad \text{for some } r'.
\]

Then, mean-field equations for each \( x_j(k) \) are given by

\[
x_j(k + 1) = \sum_{(z_1, \ldots, z_{\nu}) \in \mathcal{E}^\nu} W((z_1, \ldots, z_{\nu}) \rightarrow z^j) \prod_{i=1}^{\nu} \sum_{l=1}^{|\mathcal{E}|} \delta_{z_i,l} x_l(k)
\]

\[
= H_j(x(k)) , \quad x^T(k) = (x_1(k), \ldots, x_{|\mathcal{E}|}(k)),
\]

for \( j = 1, \ldots, |\mathcal{E}| \).

**Example:** The mean-field equation for the model of ‘diffusion of innovations’ has been derived for an interaction neighbourhood template \( \mathcal{N}_0^j = \{-1, 0, 1\} \). Let \( x_0(k) \) denote the expected density of neutrals and \( x_1(k) \) the expected density of adopters. Then, with \( \mathcal{E} = \{0, 1\} \), \( x_0(k) + x_1(k) = 1 \) and the probabilistic local rule defined on page 25,

\[
x_1(k + 1) = \sum_{(z_1, z_2, z_3) \in \{0,1\}^3} W((z_1, z_2, z_3) \rightarrow 1) \prod_{i=1}^{3} (\delta_{z_i,0} x_0(k) + \delta_{z_i,1} x_1(k))
\]

\[
= \sum_{(z_1, z_2, z_3) \in \{0,1\}^3} \left[ 1 - (1 - z_2) \left( 1 - \frac{1}{2}(z_1 + z_3) \right) \right] \prod_{i=1}^{3} (\delta_{z_i,0} x_0(k) + \delta_{z_i,1} x_1(k))
\]

\[
= x_1(k) \left( x_0^2(k) + 2x_0(k)x_1(k) + x_1(k) \right) + x_0(k) \left( \frac{1}{2} x_0(k)x_1(k) + \frac{1}{2} x_0(k)x_1(k) + x_1^2(k) \right)
\]

\[
= 2x_0^2(k)x_1(k) + 3x_0(k)x_1^2(k) + x_1^3(k) = 2x_1(k) - x_1^2(k),
\]
2.3 Analytical methods

\[ x_0(k + 1) = 1 - x_1(k + 1) \]
\[ = 1 - 2x_1(k) + x_1^2(k) = x_0^2(k). \]

Note that Eqn. (2.13) only encodes the **combinatorial information** contained in the local cellular automaton rule which maps from an interaction neighbourhood configuration to the state of a single site, and that it does not reflect the structure of the lattice on which the automaton operates. Therefore, the mean-field theory does not distinguish between cellular automaton models which have the same rule with the same number of neighbours, but are defined on different (i.e. one- or two-dimensional) lattices (Gutowitz and Victor 1989). Equation (2.11) is called ‘mean-field equation’ because each site state only depends on the average value of the states of the other sites in the interaction neighbourhood. Equation (2.13) is **exact** in the case in which

- the lattice is infinitely large, and
- the site states are randomly reallocated after updating.

Although the mean-field approach is a very crude approximation, it often yields a picture of the cellular automaton dynamics which is qualitatively correct. This will be discussed in more detail in Sec. 4.2 (p. 72).

Lattice–gas cellular automaton mean–field (Boltzmann) equations

Recall that in a LGCA the state of node \( r \) is composed of Boolean occupation numbers \( \eta_i \), i.e.

\[ s(r) = \eta(r) = (\eta_1(r), \ldots, \eta_{\tilde{b}}(r)) \in \mathcal{E} = \{0, 1\}^{\tilde{b}}, \]

where \( \tilde{b} \) is the number of channels on a node (cf. p. 21).

Since quantities of interest are not so much the Boolean variables \( \eta_i \) but macroscopic quantities such as densities, we look for an expression similar to Eqn. (2.11) in terms of some average value of the \( \eta_i \)'s. These values are given by **single particle distribution functions**

\[ f_i(r, k) := E(\eta_i(r, k)) = P(\eta_i(k) = 1) \in [0, 1] \quad (2.14) \]
\[ \forall r \in \mathcal{L}, \ i = 1, \ldots, \tilde{b}, \]

where \( E(\eta_i(r, k)) \) is the expected value with respect to the initial particle distribution \( \xi_0 \in \mathcal{S} \) of the Markov stochastic process. Note that because of the Boolean nature of the occupation variable \( \eta_i(r, k) \), we can identify \( f_i(r, k) \) with
the probability of finding a particle at channel \((r, c_i)\) at time \(k\). The expected **local mass** \(\rho(r, k) \in [0, \hat{b}]\) at a node is obtained by summing over the expected occupation numbers, i.e.,

\[
\rho(r, k) := E(n(r, k)) = E \left( \sum_{i=1}^{\hat{b}} \eta_i(r, k) \right) = \sum_{i=1}^{\hat{b}} f_i(r, k),
\]

and the expected **total mass** at time \(k\) will be denoted by \(\rho(k)\), which is

\[
\rho(k) := \sum_{r \in \mathcal{L}} \rho(r, k).
\]

Furthermore, **local** and **total particle densities** are defined as

\[
\rho(r, k) := \frac{1}{\hat{b}} \rho(r, k) \in [0, 1],
\]

\[
\rho(k) := \sum_{r \in \mathcal{L}} \rho(r, k) \in [0, 1].
\]

Extending the mean–field assumption (2.10) (cf. p. 31) to on–node configurations, the single node distribution function at time \(k\) factorises to

\[
P_k(s(r)) = P_k(\eta_1(r), \ldots, \eta_\hat{b}(r)) = \hat{b} \prod_{i=1}^{\hat{b}} P_k(\eta_i(r))
\]

\[
= \hat{b} \prod_{i=1}^{\hat{b}} f_i(r, k)^{\eta_i(r)} (1 - f_i(r, k))^{(1 - \eta_i(r))}.
\]

Note that with this assumption the Boolean occupation numbers are considered as independent random variables. Therefore, it is possible to replace the average of products by the product of averages. In particular,

\[
E(\eta_i(r, k) \eta_j(r, k))
\]

\[
= \begin{cases} 
E(\eta_i(r, k))E(\eta_j(r, k)) = f_i(r, k)f_j(r, k) & \text{if } i \neq j \\
E(\eta_i(r, k)^2) = E(\eta_i(r, k)) = f_i(r, k) & \text{if } i = j \quad (*)
\end{cases}
\]

holds.

The physical (statistical mechanics) interpretation of this approach concentrates on **ensembles**\(^4\) in which each possible microscopic configuration occurs with a particular probability. Then, one assumes that appropriate space or time averages of an individual configuration agree with averages obtained from an ensemble of different configurations. In this sense, the single particle distribution function \(f_i(r, k)\) is formally treated as the average over an arbitrary

\(^4\) A large number of identically prepared systems is called an ensemble.
distribution of initial occupation numbers \( \{ \eta_i(r, 0) \} \). Then, the mean–field assumption (2.15) states that different occupation numbers are statistically independent (Rothman and Zaleski 1997, Chopard and Droz 1998). This assumption is based on Ludwig Boltzmann’s (1844–1906) famous molecular chaos hypothesis for (ideal) gases: due to the numerous gas molecules collisions, the effects of individual inter–molecular forces are relatively weak and fluctuations are negligible; they can be approximated by the average force\(^5\) (Stowe 1984).

Under mean–field assumption, according to Eqn. (2.4) on page 28, the dynamical equation for the single particle distribution function is

\[
 f_i(r + mc_i, k + 1) = E(\eta_i(r + mc_i, k + 1))
\]

\[
 = E(\eta_i^2(r, k)) = P(\eta_i^2(r) = 1) = \sum_{z \in \{0,1\}^\hat{d}} z_i P(\eta_i^2(r) = z)
\]

\[
 = \sum_{z \in \{0,1\}^\hat{d}} \sum_{\tilde{z} \in \mathcal{S}_N(r)} z_i W(\tilde{s}_{N(r)} \rightarrow z) P_k(\tilde{\eta}(r_1), \ldots, \tilde{\eta}(r_N)) ,
\]

which by neglecting off–node correlations (Eqn. (2.10)) becomes

\[
 = \sum_{z \in \{0,1\}^\hat{d}} \sum_{\tilde{z} \in \mathcal{S}_N(r)} z_i W(\tilde{s}_{N(r)} \rightarrow z) \prod_{r_i \in \mathcal{N}_i^*(r)} P_k(\tilde{\eta}(r_i)) ,
\]

and by additionally neglecting on–node correlations (Eqn. (2.15))

\[
 = \sum_{z \in \{0,1\}^\hat{d}} \sum_{\tilde{z} \in \mathcal{S}_N(r)} z_i W(\tilde{s}_{N(r)} \rightarrow z) \prod_{r_i \in \mathcal{N}_i^*(r)} \prod_{l=1}^{\hat{d}} P_k(\tilde{\eta}(r_i))
\]

\[
 = \sum_{z(r) \in \{0,1\}^\hat{d}} \sum_{\tilde{z} \in \mathcal{S}_N(r)} z_i(r) W(\tilde{s}_{N(r)} \rightarrow z) \prod_{r_i \in \mathcal{N}_i^*(r)} \prod_{l=1}^{\hat{d}} f_i(r_i, k) \tilde{\eta}(r_i) (1 - f_i(r_i, k))^{(1-\tilde{\eta}(r_i))} .
\]

The standard notation of the mean–field approximation for LGCA is the (non-linear) lattice–Boltzmann equation (Frisch et al. 1987) given by

\[
f_i(r + mc_i, k + 1) - f_i(r, k)
\]

\[
 = E(\eta_i^2(r, k) - \eta_i(r, k))
\]

\[
 = \sum_{z \in \{0,1\}^\hat{d}} \sum_{\tilde{z} \in \mathcal{S}_N(r)} (z_i - \tilde{\eta}(r)) W(\tilde{s}_{N(r)} \rightarrow z) .
\]

\(^5\)More generally, the hypothesis relies on the rapid randomisation of microscopic configurations in many particle systems.
\[ \prod_{r_i \in N'_0(r)} \prod_{l=1}^{\tilde{b}} f_l(r_i, k) \tilde{\eta}(r_i) \left( 1 - f_l(r_i, k) \right)^{1-\tilde{\eta}(r_i)} \]

\[ = \tilde{C}_i(f_{N(r)}(k)) \]

where \( f^T_{N(r)}(k) = (f(r_i, k))_{r_i \in N'_0(r)} = \left( (f_1(r_i, k), \ldots, f_{\tilde{b}}(r_i, k)) \right)_{r_i \in N'_0(r)} \).

Here, \( \tilde{C}_i(f_{N(r)}(k)) \in [0,1] \) expresses how the average number of particles with a given velocity \( mc_i \) changes, due to inter-particle interactions and propagation. Note that the lattice–Boltzmann equation can be derived from the micro-dynamical difference Eqn. (2.5) (cf. p. 28) by replacing occupation numbers \( \eta \) by average occupation numbers \( f_i \), i.e.

\[ E(\eta_i(r + mc_i, k + 1) - \eta_i(r, k)) = E(\tilde{C}_i(s_{N(r)}(k))) \]

\[ = \left[ f_i(r + mc_i, k + 1) - f_i(r, k) \right] = \tilde{C}_i(f_{N(r)}(k)), \quad i = 1, \ldots, \tilde{b}, \] (2.19)

in which the average is taken under consideration of (2.16)(*). Thus, for a multi-component system it follows from Eqn. (2.6) (cf. p. 28) that

\[ f_{\sigma,i}(r + m\sigma c_i, k + 1) - f_{\sigma,i}(r, k) = \tilde{C}_{\sigma,i}(f_{N(r)}(k)) \] (2.20)

for \( i = 1, \ldots, \tilde{b}, \sigma = 1, \ldots, \xi \) and where

\[ f^T_{N(r)}(k) = \left( (f_{\sigma_i}(r_i, k))_{r_i \in N'_0(r)} \right)_{\sigma=1}^{\xi}, \quad f_{\sigma}(r_i, k) = (f_{\sigma,1}(r_i, k), \ldots, f_{\sigma,\tilde{b}}(r_i, k)) \]

The obtained mean-field Eqns. (2.11) (cf. p. 31) and (2.19) are deterministic equations which describe the dynamics of the automaton average concentrations and have been derived neglecting all the correlations in the automaton. They encode information contained in the local cellular automaton rule. In addition, the lattice Boltzmann equation (2.19) of a LGCA model has the property that it keeps also information about the structure of the lattice on which the automaton operates (for \( m \neq 0 \)). Hence, one can expect that the analysis of the automaton (stochastic) dynamics in terms of these time- and space-dependent difference equations can provide an approximation. But how ‘good’ is this approximation? Can we properly predict important aspects of the (stochastic) automaton dynamics, such as the wave length of an observed pattern? We will try to explore answers to this question within this work.

In order to improve the mean-field approximation given by

\[ P(s_M) = P\left(s(r_1), \ldots, s(r_{|M|})\right) = \prod_{r_i \in M} P\left(s(r_i)\right), \]

probabilities of large local configurations of length \( |M| > 2 \) can be estimated by taking into account probabilities of smaller blocks with maximal length
2.3 Analytical methods

\[ 2 \leq l < |\mathcal{M}| \text{ which they contain, i.e. (Gutowitz et al. 1987)} \]

\[
P\left(s(r_1), s(r_2), \ldots, s(r_l), s(r_{l+1})\right) = \begin{cases} 
\frac{P\left(s(r_2), \ldots, s(r_{l+1})\right) P\left(s(r_1), \ldots, s(r_l)\right)}{P\left(s(r_2), \ldots, s(r_l)\right)} & \text{if } P\left(s(r_2), \ldots, s(r_l)\right) > 0 \\
0 & \text{else}.
\end{cases}
\]

Note that the resulting equations involve rational fractions, whereas the mean-field equations are polynomial equations.

**Example:** An improved mean-field approximation for the model of ‘diffusion of innovations’ is derived including probabilities of local configurations of length 1 and 2 \((l = 2)\). From Eqn. (2.9) (p. 30) and the probabilistic local rule defined on page 25 we get for the expected density of adopters

\[
x_1(k+1) = \sum_{(z_1, z_2, z_3) \in \{0,1\}^3} W\left((z_1, z_2, z_3) \rightarrow 1\right) P_k(z_1, z_2, z_3) \\
= \sum_{(z_1, z_2, z_3) \in \{0,1\}^3} W\left((z_1, z_2, z_3) \rightarrow 1\right) \frac{1}{P_k(z_2)} P_k(z_2, z_3) P_k(z_1, z_2) \\
= \sum_{(z_1, z_2) \in \{0,1\}^2} \frac{1}{P_k(1)} P_k(1, z_3) P_k(z_1, 1) \\
+ \sum_{(z_1, 0, z_2) \in \{0,1\}^3} \frac{1}{2} (z_1 + z_3) \frac{1}{P_k(0)} P_k(0, z_3) P_k(z_1, 0) \\
= 2 P_k(1) - P_k(1, 1) = 2 x_1(k) - P_k(1, 1),
\]

where we have used the assumption that \(P_k(1, 0) = P_k(0, 1)\) and the fact that \(P_k(1, 0) - P_k(0, 0) = P_k(1) - P_k(1, 1)\). Note that in order to derive a closed expression for the dynamics of the expected density of adopters, the time evolution equations for the two-block probabilities \(P_k(z_1, z_2), (z_1, z_2) \in \{0,1\}^2\), have to be analysed in a next step.

This or very similar approximation techniques are known under various names, i.e., probability path method (Kikuchi 1966), local structure theory (Gutowitz et al. 1987, Gutowitz and Victor 1989), \(l\)-step Markov approximation (Gutowitz 1990b), cluster approximation (Ben Avraham and Köhler 1992, Rieger et al. 1994, Schreckenberg et al. 1995) or the so-called BBGKY\(^6\) hierarchy (Busse-maker 1995). An approximation with blocks of size \(l \geq 2\) explicitly takes into account spatial short-range correlations between the sites, and therefore the quality of the approximation improves with increasing block size \(l\). Unfortunately, even in one dimension, approximations for \(l \geq 2\) are very hard to obtain (Rieger et al. 1994).

\(^6\)BBGKY hierarchy, after Bogoliubov, Born, Kirkwood, Green, and Yvon
2.3.2 Linear stability analysis

In order to analyse the automaton dynamics in terms of the mean–field Eqns. (2.13) (cf. p. 32) or (2.19) (cf. p. 36), standard mathematical tools, such as linear stability analysis, can be applied (i.e. Murray 1989, Kelley and Peterson 1991). We begin with a short outline of the linear stability analysis of the system of time discrete mean–field Eqn. (2.13) which is given in vectorial notation by

$$\mathbf{x}(k + 1) = \mathbf{H}(\mathbf{x}(k)),$$

where $\mathbf{x}^T = (x_i)_{i=1}^{|\mathcal{E}|}$ and $\mathbf{H}^T = (H_i)_{i=1}^{|\mathcal{E}|}$. The $H_i$’s are nonlinear functions of polynomial type. Of special interest are steady–state solutions in which $x_i$ retain the same value for all times, i.e.

$$x_i(k) = \bar{x}_i, \quad \forall k \in \mathbb{N}, \ i = 1, \ldots, |\mathcal{E}|.$$ 

These can be obtained by solving the fix–point equation for the system

$$\mathbf{x}(k + 1) = \mathbf{H}(\mathbf{x}(k)) = \mathbf{x}(k).$$

In order to characterise the behaviour of the system close to a fix point $\bar{\mathbf{x}}^T = (\bar{x}_i)_{i=1}^{|\mathcal{E}|}$, the time evolution of a small perturbation $\delta \mathbf{x}^T = (\delta x_i)_{i=1}^{|\mathcal{E}|}$ around $\bar{\mathbf{x}}$ is analysed. In particular,

$$\delta \mathbf{x}(k) := \mathbf{x}(k) - \bar{\mathbf{x}}$$

$$\delta \mathbf{x}(k + 1) = \mathbf{x}(k + 1) - \bar{\mathbf{x}} = \mathbf{H}(\mathbf{x}(k)) - \bar{\mathbf{x}} = \mathbf{H}(\bar{\mathbf{x}} + \delta \mathbf{x}(k)) - \bar{\mathbf{x}}$$

$$\simeq \mathbf{J} \delta \mathbf{x}(k),$$

where a first–order Taylor expansion of $\mathbf{H}(\bar{\mathbf{x}} + \delta \mathbf{x}(k))$ is used to obtain a linear approximation of $\delta \mathbf{x}(k + 1)$. The Jacobian matrix $\mathbf{J}$ is defined as

$$J_{ij} = \left. \frac{\partial H_i(\mathbf{x}(k))}{\partial x_j(k)} \right|_{\mathbf{x}} \quad i, j = 1, \ldots, |\mathcal{E}|.$$ 

Equation (2.21) is a linear first–order homogeneous difference equation with constant coefficients, whose general solution is

$$\delta \mathbf{x}(k) = \mathbf{J}^k \delta \mathbf{x}(0) \quad \text{or}$$

$$\delta x_i(k) = \sum_{i=1}^{n} p_i(k) \lambda_i^k \quad i = 1, \ldots, |\mathcal{E}|.$$ 

Here, $\Lambda_J = \{\lambda_1, \ldots, \lambda_n\}$ is the set of distinct eigenvalues (spectrum) of $\mathbf{J}$ and $p_i(k)$ is a polynomial of degree less than $\alpha_i$ which is given by the minimal polynomial $\prod_{i=1}^{n} (x - \lambda_i)^{\alpha_i}$ of $\mathbf{J}$ (Kelley and Peterson 1991). If $\mathbf{J}$ has $|\mathcal{E}|$
linearily independent eigenvectors $v_i$, which means that $J$ is diagonalisable, then Eqn. (2.22) reduces to
\[
\delta x_i(k) = \sum_{i=1}^{\mathcal{E}} d_i v_i \lambda_i^k \quad i = 1, \ldots, |\mathcal{E}|,
\] (2.23)

where $v_{i\ell}$ is the $i$'th component of $v_\ell$ and the coefficient $d_i \in \mathbb{C}$ is a constant which is uniquely determined by the initial condition, i.e. $\delta \mathbf{x}(0) = d_1 v_1 + \cdots + d_{|\mathcal{E}|} v_{|\mathcal{E}|}$.

Hence, the dynamics of the perturbation $\delta \mathbf{x}(k)$ is determined by the eigenvalues of $J$, especially by the spectral radius
\[
\mu := \max \{|\lambda| : \lambda \in \Lambda_J\}.
\]

Typical behaviours\footnote{for details and proofs see for example Kelley and Peterson (1991)} are summarised as follows:

- If $\mu < 1$, then all perturbations $\delta \mathbf{x}(k)$ decrease, i.e. $\lim_{k \to \infty} \delta \mathbf{x}(k) = 0$, which means the stationary state $\bar{\mathbf{x}}$ is locally stable.

- If $\mu = 1$ and real or complex conjugate eigenvalues $\lambda$ with $|\lambda| = 1$ are simple\footnote{This means that the multiplicity of $\lambda$ as a root of the characteristic equation is 1.}, then there is a constant $C$ such that $|\delta \mathbf{x}(k)| \leq C |\delta \mathbf{x}(0)|$ for all times $k \in \mathbb{N}$. Hence, all perturbations are bounded, which is a weaker form of stability of the stationary state $\bar{\mathbf{x}}$.

- If $\mu \geq 1$, then perturbations $\delta \mathbf{x}(k)$ exist which do not decay. If $\mu > 1$, then perturbations can become very large in time such that the approximate Eqn. (2.21) will no longer be valid. In this case the stationary state $\bar{\mathbf{x}}$ is called locally unstable.

- An eigenvalue less than zero, $\lambda < 0$, implies a converging ($\lambda > -1$) or diverging ($\lambda < -1$) sawtooth oscillation\footnote{Note that this can not occur in analogous continuous–time systems.} in one of the r.h.s. expressions in Eqn. (2.22), since $\lambda^k = (-1)^k |\lambda|^k$. As all eigenvalues can have different signs, a variety of possibilities exists for the linear combination of solutions. In the linear system (2.22), the eigenvalue corresponding to the spectral radius determines the qualitative behaviour for $k \to \infty$.

Next, we outline the linear stability analysis of the lattice–Boltzmann equation (2.19) which is not only time– but also space–dependent.
Stability analysis of the lattice–Boltzmann equation

In a first attempt to understand the solutions of the time– and space–discrete lattice–Boltzmann equation (2.19) (cf. p. 36), we analyse the stability of **spatially uniform steady states**

\[ f_i(r, k) = \tilde{f}_i, \quad \forall r \in \mathcal{L}, \forall k \in \mathbb{N}, \]

with respect to small, spatially heterogeneous local fluctuations

\[ \delta f_i(r, k) := f_i(r, k) - \tilde{f}_i, \quad i = 1, \ldots, \hat{b}. \]

The homogeneous stationary states \( \tilde{f}_i \) are obtained under the assumption that the automaton is in an equilibrium locally with regard to its interactions, i.e. they satisfy the equations

\[ \tilde{\mathcal{C}}_i(\tilde{f}_N) = 0, \quad i = 1, \ldots, \hat{b}, \]

where

\[ \tilde{f} = (\tilde{f}_1, \ldots, \tilde{f}_\hat{b}) \quad \text{and} \quad \tilde{f}_N^T = (\tilde{f}, \ldots, \tilde{f}), \quad \nu = |\mathcal{N}_r| \]

If Eqn. (2.19) contains **nonlinearities**, linearisation around \( \tilde{f} \) yields the **linear lattice–Boltzmann equation**

\[
\begin{align*}
\delta f_i(r + mc_i, k + 1) &= \delta f_i(r, k) + \sum_{j=1}^{\hat{b}} \Omega_{ij}^0 \delta f_j(r, k) \\
&\quad + \sum_{r_n \in \mathcal{N}_r} \sum_{j=1}^{\hat{b}} \Omega_{ij}^0 \delta f_j(r_n, k),
\end{align*}
\]

(2.24)

where the elements of the \( \hat{b} \times \hat{b} \) – matrices \( \Omega^p \) are defined as

\[
\Omega_{ij}^p := \left. \frac{\partial \hat{\mathcal{C}}_i(\delta f_N(k))}{\partial \delta f_j(r, k)} \right|_{\tilde{f}} \quad \text{and} \quad \Omega_{ij}^n := \left. \frac{\partial \hat{\mathcal{C}}_i(\delta f_N(k))}{\partial \delta f_j(r_n, k)} \right|_{\tilde{f}}, \quad i = 1, \ldots, \hat{b}.
\]

To determine the stability of the spatially uniform steady state \( \tilde{f} \), we have to find solutions \( \delta f_i(r, k) \) of the set of spatially coupled linear difference Eqn. (2.24). If fluctuations decrease to zero when \( k \to \infty \), then \( \tilde{f} \) is stable with respect to spatially heterogeneous local fluctuations \( \delta f_i(r, 0) \). Equation (2.24) can be solved explicitly under the assumption that the fluctuations have a spatial dependence of sinusoidal shape (Press et al. 1988).
2.3 Analytical methods

Therefore, solutions for a one-dimensional periodic lattice with $L$ nodes are all of the form

$$\delta f_i(r, k) \propto \lambda^k \cos(\hat{q} \cdot r) . \quad (2.25)$$

As $\lambda^k \cos(\hat{q} \cdot r) = \delta f_i(r, k) = \delta f_i(r + L, k) = \lambda^k \cos(\hat{q} \cdot (r + L))$, we find that $\hat{q} = \frac{2\pi}{L} q$, where $q$ is an integer, $q = 0, \ldots, L - 1$; $L/q$ gives the wave length of the fluctuation and from now on we shall refer to $q$ as the wave number. In other words, $q$ is the number of sine or cosine waves which can ‘fit’ into a domain of a given size.

Similarly, for a two-dimensional lattice with $|\mathcal{L}| = L_1 \cdot L_2$ nodes $r = (r_1, r_2)$ we consider fluctuations of the form

$$\delta f_i(r, k) \propto \lambda^k \cos(\hat{q}_1 \cdot r_1) \cos(\hat{q}_2 \cdot r_2) . \quad (2.26)$$

Again, implying periodic boundary conditions we find that $\hat{q} = (\hat{q}_1, \hat{q}_2) = \left(\frac{2\pi}{L_1} q_1, \frac{2\pi}{L_2} q_2\right)$ with the wave number $q = (q_1, q_2)$ where $q_1 = 0, \ldots, L_1$ and $q_1 = 0, \ldots, L_2$. Here, and in the sequel we solely consider two-dimensional lattices with $L_1 = L_2 = L$.

Note that fluctuations associated with the wave number $q = 0$ are spatially homogeneous.

Fourier series theory allows the representation of arbitrary fluctuations as a generalised sum of sinusoidal terms. In order to find all solutions of Eqn. (2.24), we apply the discrete finite Fourier transform $\mathcal{F}$ and its inverse $\mathcal{F}^{-1}$, which are defined as

\[
\mathcal{F}\{\delta f_i(r, k)\} = F_i(q, k) = \sum_r e^{i \frac{2\pi}{L} q \cdot r} \delta f_i(r, k) , \quad (2.27)
\]

\[
\mathcal{F}^{-1}\{F_i(q, k)\} = \delta f_i(r, k) = \frac{1}{|\mathcal{L}|} \sum_q e^{-i \frac{2\pi}{L} q \cdot r} F_i(q, k) ,
\]

where $|\mathcal{L}| = L$ in one dimension and $|\mathcal{L}| = L^2$ and $q \cdot r = q_1 r_1 + q_2 r_2$ in two dimensions.

Transforming the linear Boltzmann equation (2.24) in Fourier space we obtain

\[
\mathcal{F}\{\delta f_i(r + mc, k + 1)\} = e^{i \frac{2\pi}{L} q \cdot mc} F_i(q, k + 1) \quad (2.28)
\]

\[
= F(q, k) + \sum_{j=1}^{\hat{b}} \Omega_i^j F_j(q, k)
\]

\[
+ \mathcal{F} \left\{ \sum_{r_n \in \mathcal{N}_i^j(r)} \sum_{j=1}^{\hat{b}} \Omega_i^j \delta f_j(r_n, k) \right\} .
\]
According to the translation invariance of the interaction neighbourhood $\mathcal{N}_b'(r)$ (cf. definition on p. 22), Eqn. (2.28) can be simplified to

$$F_i(q, k + 1) = e^{-1 \frac{i \omega}{2} q \cdot mc} \{ F_i(q, k) + \sum_{j=1}^{\tilde{b}} \Omega_{ij}^0 F_j(q, k) + \sum_{n=1}^\nu \sum_{j=1}^{\tilde{b}} \Omega_{ij}^n e^{i \frac{2\pi}{k} q \cdot \hat{c}_n} F_j(q, k) \} ,$$

with $\hat{c}_n \in \mathcal{N}_b'$, $n = 1, \ldots, \nu$. Let $\mathbf{F}^T(q, k) = (F_1(q, k), \ldots, F_{\tilde{b}}(q, k))$, then each mode $\mathbf{F}(q, k)$ evolves according to the vector equation

$$\mathbf{F}(q, k + 1) = \Gamma(q) \mathbf{F}(q, k) ,$$

where the elements of the $\tilde{b} \times \tilde{b}$ matrix $\Gamma(q)$ are given by

$$\Gamma_{ij}(q) = e^{-1 \frac{i \omega}{2} q \cdot mc} \{ \delta_{ij} + \sum_{n=1}^\nu \Omega_{ij}^n e^{i \frac{2\pi}{k} q \cdot \hat{c}_n} \} .$$

In matrix notation this becomes

$$\Gamma(q) = T \{ I + \Omega^0 + \sum_{n=1}^\nu \Omega^n e^{i \frac{2\pi}{k} q \cdot \hat{c}_n} \} ,$$

with $\hat{c}_n \in \mathcal{N}_b'$, $n = 1, \ldots, \nu$, the identity matrix $I$ and the ‘transport matrix’ $T = \text{diag}(e^{-1 \frac{i \omega}{2} q \cdot mc}, \ldots, e^{-1 \frac{i \omega}{2} q \cdot mc})$.

$\Gamma(q)$ is known as the Boltzmann propagator (Frisch et al. 1987). The solution of the linear discrete–time Eqn. (2.30) for each $q$ becomes

$$\mathbf{F}(q, k) = \Gamma(q)^k \mathbf{F}(q, 0), \quad \forall k \in \mathbb{N} .$$

Therefore, each Fourier component $\mathbf{F}(q, k)$ corresponding to each wave number $q$ evolves independently of the components corresponding to other wave numbers. The general solution (2.32) can be rewritten in the form

$$F_i(q, k) = \sum_{l=1}^n p_l(q, k) \lambda_l(q)^k ,$$

where the spectrum of $\Gamma(q)$ is given by $\Lambda_{\Gamma(q)} = \{ \lambda_1(q), \ldots, \lambda_n(q) \}$ and $p_l(q, k)$ is a polynomial in $k$ with coefficients depending on $q$ defined in the same way as the polynomial in Eqn. (2.22) on page 38. Taking the inverse Fourier transform $\mathcal{F}^{-1}$ of Eqn. (2.33), we obtain that the complete solution for the linear lattice–Boltzmann equation (2.24) is given by a superposition of single $q$–mode solutions, which are the modes corresponding to the wave number $q$, i.e.

$$\delta f_i(r, k) = \frac{1}{|\mathcal{L}|} \sum_q \sum_{l=1}^n p_l(q, k) e^{-1 \frac{i \omega}{2} q \cdot r} \lambda_l(q)^k .$$
2.3 Analytical methods

Again, if $\Gamma(q)$ is diagonalisable, which means that it has $\hat{b}$ linearly independent eigenvectors $v_i(q) = (v_{il}(q))_{l=1}^{\hat{b}}$, then

$$F_i(q, k) = \sum_{l=1}^{\hat{b}} d_l(q) v_{il}(q) \lambda_l(q)^k,$$

where the constants $d_l(q) \in \mathbb{C}$ are specified by the initial condition

$$F_i(q, 0) = \sum_{l=1}^{\hat{b}} d_l(q) v_{il}(q) = \sum_r e^{i \frac{2\pi q \cdot r}{\ell}} \delta f_i(r, 0), \quad i = 1, \ldots, \hat{b},$$

and hence

$$\delta f_i(r, k) = \frac{1}{|\mathcal{L}|} \sum_q e^{-i \frac{2\pi q \cdot r}{\ell}} F_i(q, k)$$

$$= \frac{1}{|\mathcal{L}|} \sum_q e^{-i \frac{2\pi q \cdot r}{\ell}} \sum_{l=1}^{\hat{b}} d_l(q) v_{il}(q) \lambda_l(q)^k.$$

Thus, from Eqn. (2.32) it follows that Eqn. (2.24) is linearly stable with respect to perturbations of wave number $q$ if the vector $F(q, k)$ remains finite. As in space–independent discrete systems (cf. p. 39), this is the case if $\Gamma(q)$ has no eigenvalue with an absolute value larger than 1. Hence, by analysing the spectrum $\Lambda_\Gamma(q)$ of the Boltzmann propagator $\Gamma(q)$, we can predict which modes can grow with time, leading to the possible emergence of spatial patterns. The corresponding set of critical wave numbers will be denoted by

$$Q^c := \left\{ q = (q_i)_{i=1}^d, q_i \in \{0, \ldots, L_i - 1\} : \mu(q) \geq 1 \right\},$$

where the spectral radius for each wave number $q$ is given by

$$\mu(q) := \max\{|\lambda(q)| : \lambda(q) \in \Lambda_\Gamma(q)\}.$$

Consequently, the dynamics of the system (2.24) (p. 40) is determined by

$$\delta f_i(r, k) \sim \sum_{q \in Q^c} e^{-i \frac{2\pi q \cdot r}{\ell}} F_i(q, k).$$

Certain cases may be distinguished:\footnote{for these and other cases, i.e. orientation–induced pattern formation (‘swarming instability’), see also Bussemaker (1995) and Deutsch (1999)}
No spatial pattern  The spatially homogeneous stationary solution \( \bar{f} \) is stable to any perturbation if \( \mu(q) \leq 1 \) for each wave number \( q \). The LGCA model for simultaneous random movement studied in Sec. 3.4 belongs to this category.

Stationary spatial pattern  If a critical wave number \( q \in Q^c \) exists such that \( q \neq 0 \) and if the corresponding eigenvalue is real, then these \( q \)-modes grow and there is an indication of a prevailing spatial wave length \( L/q \). The \( q \)-directions (in two dimensions) determine the structure of the pattern. Pattern formation of this kind is exemplarily studied in a one- and two-dimensional LGCA model based on activator–inhibitor interactions introduced in Sec. 5.1.

Nonstationary spatial pattern  Again, a critical wave number \( q \in Q^c \) exists such that \( q \neq 0 \), but the corresponding eigenvalue has a non-zero imaginary part. In Sec. 5.2 we introduce a two-dimensional LGCA model which leads to spatial oscillating spirals.

It is important to stress here that it is a feature of linear theory that each of the various modes grows or decays independently of the other modes.

### 2.4 Summary

In this chapter deterministic, probabilistic and lattice–gas cellular automata are introduced, which are characterised by a regular lattice, an interaction neighbourhood template, the set of elementary states, and the local space–and time–independent transition rule which is applied to each cell in parallel. In Subsec. 2.3.1, we presented the so-called mean–field theory as an approximation method to study dynamic properties of cellular automata. After assigning a probability to each of the elementary states of the automaton, the probabilities of the next generation are calculated on the basis of the usual combinatorial rules of probability, assuming that the probabilities for each of the sites in a neighbourhood are independent. It turns out that mean–field equations for deterministic and probabilistic cellular automata are time–dependent difference equations, whereas mean–field equations for LGCA are space– and time–dependent difference equations, called lattice–Boltzmann equations. The space dependence in the latter case results from the propagation step that supplements the interaction dynamics in LGCA. Since the state values of cellular automaton mean–field approximations are continuous, standard analytical tools for studying the system dynamics can be applied. In this work we focus on a linear stability analysis. We outlined in Subsec. 2.3.2 the linear stability analysis for systems of time–dependent difference equations in order to determine the temporal evolution of state probabilities with respect to the stability of stationary states. We also showed how to deal with systems
of space– and time–dependent difference equations. The stability of spatially homogeneous steady states is investigated by analysing the spectrum of the linearised and Fourier transformed system of space– and time–dependent difference equations, called Boltzmann propagator. We characterised different situations in which Fourier modes can indicate the formation of spatial patterns. In the following chapters we provide examples of LGCA to demonstrate that LGCA–dynamics may indeed be analysed by means of stability analysis.
3 Particle movement

3.1 Introduction

The term particles refers to any identifiable unit, for example, physical particles like molecules, biological cells or individuals, or ‘things’ such as diseases, rumours and technologies. The motion of particles in space\(^1\) can be directed or random, independent or dependent, i.e. if the motion is biased by an interaction between particles or by the environment, and active or passive. Although it is not always obvious to distinguish essential properties of particle motion, some examples are given in Table 3.1.

<table>
<thead>
<tr>
<th>phenomenon</th>
<th>‘particle’</th>
<th>movement</th>
<th>active / passive</th>
</tr>
</thead>
<tbody>
<tr>
<td>flock of birds(^a)</td>
<td>bird</td>
<td>directed / random</td>
<td>dependent</td>
</tr>
<tr>
<td>sugar dissolution in coffee(^b)</td>
<td>molecule</td>
<td>random</td>
<td>independent</td>
</tr>
<tr>
<td>animal mobility through energy conversion(^c)</td>
<td>biological</td>
<td>random</td>
<td>dependent</td>
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<td></td>
<td>micro-object</td>
<td>i.e. bacterium,</td>
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<td>social insect</td>
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<td>city traffic(^d)</td>
<td>car</td>
<td>directed</td>
<td>dependent</td>
</tr>
<tr>
<td>evolution(^e)</td>
<td>phenotype</td>
<td>random</td>
<td>independent</td>
</tr>
<tr>
<td>opinion formation(^f)</td>
<td>individuals with opinions</td>
<td>random</td>
<td>dependent</td>
</tr>
</tbody>
</table>

Table 3.1: Examples of particle motion; references: \(^a\)Bussemaker et al. (1997), \(^b\)Alonso (1980), \(^c\)Ebeling (1999), \(^d\)Schadschneider (1999), \(^e\)Ebeling (1990), \(^f\)Helbing (1995).

Particle movement in space is one of the principal subjects of scientific interest. The point of departure is Brownian motion\(^2\). Random, independent and passive motion of particles leads to an endless irregular motion and is named after the botanist Robert Brown (1773–1858) (Brown 1828). In his botanical studies (1827), he found pollen grains in a state of continuing irregular motion.

\(^1\)The term space does not refer only to Euclidean space, but also to any abstract space such as ecological niche space, ‘social space’, i.e. space of attitudes, or fitness landscapes.

\(^2\)Some reviews are, e.g. Murray (1989), Okubo (1980) and Czárán (1998).
in water, and he explained this movement as a general phenomenon characterising small physical particles. Later, Albert Einstein recognised that the random motion observed by Brown was the result of innumerable collisions with the water molecules which are thermally driven (Einstein 1905). This explanation provided a link to the (macroscopic) physical process of molecular diffusion which is based on Fick’s phenomenological law (formulated by the physiologist Adolf Fick (1829–1901) in 1855). Fick’s law states that particle flux due to random motion is approximately proportional to the local gradient in the particle concentration. A more general definition of a diffusion concept is given by Ōkubo (1980), who states that the collective behaviour of many particles is a diffusive phenomenon, “when the microscopic irregular motion of each particle gives rise to a regularity of motion of the total particle group (macroscopic regularity)”. In his book Ōkubo provides an excellent review of diffusion models with biological applications\(^3\), for example the spread of genes (Fisher 1937) or the random dispersion of biological populations (Skellam 1951, Skellam 1973). Other applications of diffusion models are innovation and expenditure diffusion, worker migration, and price waves.\(^4\)

If particle motion is not random it is biased, either by an external, e.g. flow of the medium, or internal force, e.g. motivation to move to some ‘attractive position’ in space. In this case the collective movement of particles has a resulting directional component.

In the next section we give a brief formal description of a simple model which describes Brownian motion of a single particle as a stochastic process (i.e. Feller 1968, Haken 1978). For simplicity, we restrict our attention to the one-dimensional random motion. The common name for stochastic displacement is random walk. In the random walk model introduced here, time and space are assumed as discrete. Furthermore, the relation to the macroscopic diffusion equation will be described.

### 3.2 Discrete random walk and diffusion

Here, we assume that a single particle walks randomly on a one-dimensional periodic lattice \(\mathcal{L}_\epsilon\). Space and time are uniformly discretised such that the possible positions \(x \in \mathcal{L}_\epsilon\) of the particle at time \(t\) are given by

\[
x = x(t) = r \epsilon \quad \text{and} \quad t = k \delta,
\]

where \(|\mathcal{L}_\epsilon| = L\) spatial units of length \(\epsilon \in \mathbb{R}^+\) and temporal units of duration \(\delta \in \mathbb{R}^+\). Furthermore, we assume that besides motion no other events (i.e. death) occur. The random walk of the particle is described by choosing a new

---

\(^3\)see also Britton (1986)

\(^4\)for references and further examples of diffusion models see the book of Banks (1994)
random direction at each time $t$ and moving a step in that direction during the time interval between $t$ and $t + \delta$. The spatial steps are always of equal length $\epsilon$ in any direction and we suppose that successive moves are independent of each other. Since the particle should not be directional affected we choose equal probabilities $\alpha$ for jumps to the left and right. In this case the random walk is called isotropic\textsuperscript{5}. Furthermore, there is a probability that the particle does not move. Hence, as illustrated in Fig. 3.1, the change of the particle position is given by

$$x(t + \delta) = \begin{cases} 
  x(t) - \epsilon & \frac{\alpha}{2} \\
  x(t) & \text{with probability } 1 - \alpha, \\
  x(t) + \epsilon & \frac{\alpha}{2}
\end{cases}$$

where $\alpha \in [0,1]$ (Weimar 1995).

![Random walk model of a single particle on a one-dimensional lattice $\mathcal{L}_\epsilon$.](image)

Figure 3.1: Random walk model of a single particle on a one–dimensional lattice $\mathcal{L}_\epsilon$.

Let the particle position $x$ at time $t$ be a discrete random variable and let $P_s(x,t)$ be the probability that the single particle has reached point $x$ at time $t$. Then, the probabilistic description of the random walk model is given by

$$P_s(x,t + \delta) = \frac{\alpha}{2} P_s(x + \epsilon,t) + (1 - \alpha) P_s(x,t) + \frac{\alpha}{2} P_s(x - \epsilon,t) . \quad (3.1)$$

In order to solve this equation it is convenient to consider the corresponding equation

$$P_s\left(\frac{x}{\epsilon}, \frac{t + \delta}{\delta}\right) = P_s(r,k + 1) \quad (3.2)$$

$$= \frac{\alpha}{2} P_s(r + 1,k) + (1 - \alpha) P_s(r,k) + \frac{\alpha}{2} P_s(r - 1,k) .$$

This is a linear difference equation which can be solved by applying the discrete Fourier transformation and its inverse, as defined by (2.27) on page 41. The spatial Fourier transform of (3.2) is

$$\hat{P}_s(q,k + 1) := \mathcal{F}\{P_s(r,k)\}$$

\textsuperscript{5}from greek *isos*, the same, and *tropos*, direction
\[
\frac{\alpha}{2} e^{-\frac{1}{2} \frac{2\pi}{L} q} \hat{P}_s(q, k) + (1 - \alpha) \hat{P}_s(q, k) + \frac{\alpha}{2} e^{\frac{1}{2} \frac{2\pi}{L} q} \hat{P}_s(q, k)
\]
\[
= \left( 1 - \alpha + \alpha \cos\left(\frac{2\pi}{L} q\right) \right) \hat{P}_s(q, k)
\]

with solution
\[
\hat{P}_s(q, k) = \left( 1 - \alpha + \alpha \cos\left(\frac{2\pi}{L} q\right) \right)^k \hat{P}_s(q, 0),
\]

where
\[
\hat{P}_s(q, 0) = \sum_{r=0}^{L-1} e^{\frac{1}{2} \frac{2\pi}{L} qr} P_s(r, 0),
\]

for wave numbers \(q \in \{0, \ldots, L - 1\}\). Hence, the probability of finding the particle after \(k\) time steps at position \(r\) is given by

\[
P_s(r, k) = \mathcal{F}^{-1} \left\{ \hat{P}_s(q, k) \right\}
= \frac{1}{L} \sum_{q=0}^{L-1} \hat{P}_s(q, 0) e^{-\frac{1}{2} \frac{2\pi}{L} qr} \left( 1 - \alpha + \alpha \cos\left(\frac{2\pi}{L} q\right) \right)^k.
\]

(3.3)

If the particle starts at time step \(k = 0\) at position \(r^*\), i.e.
\[
P_s(r, 0) = \begin{cases} 1 & r = r^* \\ 0 & \text{else} \end{cases},
\]

the solution (3.3) becomes
\[
P_s(r, k) = \frac{1}{L} \sum_{q=0}^{L-1} e^{-\frac{1}{2} \frac{2\pi}{L} q(r - r^*)} \left( 1 - \alpha + \alpha \cos\left(\frac{2\pi}{L} q\right) \right)^k,
\]

and hence
\[
P_s(x, t) = \frac{1}{L} \sum_{q=0}^{L-1} e^{-\frac{1}{2} \frac{2\pi}{L} q(x - x^*)} \left( 1 - \alpha + \alpha \cos\left(\frac{2\pi}{L} q\right) \right)^{\frac{t}{\delta}},
\]

(3.4)

for \(x \in \{0, \epsilon, 2\epsilon, \ldots, L \epsilon\}\), \(x^* = r^* \epsilon\) and \(t = 0, \delta, 2\delta, \ldots\). Figure 3.2 shows this probability distribution \(P_s(x, t)\) at different times.

If a large number of particles follows the same random walk rule independently of each other, the probabilities \(P_s(x, t)\) for each walker can simply be added. In this sense, \(P(x, t) \equiv P_s(x, t)\) also represents the probability density of particles at position \(x = r \epsilon\) at time \(t = k \delta\).
In order to derive a description of the random walk in continuous time and space we assume that the density of particles within a small spatial interval of length $\varepsilon$ is large enough to neglect spatial and temporal random fluctuations in density. With this assumption, $P(x,t)$ can be considered as a smooth function in $x$ and $t$ such that it can be approximated using its Taylor expansion. We can rewrite Eqn. (3.1) as

$$P(x,t) = \frac{\alpha}{2} P(x + \varepsilon, t - \delta) + (1 - \alpha) P(x, t - \delta) + \frac{\alpha}{2} P(x - \varepsilon, t - \delta)$$  \hspace{1cm} (3.5)

and approximate $P(x, t - \delta)$ and $P(x \pm \varepsilon, t - \delta)$ by

$$P(x, t - \delta) = P(x, t) - \varepsilon \frac{\partial P(x, t)}{\partial t} + O(\delta^2)$$  \hspace{1cm} (3.6)

$$P(x \pm \varepsilon, t - \delta) = P(x, t) - \delta \frac{\partial P(x, t)}{\partial t} \pm \varepsilon \frac{\partial P(x, t)}{\partial x} + \frac{\varepsilon^2}{2} \frac{\partial^2 P(x, t)}{\partial x^2} + O(\varepsilon^2 \delta, \varepsilon \delta^2)$$  \hspace{1cm} (3.7)

Substituting Eqns. (3.6) and (3.7) in Eqn. (3.5) and rearranging terms yields

$$\frac{\partial P(x, t)}{\partial t} = \frac{\alpha}{2} \frac{\varepsilon^2}{\delta} \frac{\partial^2 P(x, t)}{\partial x^2} + O(\delta^2) + O(\varepsilon^2 \delta, \varepsilon \delta^2)$$  \hspace{1cm} (3.8)

Hence, in the limit for $\varepsilon \to 0$ and $\delta \to 0$ but with the requirement

$$\lim_{\varepsilon \to 0} \frac{\varepsilon^2}{\delta} = \text{constant} \neq 0$$  \hspace{1cm} (3.9)

Eqn. (3.8) becomes
\[ \frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial x^2} \quad \text{with} \quad D := \frac{\alpha}{2} \lim_{\epsilon \to 0} \frac{\epsilon^2}{\delta}, \quad (3.10) \]

for \( x \in \mathbb{R}, t \in \mathbb{R}^+ \). This is the (partial differential) equation of diffusion for the random walk that results from the limiting process. If \( P(x,t) \), the probability density, is multiplied by the total number of particles in the system, then the resulting equation for the particle density is known as Fick’s diffusion equation or heat equation. The analytic solvability of Eqn. (3.10) strongly depends on the imposed initial and boundary conditions. An extensive mathematical treatment of this equation can be found in Crank (1975). For example, if all particles start their walk at time \( t = 0 \) from the same position \( x^* \), i.e.

\[ P(x,0) = \begin{cases} 1 & x = x^* \\ 0 & \text{else} \end{cases}, \]

the solution of (3.10) for an infinite domain is given by

\[ P(x,t) = \frac{1}{\sqrt{4 \pi D t}} e^{- \frac{(x-x^*)^2}{4 D t}}, \quad t > 0. \quad (3.11) \]

A comparison of the approximated solution (3.11) with the exact solution of the random walk model (3.4) (cf. p. 50) for \( t = 1 \) is shown in Fig. 3.2 (cf. p. 51). Note that \( D \), which is the diffusion coefficient, has dimensions \((\text{length})^2 / (\text{time})\) and is not the speed of the particle motion. The speed \( c = \epsilon / \delta \) approaches positive infinity as \( \epsilon \to 0 \) and \( \delta \to 0 \). In other words, the continuous diffusion equation predicts that in an arbitrarily short time some particle will be found at an arbitrarily large distance from its starting point, which for most problems is a rather unrealistic assumption. Particles in the discrete random walk model have a finite speed. Note further that the derivation of the diffusion equation relies on \( \epsilon \) and \( \delta \) approaching zero in a rather specific way (cf. Eqn. (3.9)). As Okubo (1980) observes, the use of the continuous diffusion approximation is justified when “the time of observation \( t \) is much greater than the duration time \( \delta \) of each random step, and when the scale of observation \( x \) is much greater than the length of each random step \( \epsilon \).”

### 3.3 Movement in probabilistic cellular automaton models

The implementation of a random walk of many particles in a cellular automaton may cause problems. Since all (independent) particles move synchronously in a classical cellular automaton, several of them possibly choose to move at the same time to the same cell of the lattice. This may lead to an arbitrarily
3.3 Movement in probabilistic cellular automaton models

large number of particles in some lattice cells, which is in conflict with the requirement that the set of elementary states should be small and finite (cf. def. p. 20). In the following we present some solutions to this problem based on space–time dependent local rules (Subsec. 3.3.1) and asynchronous update (Subsec. 3.3.2).

3.3.1 One–dimensional random walk rule according to Toffoli and Margolus

The random walk rule of Toffoli and Margolus (1987) for particles is based on the assumptions that (i) Brownian motion does not occur in vacuum, i.e. pollen grain molecules interact with water molecules, and (ii) particles are impenetrable. Hence, when a particle moves it swaps places with other particles. In order to deal with a synchronous swapping of all particles the lattice is partitioned in non-overlapping ‘blocks’ (pairs) of two adjacent cells. As shown in Fig. 3.3, two partitions of lattice nodes are defined – one for even times and one for odd times. Each cell can be empty or can host one particle. At each

\[
\begin{align*}
  r : & \quad 9 \quad 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 0 \\
  k : & \quad \boxed{\text{-----------}} \\
  k + 1 : & \quad \boxed{\text{-----------}} \\
  k + 2 : & \quad \boxed{\text{-----------}} 
\end{align*}
\]

Figure 3.3: Example of time–dependent \( k \) block–partitioning of cells \( r \) for a one–dimensional periodic lattice \( L \) with \( L = 10 \) nodes.

time step \( k \) the contents of each block of cells is randomly swapped according to the actual partitioning of the lattice. This swapping rule is data blind since, if particles are present in both cells of a block, both will exchange places. Note that this random work algorithm leads to a time– and space–dependent local transition rule. Thus the Toffoli and Margolus model is not a probabilistic cellular automaton according to the definition given previously (Sec. 2.1, p. 23).

This model is formally defined as follows: the state of each cell is composed of two components \( s(r,k) = (s_1(r,k), s_2(r,k)) \in \mathcal{E} = \{0,1\}^2 \) where \( s_1(r,k) = 1 \) or 0 with equal probability and \( s_2(r,k) \) denotes the presence \( s_2(r,k) = 1 \) or absence \( s_2(r,k) = 0 \) of a particle in cell \( r \) at time \( k \). The random bit \( s_1 \) is used to model the randomness of swapping in such a way that whenever two cells \( r_1 \) and \( r_2 \) belonging to the same block have equal random bits, i.e. \( s_1(r_1,k) = s_1(r_2,k) \), then they exchange their contents, i.e. \( s_2(r_1,k+1) = s_2(r_2,k) \) and \( s_2(r_2,k+1) = s_2(r_1,k) \). With an interaction neighbourhood template given
by $A'_4 = \{-1, 0, 1\}$, the local interaction rule $R$ (cf. Eqn. (2.1) on p. 25) can be defined as

$$s(r, k + 1) = R(s_{N(1)}(k), r, k) = (R_1(r, k), R_2(s_{N(0)}(k), r, k))$$

with

$$s_1(r, k + 1) = R_1(r, k) = \xi(r, k + 1)$$

and

$$s_2(r, k + 1) = R_2 \left( (s(r - 1, k), s(r, k), s(r + 1, k)), r, k \right)$$

$$= ((r + k) \text{mod } 2) \left\{ \left( 1 - (s_1(r, k) - s_1(r + 1, k))^2 \right) s_2(r - 1, k) + (s_1(r, k) - s_1(r - 1, k))^2 s_2(r, k) \right\}$$

$$+ (1 - (r + k) \text{mod } 2) \left\{ \left( 1 - (s_1(r, k) - s_1(r + 1, k))^2 \right) s_2(r + 1, k) + (s_1(r, k) - s_1(r + 1, k))^2 s_2(r, k) \right\},$$

where $\xi(r, k) \in \{0, 1\}$ are time- and cell-independent random variables taken from a uniform distribution, i.e. $P(\xi(r, k) = 1) = 1/2$. Note that the resulting random walk of a single particle is not isotropic, as can be seen from the example given in Fig. 3.4.

![Diagram of random walk](image)

**Figure 3.4:** Example of a random walk of one particle; a number below a lattice cell $r$ denotes the probability of the particle starting from position $r^* = 4$ to reach position $r$ at time $k$. It can be seen that the random walk is not isotropic since the particle has a drift to the right.

The repeated application of this cellular automaton rule leads to a random walk of many particles, as shown in Fig. 3.5.
3.3 Movement in probabilistic cellular automaton models

Figure 3.5: Space–time–dynamics of the one–dimensional random walk model on a periodic lattice according to Toffoli and Margolus (1987); parameters: \( L = 100, k = 0, \ldots, 200 \) and initial particle distribution \( s_2(r, 0) = 1 \) for \( r = 45, \ldots, 55 \) and \( s_2(r, 0) = 0 \) else.

An extension of this model to two dimensions is straightforward (see Toffoli and Margolus 1987). The resulting partitioning of the two–dimensional lattice is known as the Margolus neighbourhood (see Fig. 3.6(a)).

(a) ‘Margolus neighbourhood’: Part of time–dependent block–partitioning of cells for a two–dimensional lattice. The solid frame belongs to the partition at time \( k \) and the dashed frame to the partition at time \( k + 1 \).

(b) Clockwise and counter–clockwise rotation of the contents of a Margolus block

Figure 3.6: Two–dimensional random walk model using the ‘Margolus neighbourhood’.

The contents of such a \( 2 \times 2 \) block of adjacent cells can be shuffled in \( 4! \) different ways. Chopard and Droz (1990) showed that a shuffling algorithm which considers only clockwise and counter–clockwise block–rotations with equal probability is sufficient to model diffusive behaviour on appropriate continuum space– and time–scales (cf. Fig. 3.6(b)).
3.3.2 One-dimensional random walk in probabilistic cellular automata with asynchronous updating

If we allow the updating procedure to be **asynchronous**, a common way\(^6\) to model a random walk of many particles is as follows: Each cell can be empty or occupied by at most one particle. A particle is selected at random and may move to a cell in its interaction neighbourhood also chosen at random. If this cell is empty the particle will move to it, otherwise the particle will not move. This is equivalent to exchanging the contents of each selected pair of cells since the particles are indistinguishable\(^7\). The interaction neighbourhood defines the range of the move. Note that this sequential procedure allows some particles to move more than others. Let \(N\) be the total number of particles in the system. If in one unit of time \(k\) to \(k + 1\), \(\tau N, \tau > 0\), particles are sequentially selected at random to perform a move, then the probability that \(\bar{N}\) particles are not selected to move is \((1 - \bar{N}/N)^\tau\). In particular, for a large number of particles we get

\[
\lim_{N \to \infty} (1 - \frac{\bar{N}}{N})^{\tau N} = e^{-\tau \bar{N}},
\]

and therefore the probability that a single cell, i.e. \(\bar{N} = 1\), is updated at least once in one unit of time is given by \(1 - e^{-\tau}\) in this limit. Hence, \(\tau\) represents the average number of **tentative** moves per particle during a unit of time. These considerations are the link to **continuous time** Markov chains (interacting particle systems). Herein, the probability that an event occurs with a rate \(\alpha\) at least once between times \(t\) and \(t + dt\), where \(t, dt \in \mathbb{R}^+\) and \(dt\) is small, follows \(1 - e^{-\alpha dt}\) (Durrett 1995). Then, the rate \(\alpha\) corresponds to \(\alpha = \tau \rho\), where \(\rho\) is the density of particles. One can identify \(\tau N = \alpha/\rho\) \(N = \alpha L\) steps with one unit of time, where \(L\) is the number of cells in the lattice.\(^8\)

From now on we set the range of the move to one (outer von Neumann interaction neighbourhood) and measure the degree of mixing with the parameter \(\tau\). Figure 3.7 shows a space-time plot of this asynchronous random walk for \(\tau = 1\) and \(\tau = 5\). Note that models of this type are also named ‘probabilistic automata networks’ (Boccara and Cheong 1992).

In the following sections, movement in deterministic and probabilistic cellular automaton models will always be defined according to the asynchronous random walk implementation (cf. Subsec. 3.3.2) because of its wide applications in many cellular automaton models.


\(^7\)Note that automata, in which the new states of two neighbouring cells are functions of the states of these cells, are known as ‘dimer automata’ (Schönfisch and Hadeler 1996).

\(^8\)Note that algorithms for (discrete) simulations of continuous Markov chains are defined similar to the asynchronous updating rule.
Figure 3.7: Space–time–dynamics of the one–dimensional asynchronous random walk model on a periodic lattice; parameters: $L = 100, k = 0, \ldots, 200$ and initial particle distribution $s_2(r, 0) = 1$ for $r = 45, \ldots, 55$ and $s_2(r, 0) = 0$ else.

3.4 Movement in lattice–gas cellular automaton models

The independent random walk of many particles within the framework of LGCA is modelled by a shuffling (mixing) operator $\mathcal{M}$ which acts as follows (Lawnickzak 1997): Before particles move from one node to a neighbouring node according to the propagation step (defined on page 27), each particle randomly selects a new velocity among the values permitted by the lattice. In order to avoid two or more particles occupying the same channel, a random permutation of the velocity vectors is performed, at each lattice node, independently of the node configuration (data–blind) and at each time step. This interaction step called shuffling step does not take into account the configuration of neighbouring nodes, i.e. $\mathcal{N}_b^o(r) = \{r\}$. Since $\hat{b}$ channels are assigned to each node, they can be shuffled in $\hat{b}$! ways, which is the number of permutations of $\hat{b}$ objects. Figure 3.8 shows all possible node configurations for a one–dimensional lattice with two velocity channels and one rest channel, i.e. $\hat{b} = 3$. Note that the shuffling operation conserves the number of particles but not the momentum.

The local shuffling process can be formally described as follows: If $u^j, j = 1, \ldots, \hat{b}$, are unit vectors with $\hat{b}$ components, $\mathcal{A}_b^\hat{b}$ denotes the set of all orthonor-
\[ n(r) = 0 \quad \bullet \circ \circ \quad \bullet \circ \circ \quad \bullet \circ \circ \]
\[ n(r) = 1 \quad \bullet \circ \circ \quad \bullet \circ \circ \quad \bullet \circ \circ \]
\[ n(r) = 2 \quad \bullet \circ \circ \quad \bullet \circ \circ \quad \bullet \circ \circ \]
\[ n(r) = 3 \quad \bullet \bullet \bullet \quad \bullet \bullet \bullet \quad \bullet \bullet \bullet \]

Figure 3.8: Possible node configurations for nodes of a one-dimensional lattice with \( \hat{b} = 3 \); \( n(r) \) denotes the total number of particles present at node \( r \).

Formal permutation matrices \( A \), given by
\[
\mathcal{A}_{\hat{b}} := \left\{ A \in \mathbb{R}^{\hat{b} \times \hat{b}} : \exists \pi \in \Pi_{\hat{b}} \ a^i = u^{\pi(i)} \ \forall i = 1, \ldots, \hat{b} \right\} = \left\{ A_1, \ldots, A_{\hat{b}} \right\},
\]
where \( a^i \) is the \( i \)th column vector of \( A \) and \( \Pi_{\hat{b}} \) is the set of all permutations of \( \hat{b} \) elements. In order to select a permutation matrix \( A_j \in \mathcal{A}_{\hat{b}} \), \( \{ \xi_j(r, k) \}_{r \in \mathcal{L}, k \in \mathbb{N}} \) is defined for each \( j = 1, \ldots, \hat{b}! \) as an independent sequence of independent, identically distributed Bernoulli-type random variables \( \xi_j \in \{0, 1\} \) such that for every \( k \) the random variables \( \{ \xi_j(r, k) \}_{r \in \mathcal{L}} \) are independent of the past evolution of the automaton,
\[
p_j := P(\xi_j(r, k) = 1) \quad j = 1, \ldots, \hat{b}! \quad \text{and} \quad (3.12)
\]
\[
\sum_{j=1}^{\hat{b}!} \xi_j(r, k) = \sum_{j=1}^{\hat{b}!} p_j = 1 \quad \forall r \in \mathcal{L}, \ k \in \mathbb{N}. \quad (3.13)
\]

Then, the microdynamics can be described by
\[
\eta_i^p(r, k) = R_i^p(\eta(r, k)) = \sum_{j=1}^{\hat{b}!} \xi_j(r, k) \sum_{l=1}^{\hat{b}} \eta_l(r, k) a^j_{il}, \quad (3.14)
\]
where \( a^j_{il} \) is a matrix element of \( A_j \in \mathcal{A}_{\hat{b}} \). Note that at a given node \( r \) and time step \( k \) only one of the \( \xi_j \)'s is equal to 1.

As an example consider again a LGCA with \( \hat{b} = 3 \). Then, \( \mathcal{A}_3 \) is given by
\[
\mathcal{A}_3 = \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}
\]

and therefore
\[
\eta_1^p = \xi_1 \eta_1 + \xi_2 \eta_1 + \xi_3 \eta_2 + \xi_4 \eta_2 + \xi_5 \eta_3 + \xi_6 \eta_3, \quad (3.15)
\]
\[ \eta_2 = \xi_2 \eta_2 + \xi_3 \eta_3 + \xi_4 \eta_4 + \xi_5 \eta_5 + \xi_6 \eta_6, \]
\[ \eta_3 = \xi_1 \eta_1 + \xi_2 \eta_2 + \xi_3 \eta_3 + \xi_4 \eta_4 + \xi_5 \eta_5 + \xi_6 \eta_6, \]

where we have neglected the \((r, k)\) dependence for simplicity.

Hence, the complete dynamics is governed by the composition of the shuffling step (Eqn. (3.14)) with the propagation step (Eqn. (2.3) on page 27) and can be described by the microdynamical difference–equation

\[
\eta_i(r + mc_i, k + 1) - \eta_i(r, k) = \eta_i^w(r, k) - \eta_i(r, k)
\]
\[
= \sum_{j=1}^{\hat{k}} \xi_j(r, k) \sum_{l=1}^{\hat{b}} \eta_l(r, k) a_{li}^j - \eta_i(r, k)
\]
\[
= C_i(\eta(r, k)).
\]

The repeated application of propagation and the shuffling operators leads to a random walk for each particle as shown in Fig. 3.9, where each particle moves a distance \(m\) in a random direction within each time step.

![Diagram](image)

**Figure 3.9:** Space–time–dynamics of the one-dimensional LGCA random walk model with one rest particle on a periodic lattice for different speeds \(m \in \{1, 2\}\); **parameters:** \(L = 100, k = 0, \ldots, 200\) and initial particle distribution \(P(\eta_i(r, 0) = 1) = 1/3\) for \(r = 45, \ldots, 55\) and \(P(\eta_i(r, 0) = 1) = 0\) else.

This random walk performed by different particles is **not completely independent** because the exclusion principle does not allow independent changes of
velocities of different particles at the same node. Nevertheless, since the interaction between random walkers is strictly local, the macroscopic behaviour of the particle density can be expected to be **diffusive**. For example, Lawniczak (1997) showed that the presented automaton rules lead to correct diffusive behaviour in a continuous limit which can be reached using appropriate time- and space-scaling assumptions\(^9\).

In order to analyse the diffusive dynamics, we study the corresponding lattice–Boltzmann equation which is obtained by taking the expectation of the microdynamical Eqn. (3.16) as described in Section 2.3.2 on page 40. Note that the right-hand side of Eqn. (3.16) is **linear**. Therefore, the lattice–Boltzmann equation can be solved explicitly.

To be more specific, we shall now consider the one-dimensional \((b = 2)\) case with one rest channel \((\beta = 1)\), i.e. \(\hat{b} = 3\).

Several other LGCA models for the simultaneous random walk of many particles are conceivable. For example, in the case of isotropic random walk, the shuffling operator \(M\) can be restricted to cyclic permutations of the velocity vectors (Boon et al. 1996, Lawniczak 1997, Chopard and Droz 1998). Qian et al. (1992) study a one-dimensional LGCA model for unsteady flows, in which each node is associated with four velocity channels \(c_1 = 1, c_2 = 2, c_3 = -1\) and \(c_4 = -2\). The shuffling step defines deterministic particle collisions which satisfy the conservation of mass and momentum.

### 3.4.1 Stability analysis for the one-dimensional random walk with one rest channel

By definition, the random variables \(\xi_j\)'s are mutually independent. Therefore, according to Eqn. (2.19) on page 36, the lattice–Boltzmann equation can be derived from (3.16) as

\[
f_i(r + mc_i, k + 1) - f_i(r, k) = \mathcal{C}_i(f(r, k)) = \sum_{j=1}^{\hat{b}} \sum_{l=1}^{\hat{b}} p_j f_i(r, k) a_{ij}^l - f_i(r, k),
\]

where we used Eqns. (3.12) and (3.13). This is equivalent to

\[
f_i(r + m, k + 1) - f_i(r, k) = (p_1 + p_2 - 1)f_1(r, k) + (p_3 + p_4)f_2(r, k) + (p_5 + p_6)f_3(r, k),
\]

\[
f_i(r - m, k + 1) - f_i(r, k) = (p_3 + p_6)f_1(r, k) + (p_1 + p_5 - 1)f_2(r, k) + (p_2 + p_4)f_3(r, k),
\]

\(^9\)see also Subsec. 5.1.5 (p. 110), where we derive a macroscopic description of a LGCA model.
\[ f_3(r, k + 1) - f_3(r, k) = (p_4 + p_5) f_1(r, k) + (p_2 + p_6) f_2(r, k) + (p_1 + p_3 - 1) f_3(r, k) . \]

Note that in the special case in which all configurations have equal probabilities, i.e. \( p_i = p_j, i, j = 1, \ldots, \hat{b} \) and therefore \( p_i = 1/\hat{b} \) due to constraint (3.13), the following expression can be obtained from Eqn. (3.17)

\[
\begin{align*}
  f_i(r + m c_i, k + 1) - f_i(r, k) &= \frac{(\hat{b} - 1)!}{\hat{b}!} \sum_{l=1}^{\hat{b}} f_i(r, k) - f_i(r, k) \\
  &= \frac{1}{\hat{b}} \sum_{l=1}^{\hat{b}} f_i(r, k) - f_i(r, k) .
\end{align*}
\]

(3.18)

Since the right-hand side of Eqn. (3.17) is linear and the interaction neighbourhood of a node \( r \) was defined to be the node itself, i.e. \( N^f_2(r) = \{r\} \) and therefore \( \nu = 1 \), the Boltzmann propagator (2.31) (cf. p. 42) simply becomes

\[
\Gamma(q) = T \{ I + \Omega^0 \} \\
= \left( \begin{array}{ccc}
  e^{-\frac{2\pi i}{L} q \cdot m} & 0 & 0 \\
  0 & e^{\frac{2\pi i}{L} q \cdot m} & 0 \\
  0 & 0 & 1
\end{array} \right) \left( \begin{array}{cccc}
  p_1 + p_2 & p_3 + p_4 & p_5 + p_6 \\
  p_3 + p_6 & p_1 + p_5 & p_2 + p_4 \\
  p_4 + p_5 & p_2 + p_6 & p_1 + p_3
\end{array} \right),
\]

with \( |\mathcal{L}| = L \). In the following, we will consider only isotropic diffusion processes, i.e. \( p_i = \frac{1}{6}, i = 1, \ldots, 6 \). Under this assumption, \( \Gamma(q) \) has a very simple structure such that we can determine the spectrum \( \Lambda_{\Gamma(q)} = \{\lambda_1(q), \lambda_2(q)\} \) as

\[
\lambda_1(q) = \frac{1}{3} \left( \frac{2\pi}{L} q m \right) \cos\left( \frac{2\pi}{L} q m \right) \approx 1 - \frac{1}{3} \left( \frac{2\pi}{L} q m \right)^2 + \frac{1}{36} \left( \frac{2\pi}{L} q m \right)^4 + O(q^6),
\]

\[
\lambda_2(q) = \lambda_3(q) = 0,
\]

and corresponding eigenvectors as

\[
v_1^T(q) = \left( e^{-\frac{2\pi i}{L} q \cdot m}, e^{\frac{2\pi i}{L} q \cdot m}, 1 \right), \quad v_2^T(q) = (1, -1, 0) \quad \text{and} \quad v_3^T(q) = (1, 0, -1).
\]

\( \Gamma(q) \) is diagonalisable because the dimension of the eigenspace of the multiple eigenvalue \( \lambda_2(q) = \lambda_3(q) = 0 \) is \( 3 - \text{rank}(\Gamma(q)) = 2 \), and therefore, according to Eqn. (2.36) (cf. p. 43), the general solution of the lattice–Boltzmann equation (3.17) is given by

\[
\delta f_i(r, k) = \frac{1}{L} \sum_{q=0}^{L-1} e^{-\frac{2\pi i}{L} q \cdot r} F_i(q, k),
\]

(3.20)

with

\[
F_i(q, k) = d_1(q) v_{i1}(q) \lambda_1(q)^k
\]

(3.21)
and

\[ F_i(q, 0) = d_1(q) v_{1i}(q) + d_2(q) v_{2i}(q) + d_3(q) v_{3i}(q) \]  \hspace{1cm} (3.22)
\[ = \sum_{r=0}^{L-1} e^{i \frac{2\pi}{L} q r} \delta f_i(r, 0) . \]

Hence, solutions corresponding to the eigenvalues \( \lambda_2(q) = \lambda_3(q) = 0 \) decrease to zero in one time step independently of the value of \( q \). Because \( \mu(q) = |\lambda_1(q)| \leq 1 \ \forall q \), no modes can grow with time, i.e. pattern formation is not possible since all instabilities (with \( q \neq 0 \)) are damped out. A spectral radius with \( \mu(q) = 1 \) indicates the existence of invariants in the system. Here, the spectral radius \( \mu(q) = |\lambda_1(q)| \) converges to one if \( q \) converges to zero, i.e. when the wave length becomes very large. In this case, there exists a dominant projection of the eigenvector \( v_1(q) \) on the ‘mass vector’ \( v_1^T(0) = (1, 1, 1) \) since

\[
\begin{pmatrix}
1 & 1 & 1 \\
1 & -1 & 0 \\
1 & 0 & -1 \\
\end{pmatrix}^{-1} v_1(q) \approx (1 + O(q^2), -i O(q), O(q^2)) .
\]

According to Eqn. (3.21), we find that for \( q = 0 \)

\[
F_1(0, k) = F_2(0, k) = F_3(0, k) = d_1(0) \quad \forall k \in \mathbb{N},
\]

since \( \lambda_1(0) = 1 \) and \( v_1^T(0) = (1, 1, 1) \). \( d_1(0) \) is determined by Eqn. (3.22), i.e.

\[
d_1(0) + d_2(0) + d_3(0) = \sum_{r=0}^{L-1} \delta f_1(r, 0)
\]

\[
\wedge 
\]

\[
d_1(0) - d_2(0) = \sum_{r=0}^{L-1} \delta f_2(r, 0)
\]

\[
\wedge 
\]

\[
d_1(0) - d_3(0) = \sum_{r=0}^{L-1} \delta f_3(r, 0)
\]

\[
\Rightarrow 
\]

\[
3 d_1(0) = \sum_{r=0}^{L-1} \sum_{i=0}^{3} \delta f_i(r, 0) ,
\]

and hence

\[
\sum_{i=1}^{3} F_i(0, k) = 3 d_1(0) = \sum_{r=0}^{L-1} \sum_{i=0}^{3} \delta f_i(r, 0) . \hspace{1cm} (3.23)
\]

Therefore, persisting modes, which are associated with long wave lengths, describe diffusion of the particles initially present in the system.
3.4 Movement in lattice–gas cellular automaton models

In particular, a closed equation for the average local mass of particles at node $r$ at time $k$, denoted by $q(r,k) := \delta f_1(r,k) + \delta f_2(r,k) + \delta f_3(r,k) \in [0,3]$, can be derived as (cf. Eqn. (3.20))

$$q(r,k) = \frac{1}{L} \sum_{q=0}^{L-1} \left( \sum_{i=1}^{3} F_i(q,0) \right) e^{-i \frac{2\pi}{L} q \cdot r} \left( \frac{1}{3} + \frac{2}{3} \cos\left( \frac{2\pi}{L} q m \right) \right)^k , \quad (3.24)$$

with the Fourier transformed initial conditions $\sum_{i=1}^{3} F_i(q,0)$. Note that the solution of the one–dimensional simultaneous random walk LGCA model with one rest particle given by Eqn. (3.24) is equivalent to the solution (3.3) (cf. p. 50) which we derived for the random walk model in Sec. 3.2 with $\alpha = \frac{2}{3}$ and $m = 1$.

In the next subsection we explain the importance of rest particles in LGCA models by means of the one–dimensional simultaneous random walk.

3.4.2 Checkerboard artefact

The linear stability analysis for the one–dimensional isotropic random walk model with an arbitrary number ($\beta > 0$) of zero–velocity channels is straightforward. A special situation is the LGCA–random walk model without rest particles, i.e. $\beta = 0$. The corresponding Boltzmann propagator (cf. Eqn. (3.19), p. 61) is given by

$$\Gamma(q) = \frac{1}{2} \begin{pmatrix} e^{-i \frac{2\pi}{L} q \cdot m} & e^{-i \frac{2\pi}{L} q \cdot m} \\ e^{i \frac{2\pi}{L} q \cdot m} & e^{i \frac{2\pi}{L} q \cdot m} \end{pmatrix},$$

with eigenvalues

$$\lambda_1(q) = \cos\left( \frac{2\pi}{L} q m \right), \quad \lambda_2(q) = 0 , \quad (3.25)$$

and linear independent eigenvectors

$$v_1^T(q) = (e^{-i \frac{\pi}{L} q m}, 1), \quad v_2^T(q) = (-1, 1) . \quad (3.26)$$

Due to possible simplifications in the mathematical derivations, we examine the special case $m = 1$ in the following.

Here, another invariant is present in the system, because

$$\mu(\tilde{q}) = |\lambda_1(\tilde{q})| = |-1| = 1 \quad \text{for} \quad \tilde{q} = \frac{L}{2} .$$

Note that $\tilde{q}$ is an integer only for even lattice sizes $L$. The corresponding eigenvector is $v_1^T(\tilde{q}) = (1, 1)$, and hence modes

$$F_i(\tilde{q},k) = (-1)^k d_1(\tilde{q})$$
perform undamped oscillations over time with period 2. Using the initial condition we get

\[
d_1(\tilde{q}) - d_2(\tilde{q}) = \sum_{\mathcal{L}} e^{i\pi r} \delta f_1(r, 0)
\]

\[
\land \quad d_1(\tilde{q}) + d_2(\tilde{q}) = \sum_{\mathcal{L}} e^{i\pi r} \delta f_2(r, 0)
\]

\[
\Rightarrow \quad 2d_1(\tilde{q}) = \sum_{\mathcal{L}} e^{i\pi r}(\delta f_1(r, 0) + \delta f_2(r, 0)).
\]

Hence,

\[
\sum_{i=1}^{2} F_i(\tilde{q}, k) = (-1)^k 2d_1(\tilde{q})
\]

\[
= (-1)^k \sum_{\mathcal{L}} e^{i\pi r} \varrho(r, 0)
\]

\[
= (-1)^k \left( \sum_{r \text{ even}} e^{i\pi r} \varrho(r, 0) + \sum_{r \text{ odd}} e^{i\pi r} \varrho(r, 0) \right)
\]

\[
= (-1)^k \left( \sum_{r \text{ even}} \varrho(r, 0) - \sum_{r \text{ odd}} \varrho(r, 0) \right),
\]

where \( \tilde{q} = L/2 \). This invariant, which obviously does not have any interpretable meaning in the real system, i.e. it is artificial (spurious)\(^{10}\), is known as the **checkerboard invariant** in the context of LGCA models (d’Humières et al. 1989) and as **mesh–drift instability** in the context of numerical treatment of partial differential equations (Press et al. 1988). Note, that it is straightforward to find checkerboard invariants in higher dimensional systems with square symmetries (d’Humières et al. 1989, Boon et al. 1996, Deutsch 1999). This invariant with wave length 2 = \( L/\tilde{q} \) is related to the fact that odd and even lattice nodes are completely decoupled, i.e. there is no interaction at any time between particles that are not located on the same even or odd sublattice. This can be seen more clearly in Table 3.2 which we derive next. According to Eqn. (2.36) (cf. p. 43) we get

\[
\varrho(r, k) = \frac{1}{L} \sum_{i=1}^{2} \sum_{q=0}^{L-1} e^{-i\pi r \tilde{q} q} F_i(q, k)
\]

\[
= \frac{1}{L} \sum_{i=1}^{2} \left( F_i(0, k) + e^{-i\pi r \tilde{q} k} F_i(\tilde{q}, k) + \sum_{q=1}^{L-1} e^{-i\pi r \tilde{q} q} F_i(q, k) \right)
\]

\(^{10}\)in contrast to the diffusion of mass
\[
\frac{1}{L} \left( \sum_{\tilde{r} \in \mathcal{L}} g(\tilde{r}, 0) + (-1)^{k} e^{-i \pi r} \left( \sum_{\tilde{r} \in \mathcal{L} \text{ even}} g(\tilde{r}, 0) - \sum_{\tilde{r} \in \mathcal{L} \text{ odd}} g(\tilde{r}, 0) \right) + \sum_{q=1}^{L-1} e^{-i \frac{2\pi}{L} qr} \sum_{i=1}^{2} F_i(q, k) \right),
\]

where \( q = L/2 \) and \( F_1(0, k) + F_2(0, k) = \sum_{r \in \mathcal{L}} g(r, 0) \), which follows with similar arguments as used in (3.23) (cf. p. 62). Furthermore, since the spectral radius \( \mu(q) < 1 \) for every \( q \not\in \{0, L/2\} \), all corresponding modes \( F_i(q, k) \) will decay with time and accordingly their sum. Therefore, using the fact that

\[
\sum_{\tilde{r} \in \mathcal{L}} g(\tilde{r}, 0) = \sum_{\tilde{r} \in \mathcal{L} \text{ even}} g(\tilde{r}, 0) + \sum_{\tilde{r} \in \mathcal{L} \text{ odd}} g(\tilde{r}, 0),
\]

we get

\[
g(r, k) \approx \frac{1}{L} \left( 1 + (-1)^{k} e^{-i \pi r} \sum_{\tilde{r} \in \mathcal{L} \text{ even}} g(\tilde{r}, 0) + (1 - (-1)^{k} e^{-i \pi r}) \sum_{\tilde{r} \in \mathcal{L} \text{ odd}} g(\tilde{r}, 0) \right),
\]

and hence, as summarised in Table 3.2, at even lattice nodes and even time steps the expected mass depends solely on the mass of nodes in the even sublattice while at odd time steps it depends solely on the nodes on the odd sublattice.

<table>
<thead>
<tr>
<th></th>
<th>( k \text{ even} )</th>
<th>( k \text{ odd} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r \text{ even} )</td>
<td>( g(r, k) \approx \frac{2}{L} \sum_{\tilde{r} \in \mathcal{L} \text{ even}} g(\tilde{r}, 0) )</td>
<td>( g(r, k) \approx \frac{2}{L} \sum_{\tilde{r} \in \mathcal{L} \text{ odd}} g(\tilde{r}, 0) )</td>
</tr>
<tr>
<td>( r \text{ odd} )</td>
<td>( g(r, k) \approx \frac{2}{L} \sum_{\tilde{r} \in \mathcal{L} \text{ even}} g(\tilde{r}, 0) )</td>
<td>( g(r, k) \approx \frac{2}{L} \sum_{\tilde{r} \in \mathcal{L} \text{ odd}} g(\tilde{r}, 0) )</td>
</tr>
</tbody>
</table>

Table 3.2: Time- and (even/odd) sublattice-dependence of the expected local mass \( g(r, k) \); this table is based on Eqn. (3.28).

If the lattice size \( L \) is odd the checkerboard invariant is absent, because in this case no integer solution of the equation \( \lambda_{1}(q) = -1 \) (cf. (3.25)) exists. But modes corresponding to wave numbers close to \( L/2 \) decay very slowly, due to their sign-oscillating nature. Therefore, also in this case, a local decoupling of odd and even lattice nodes can persist for a while (Boon et al. 1996).
One possibility to avoid a checkerboard invariant is the introduction of rest particles\textsuperscript{11}. Their effect is a coupling of the two (even and odd) sublattices with each other. It is easy to show that for any number $\beta > 0$ of rest particles the $(2 + \beta) \times (2 + \beta)$–Boltzmann propagator is given by

$$
\Gamma(q) = \frac{1}{2 + \beta} \begin{pmatrix}
    e^{-i \frac{2\pi}{L} q \cdot m} & \cdots & e^{-i \frac{2\pi}{L} q \cdot m} \\
    e^{i \frac{2\pi}{L} q \cdot m} & \cdots & e^{i \frac{2\pi}{L} q \cdot m} \\
    1 & \cdots & 1 \\
    \vdots & \ddots & \vdots \\
    1 & \cdots & 1
\end{pmatrix}.
\tag{3.29}
$$

The eigenvalues of (3.29) are

$$
\lambda_1(q) = \frac{1}{2 + \beta} \left( \beta + 2 \cos \left( \frac{2\pi}{L} q m \right) \right),
\tag{3.30}
$$
$$
\lambda_2(q) = \ldots = \lambda_{2+\beta}(q) = 0,
$$

and eigenvectors are

$$
v_1^T(q) = (e^{-i \frac{2\pi}{L} q \cdot m}, e^{i \frac{2\pi}{L} q \cdot m}, 1, \ldots, 1),
$$
$$
v_j^T(q) = (-1, 0, \ldots, 0, \underbrace{1}_{j\text{th position}}, 0, \ldots, 0) \quad \text{for} \quad j = 2, \ldots, 2 + \beta.
\tag{3.31}
$$

Hence, $\Gamma(q)$ is always diagonalisable. As illustrated in Fig. 3.10, the magnitude of the minimum of the dominant eigenvalue $\lambda_1(q)$ depends on the number $\beta$ of rest particles. Note that all sign–oscillating modes can be eliminated by introducing at least two zero velocity channels.

Later on in Sec. 5.1 we present a further one–dimensional LGCA model with one zero velocity channel in which unstable modes which change sign at each time step are present and also become visible.

If we compare the solution for the expected local mass of particles for $m = 1$, given by

$$
q(r, k) = \frac{1}{L} \sum_{q=0}^{L-1} \left( \sum_{i=1}^{2+\beta} F_i(q, 0) \right) e^{-i \frac{2\pi}{L} q \cdot r} \left( \frac{1}{2 + \beta} \left( \beta + 2 \cos \left( \frac{2\pi}{L} q \right) \right) \right)^k,
\tag{3.32}
$$

with the solution (3.3) (cf. p. 50) for the stochastic random walk model derived in Section 3.2, we get the following relationship between the number of rest particles...
3.5 Summary

Figure 3.10: Dominant eigenvalues for one-dimensional LGCA random walk models given by Eqn. (3.30); small dashed line: no rest particle ($\beta = 0$), solid line: one rest particle ($\beta = 1$) and large dashed line: two rest particles ($\beta = 2$); parameters: $L = 100, m = 1$.

particles $\beta$ and the jump probability $\alpha$ (cf. p. 56):

<table>
<thead>
<tr>
<th># rest particles</th>
<th>jump probability ($\alpha$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>2/3</td>
</tr>
<tr>
<td>2</td>
<td>1/2</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$\vdots$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$\frac{2}{2 + \beta}$</td>
</tr>
</tbody>
</table>

In the interpretation of the stochastic random walk model introduced in Sec. 3.2, a jump probability of $\alpha = 1$ implies that a particle jumps with probability 1/2 either to the left or to the right, which implies that particles starting at even lattice nodes can only be on even lattice nodes after an even number of time steps (checkerboard artefact, Weimar 1995).

3.5 Summary

In this chapter we presented a short overview of mainly one-dimensional random walk models, discrete in time and space. In particular, we introduced three approaches to model a random walk in the framework of cellular automata. Rules usually defined for random movement in probabilistic cellular automaton models are either time- and space-dependent (cf. Subsec. 3.3.1) or asynchronous (cf. Subsec. 3.3.2), while rules defined for LGCA models (cf. Sec. 3.4) are time- and space-independent and applied synchronously. We
showed that the same equations for the evolution of the average total mass of particles describe the stochastic random walk model (cf. Eqn. (3.3), p. 50) and the LGCA model (cf. Eqn. (3.32), p. 66) if the jump probability and the number of rest particles are adjusted appropriately. The diffusive dynamics of the LGCA is well captured by the corresponding linear lattice–Boltzmann equations, which can be solved explicitly. Moreover, the existence of an artificial (geometrical) invariant, known as the checkerboard invariant, can be identified with the help of the lattice–Boltzmann model. This artefact, not necessarily obvious in simulations can also be observed in stochastic random walk models without exclusion principle. Checkerboard artefacts do not occur in analogous continuous–space systems.
4 One–component interaction and movement: Growth processes

The term ‘growth’ is used to indicate both increase in size, i.e. volume of an individual organism, area of a city or height of a tree, and increase in numbers i.e. number of individuals in a population, number of people in a city or dry biomass of trees. Other phenomena related to the increase of some quantity are the spread of rumors, innovations or epidemics or the transmission of heat or information. In the following we will use the term growth in a rather abstract way. Whenever the number of particles1 increases we refer to this phenomenon to the growth of particles.

4.1 Classical growth models

A very detailed study of various growth models together with applications can be found in Doucet and Sloep (1992) and Banks (1994). Following these authors, we shortly present some basic aspects of different growth processes. In the history of modelling growth phenomena the English clergyman Thomas R. Malthus (1798), Benjamin Gompertz (1825) and the Belgian mathematician Pierre F. Verhulst (1838) are three especially noteworthy researchers whose basic frameworks are still adequate for handling many kinds of practical problems. They all studied growth processes of (human) populations. In present-day vocabulary, the main proposals are as follows: Let $N(t)$ be the number of individuals in a population at continuous time $t$. Then Malthus assumed that the relative growth rate, or growth rate per capita, is constant2, i.e.

$$\frac{N'(t)}{N(t)} = \gamma ,$$

(4.1)

where $N'(t) = dN(t)/dt$. In other words, this Eqn. expresses that the rate at which the quantity $N$ changes in time is directly proportional to the amount

---

1In the sense defined previously (cf. p. 47)
2A synonym for the relative growth rate is specific growth rate. But this term might be misleading, since the term ‘specific’ carries the connotation of being constant - which is not always true as the upcoming examples show.
of \( N \) present. The solution of Eqn. (4.1) is
\[
N(t) = N(0) e^{\gamma t}.
\]
Accordingly, this simplest law of growth is also known as exponential growth because the quantity of interest performs an unlimited growth. For example, under suitable conditions, the growth of bacterial cells follows Malthusian growth, at least for short times, since it is characterised by independent cell divisions. But exponential growth cannot go on forever. A more realistic approach takes limitations of the growth process into account, for example, a shortage of food and other resources or 'crowding effects'. A suggestion to account for such effects, was originally proposed by Verhulst. He stated that the relative growth rate is density-dependent in such a way that it decreases linearly with the size of the population, i.e.
\[
\frac{N'(t)}{N(t)} = \gamma - \frac{\gamma}{K} N(t) = \gamma \left( 1 - \frac{N(t)}{K} \right),
\]
where \( K \) (carrying capacity) is the population size which will be reached after a long time. The solution of Eqn. (4.2) is
\[
N(t) = K \left( 1 + \left( \frac{K}{N(0)} - 1 \right) e^{-\gamma t} \right)^{-1}.
\]
Verhulst's growth model is also known as the logistic growth model. The solution curve is \( S \)-shaped which is for 'short' times and low values of \( N(0) \) almost exponential. A third growth law that frequently appears in models of single component growth is the Gompertz law. Gompertz proposed that the relative growth rate decreases exponentially with time, i.e.
\[
\frac{N'(t)}{N(t)} = \gamma e^{-\alpha t}.
\]
Using the solution given by
\[
N(t) = N(0) e^{\beta \left(1-e^{-\gamma t}\right)} \quad \text{as} \quad t \to \infty \quad K = N(0) e^{\beta},
\]
a formally equivalent version of the relative growth rate can be derived as
\[
\frac{N'(t)}{N(t)} = \gamma \left( \ln(K) - \ln(N) \right).
\]
This growth model is widely used to describe the growth of solid tumors in mice, rats, and rabbits (i.e. Casey 1934).

In Fig. 4.1 a comparison of exponential, logistic, and Gompertz growth curves is shown. Note that for all these models it is assumed that the relative growth rate is maximal if no other individuals are around.

In the models presented so far space is not explicitly considered. But, space plays an important role in the growth of aggregates, which is the collection of particles in space. Here, basically two classes can be distinguished (Williams et al. 1998):
4.1 Classical growth models

\[ N(t) \]

\[ N'(t)/N(t) \]

(a) Temporal dynamics

(b) Relative growth rates

Figure 4.1: Comparison of exponential (Eqn. (4.1)), logistic (Eqn. (4.2)) and Gompertz (Eqn. (4.4)) growth curves; parameters: \( N(0) = 100, K = 10000, \gamma = 0.1 \) and \( \alpha = 0.0217 \).

1. growing aggregates due to a particle reproduction which is limited to points adjacent to the aggregate (e.g. Eden 1961, Richardson 1973) and

2. growing aggregates by sticking together of diffusing particles if they meet. A prototype model for this process is the so-called ‘diffusion-limited aggregation’, introduced by Witten and Sander (1983).

Originally, these growth models are considered as discrete time stochastic Markov processes (i.e. asynchronous updating). But recently, also cellular automaton models have been constructed to study these phenomena (e.g. Packard and Wolfram 1985, Eloranta 1997, Chopard and Droz 1998, Williams et al. 1998).

In the following, we consider particle-growth processes related to the first category modelled in the framework of cellular automata.

Since time \( k \) is discrete, the relative growth rate for a difference equation is given by

\[ \frac{\Delta N(k)}{N(k)} := \frac{N(k + 1) - N(k)}{N(k)}. \] (4.5)

We restrict our analysis to cellular automata defined on a two-dimensional square lattice, i.e. \( \mathcal{N}_4 \) (cf. p. 17), with periodic boundary conditions.
4.2 Growth processes in cellular automata

A particle population is represented by particles occupying cells of the lattice. Each cell is either vacant \((s(r, k) = 0)\) or occupied \((s(r, k) = 1)\) by one particle, i.e. \(E = \{0, 1\}\). An empty cell becomes occupied with a certain time-independent transition probability \(W(s_{N(r)} \to 1)\) which depends on the local configuration \(s_{N(r)}\) of the interaction neighbourhood \(N_{4}^{i}\). In simple growth processes particles do not disappear, i.e. occupied cells remain occupied for all times. In conclusion, the general formal definition of a local rule for a growth process in a cellular automaton is given by

\[
    s(r, k + 1) = R(s_{N(r)}(k)) = \begin{cases} 
    1 & \text{if } s(r, k) = 1 \\
    \zeta(s_{N(r)}(k)) & \text{if } s(r, k) = 0 
    \end{cases} \quad (4.6)
\]

where \(\zeta(s_{N(r)}(k)) \in \{0, 1\}\) is a space- and time-independent random variable with probability distribution

\[
    P(\zeta(s_{N(r)}(k)) = 1) = W(s_{N(r)}(k) \to 1) \\
    P(\zeta(s_{N(r)}(k)) = 0) = 1 - W(s_{N(r)}(k) \to 1) \quad (4.7)
\]

We will consider only growth processes which are not directionally biased. Hence, the transition probability \(W\) should depend solely on the total number of particles in the outer interaction neighbourhood, which will be denoted by

\[
    n_{N(r)}(k) := \sum_{\tilde{r} \in N_{4}^{i}(r), \tilde{r} \neq r} s(\tilde{r}, k) \in [0, \nu - 1], \quad \nu = |N_{4}^{i}| > 1.
\]

Next we give some examples for the transition probability \(W\). Boccara et al. (1994b) consider a generalised ‘game of life’ model (see also Sec. 1.2, p. 7), in which the interaction neighbourhood is \(R\)-axial (cf. p. 23). The growth–part of their automaton rule is defined as follows: A vacant cell becomes occupied with probability \(\gamma = 1\), if at least \(B_{\min}\) and maximal \(B_{\max}\) particles are in the interaction neighbourhood, i.e. \([B_{\min}, B_{\max}]\) represents an interval of ‘fertility’. Hence,

\[
    W(s_{N(r)}(k) \to 1) = \begin{cases} 
    \gamma & \text{if } n_{N(r)}(k) \in [B_{\min}, B_{\max}] \\
    0 & \text{else} \quad (4.8)
    \end{cases}
\]
4.2 Growth processes in cellular automata

Note that the growth-part of the classical ‘game of life’ model\(^3\) suggested by John Conway corresponds to \(R = 1\) and \(B_{\text{min}} = B_{\text{max}} = 3, \gamma = 1\). A comprehensive treatment of ‘game of life’–like models can be found, for example, in Chaté and Manneville (1992) or de la Torre and Martín (1997). Figure 4.3(a) shows an example for the spatial distribution of particles resulting from a growth process after \(k = 200\) steps with initially two seeds in the center. Since the growth process described by this rule is very restrictive and strongly dependent on the initial conditions we do not go into further details.

For many infection or excitation processes\(^4\) a lower bound \(B\) is defined, such that a susceptible/resting cell (‘empty’ cell) becomes infected/excited (cell occupied by a particle) with probability \(\gamma\), if at least \(B\) cells in state 1 are in the interaction neighbourhood, i.e.

\[
W(s_{\mathcal{N}_c}(k) \rightarrow 1) = \begin{cases} 
\gamma & \text{if } n_{\mathcal{N}_c}(k) \geq B \\
0 & \text{else}.
\end{cases}
\]  

(4.9)

For example, Greenberg et al. (1978) studied an excitation process. They use a von Neumann interaction neighbourhood (cf. p. 22), i.e. \(\nu = |\mathcal{N}_c| = 5\), and take the threshold to be \(B = 1\) with \(\gamma = 1\). Further examples are forest fire models, e.g., Chen et al. (1990). A ‘green tree’ (‘empty’ cell) becomes a burning tree (cell occupied by a particle) if at least one of its nearest neighbours is burning, i.e. \(B = 1\) and \(\gamma = 1\).

An automaton for the spread of innovations is introduced and studied by Boccara and Fukš (1998). They study a one–dimensional automaton with \(R\)-axial interaction neighbourhood. Here, we state the rule for the two–dimensional lattice, i.e. \(\nu = |\mathcal{N}_c| = (2R + 1)^2\). A neutral individual (‘empty’ cell) becomes an adopter (cell occupied by a particle) with a probability depending on the local density of adopters, i.e.

\[
W(s_{\mathcal{N}_c}(k) \rightarrow 1) = \frac{\gamma}{\nu - 1} n_{\mathcal{N}_c}(k).
\]  

(4.10)

Another approach assumes that each particle produces an ‘offspring’ with probability \(\gamma\). Then, the probability for an empty cell to become occupied is given by

\[
W(s_{\mathcal{N}_c}(k) \rightarrow 1) = 1 - (1 - \gamma)^{n_{\mathcal{N}_c}(k)}.
\]  

(4.11)

\(^3\)The complete rule for the ‘game of life’ model includes a death–part, where a particle ‘dies’ if \(n_{\mathcal{N}_c}(k) \neq 3\).

\(^4\)Reviews of epidemic models and excitable media in the framework of cellular automata are given in Schönfisch (1993) and Kapral et al. (1991).
In the context of epidemics, $\gamma$ is interpreted as the probability to become infected by contact with one individual (Bocca and Cheong 1993, Duryea et al. 1999). This rule is also used for predator–prey systems (Bocca et al., 1994a, Hiebeler 1997, Rozenfeld and Albano 1999).

Figure 4.2 illustrates the transition probabilities $W$ and Fig. 4.3 shows snapshots of the particle distribution in space for each growth model.

![Diagram](image)

Figure 4.2: Transition probability $W(n_{N(c)} \rightarrow 1)$ for $\gamma = 0.1$ and a von Neumann interaction neighbourhood; the solid line refers to Eqn. (4.8) with $B_{\min} = 2, B_{\max} = 3$, the large dashed line to Eqn. (4.9) with $B = 1$, the intermediate dashed line to Eqn. (4.10) and the small dashed line to Eqn. (4.11), respectively.

In order to study the temporal evolution of the number of particles $N(k)$ in the described growth processes, we focus on the model defined by Eqn. (4.9) for $B = 1$. First, let us consider the growth process resulting from a single seed in the center of the lattice, i.e. $N(0) = 1$. A snapshot of the particle distribution in space after $k = 200$ steps with the von Neumann interaction neighbourhood and $\gamma = 0.1$ is shown in Fig. 4.3(b). A crude approximation of this growth process is given by the following difference equation

$$N(k+1) = N(k) + (\nu - 1) \gamma k$$

$$\Rightarrow N(k) = 1 + \frac{\nu - 1}{2} \gamma k(k - 1) ,$$

(4.12)

where $\nu = 5$ for the von Neumann neighbourhood and $\nu = 9$ for the Moore neighbourhood. Equation (4.12) is exact for $\gamma = 1$ and an infinite lattice. If we place $N_0 > 1$ seeds on the lattice and assume independent growth from each seed, then

$$N(k) = N_0 + N_0 \frac{\nu - 1}{2} \gamma k(k - 1) ,$$

or in terms of spatial averages $\rho := \frac{1}{L} N \in [0, 1] ,$

$$\rho(k) = \rho(0) + \rho(0) \frac{\nu - 1}{2} \gamma k(k - 1)$$

(4.13)
4.2 Growth processes in cellular automata

(a) Growth according to Rule (4.8): Moore neighbourhood, two seeds in the center at \( k = 0 \) and \( B_{\text{min}} = 2, B_{\text{max}} = 3 \)

(b) Growth according to Rule (4.9): von Neumann neighbourhood, one seed in the center at \( k = 0 \) and \( B = 1 \)

(c) Growth according to Rule (4.10): von Neumann neighbourhood, one seed in the center at \( k = 0 \)

(d) Growth according to Rule (4.11): von Neumann neighbourhood, one seed in the center at \( k = 0 \)

Figure 4.3: Two-dimensional growth processes in cellular automaton models shown after \( k = 200 \) steps; parameters: \( L = 100 \times 100, \gamma = 0.1 \).

is an upper bound for the growth process. As shown in Fig. 4.4(a) the relative growth rate predicted by Eqn. (4.13) for \( \rho(0) = \frac{1}{L} \) (single seed) is in good correspondence with simulation data. Furthermore, the simulated growth process is qualitatively similar to the predicted (Eqn. (4.13)), because the double logarithmic plot 4.4(b) shows a linear relationship for intermediate times, which is typical for polynomial processes. For higher initial densities, i.e. \( \rho(0) > \frac{1}{L} \), the prediction given by Eqn. (4.13) is not useful. The predicted relative growth rate overestimates the growth process (cf. Fig. 4.4(a)), since we did not take into account crowding effects of the agglomerations growing from each seed. In addition, although the shape of the predicted relative growth rate is similar to the relative growth rate obtained from simulation data the simulated growth process is qualitatively different as can be seen in Fig. 4.4(b).
Mean–field approximation

We continue with an approximation of the given ‘growth’–rules by mean–field theory (cf. Subsec. 2.3.1, p. 31). In particular the mean–field equation for Rule (4.9) is derived, while we simply state the mean–field equations for the other rules. According to Eqn. (2.12) (p. 32) the evolution equation for the spatial averaged density of particles \(x_1(k)\) is given by

\[
x_1(k+1) = \sum_{\{z_1, \ldots, z_\nu\} \in \{0,1\}^\nu} W((z_1, \ldots, z_\nu) \to 1) \prod_{i=1}^{\nu} \sum_{l=0}^{1} \delta_{z_i,l} x_1(k),
\]

(4.14)

where \(x_0(k)\) denotes the spatial averaged density of empty cells and \(z^0 = 0\) and \(z^1 = 1\). For Rule (4.9) this equation becomes

\[
x_1(k+1) = x_1(k) + x_0(k) \sum_{i=B}^{\nu-1} \left(\frac{\nu - 1}{i}\right) \gamma (x_1(k))^i (x_0(k))^{\nu-1-i}.
\]

(4.15)

For \(B = 1\), with the substitution \(\rho(k) \equiv x_1(k), 1 - \rho(k) \equiv x_0(k)\) and with the identity

\[
\sum_{i=0}^{\nu-1} \left(\frac{\nu - 1}{i}\right) \rho^i(k) (1 - \rho(k))^{\nu-1-i} = (\rho(k) + 1 - \rho(k))^{\nu-1} = 1,
\]
4.2 Growth processes in cellular automata

Eqn. (4.15) simplifies to

Rule (4.9):

\[
\rho(k + 1) = \rho(k) + \gamma (1 - \rho(k)) \left(1 - (1 - \rho(k))^{q^{-1}}\right).
\]  
(4.16)

Mean-field equations for Rules (4.10) and (4.11) are obtained in a similar way, i.e.

Rule (4.10):

\[
\rho(k + 1) = \rho(k) + \gamma \rho(k) (1 - \rho(k))
\]  
(4.17)

and

Rule (4.11):

\[
\rho(k + 1) = \rho(k) + (1 - \rho(k)) \left(1 - (1 - \gamma \rho(k))^{q^{-1}}\right).
\]  
(4.18)

For a comparison of these growth laws see Fig. 4.5. The basic assumption underlying the derivation of mean-field equations is the neglect of any correlations. Since random independent particle movement destroys correlations, we expect that the mean-field equations are good approximations for processes which combine interaction with motion. Therefore, we impose an asynchronous
random walk step (cf. Subsec. 3.3.2, p. 56) after each growth step. As it is summarised in Fig. 4.6, the qualitative evolution of these automata is correctly predicted by mean-field theory. As the degree of mixing (\(\tau\)) increases, the prediction becomes also quantitatively correct (Boccara et al. 1994). Note that particle-motion leads also to an increase of the relative growth rate. Furthermore, these examples indicate that the evolution of cellular automaton models lacking any correlation destroying mechanism can neither qualitatively nor quantitatively captured by mean field approximation.

\[ \frac{\Delta \rho(k)}{\rho(k)} \]

\[ \rho(k) \]

(a) Rule (4.9) \(\text{i: Eqn. (4.16)}\)

\[ \frac{\Delta \rho(k)}{\rho(k)} \]

\[ \rho(k) \]

(b) Rule (4.10) \(\text{i: Eqn. (4.17)}\)

\[ \frac{\Delta \rho(k)}{\rho(k)} \]

\[ \rho(k) \]

(c) Rule (4.11) \(\text{i: Eqn. (4.18)}\)

Figure 4.6: Comparison of relative growth rates; legend: i: mean-field equation, ii: no movement, iii: asynchronous movement (\(\tau = 1\)), iv: asynchronous movement (\(\tau = 10\)); parameters: \(L = 100 \times 100\), von Neumann interaction neighbourhood, i.e. \(\nu = 5\), \(\rho(0) = 0.01\) and \(\gamma = 0.1\).
4.3 Growth processes in lattice–gas cellular automata

Lattice–gas cellular automata are especially designed to model processes of interaction (I) and movement (propagation operator P) (cf. p. 27). In the case of growth the interaction step is split into two parts: the ‘growth’ mechanism (operator G) and the shuffling operator (M) which was introduced to model a random walk of many particles (cf. Sec. 3.4, p. 57). Therefore, the dynamics is given by repeated application of operators $P \circ M \circ G$. We consider a two–dimensional lattice with coordination number $b = 4$ and introduce one additional rest particle $\beta = 1$, i.e. $\tilde{b} = 5$. Hence, the state at node $r$ at time $k$ is given by $\eta(r, k) \in \{0,1\}^5 = \mathcal{E}$. For simplicity, we restrict the interaction neighbourhood for the growth and shuffling part to the node itself, i.e. $\mathcal{N}_i^g(r) = \{r\}$. The propagation step ensures the local interaction with neighbouring nodes. Furthermore, we consider isotropic growth rules, which means that they are independent on the particle distribution in channels and solely depend on the total number of particles $n(r, k)$ at the node. Hence, the pre–interaction state $\eta_i(r, k)$ is replaced by the post–growth–interaction state $\eta_i^g(r, k)$ determined by

$$
\eta_i^g(r, k) = \mathcal{R}_i^g(\eta(r, k)) = \eta_i(r, k) + (1 - \eta_i(r, k)) \zeta_i(\eta(r, k)).
$$

(4.19)

$\zeta_i(\eta(r, k)) \in \{0,1\}, i = 1, \ldots, 5$, are space– and time–independent random variables with probability distribution

$$
P\left(\zeta_i(\eta(r, k)) = 1\right) = W_i(\eta(r, k) \rightarrow (z_1, \ldots, z_5)|_{z_i=1}),$$

$$P\left(\zeta_i(\eta(r, k)) = 0\right) = 1 - W_i(\eta(r, k) \rightarrow (z_1, \ldots, z_5)|_{z_i=1}),
$$

(4.20)

where $z_j \in \{0,1\}, j = 1, \ldots, 5$ and $y|_{y=a}$ denotes any vector $y$ for which the $i$–th component has the value $a$. Hence, using Eqn. (4.19), Eqn. (3.14) (p. 58) and Eqn. (2.4) (p. 28), the complete dynamics can be described by the microdynamical equation

$$
\eta_i(r + mc_i, k + 1) = \mathcal{R}_i^g(\eta^g(r, k)).
$$

(4.21)

A growth rule similar to Rule (4.9) (cf. p. 73), defined for probabilistic cellular automata, could be formulated as follows: An empty channel $(r, c_i)$ gains a particle with probability $\gamma$ if at least $B$ particles are present at the node, i.e.

$$W_i(\eta(r, k) \rightarrow (z_1, \ldots, z_5)|_{z_i=1}) = \begin{cases} \gamma & \text{if } n(r, k) \geq B \\ 0 & \text{else}. \end{cases}
$$

(4.22)

Mean–field approximation

We now derive the mean–field equation for the growth process defined by Eqn. (4.22). Since the growth–interaction operator $G$ depends only on the
number of particles at a node \((n(r, k))\), it is convenient to define indicator functions \(\Psi_a : \{0, 1\}^b \rightarrow \{0, 1\}\), for \(a = 0, \ldots, \hat{b}\), such that

\[
\Psi_a (\boldsymbol{\eta}(r, k)) = \begin{cases} 
1 & \text{if } n(r, k) = a \\
0 & \text{else}.
\end{cases}
\]  

(4.23)

These can be formulated as

\[
\Psi_a (\boldsymbol{\eta}(r, k)) := \sum_{i=1}^{\hat{b}} \prod_{i \in \mathcal{M}_a^i} \eta_i(r, k) \prod_{j \in \mathcal{M}_{a, l}^i} (1 - \eta_j(r, k)),
\]

(4.24)

with the index set \(\mathcal{M} := \{1, \ldots, \hat{b}\}\) and with \(\mathcal{M}_a^i\) denoting the \(a\)-th subset of \(\mathcal{M}\) with \(l\) elements. Now, the transition probability defined in Eqn. (4.22) can be rewritten as

\[
W_t(\boldsymbol{\eta}(r, k) \rightarrow (z_1, \ldots, z_5)|_{z_i=1}) = \gamma P \left( \Psi_B(\boldsymbol{\eta}(r, k)) + \cdots + \Psi_a(\boldsymbol{\eta}(r, k)) = 1 \right).
\]

(4.25)

Taking expectation values of Eqn. (4.21) we get

\[
f_i(r + mc_i, k + 1) = E \left( R^5 (n^5(r, k)) \right)
\]

(4.26)

\[
= \frac{1}{5} \sum_{l=1}^{5} E(\eta^5(r, k)) \quad \text{(isotropic random walk)}
\]

\[
= \frac{1}{5} \sum_{l=1}^{5} \left[ f_i(r, k) + E \left( (1 - \eta_l(r, k)) \zeta(\boldsymbol{\eta}(r, k)) \right) \right]
\]

\[
= \frac{1}{5} \sum_{l=1}^{5} \left[ f_i(r, k) + \gamma E \left( (1 - \eta_l(r, k)) \cdot \left( \Psi_B(\boldsymbol{\eta}(r, k)) + \cdots + \Psi_a(\boldsymbol{\eta}(r, k)) \right) \right) \right]
\]

where we used Eqn. (3.18) (p. 61) and Eqns. (4.19), (4.25). Furthermore, as we show in Appendix A, the following simplified LGCA growth rule leads to the same mean-field Eqn. (4.26): All empty channels \((r, c_i)\) simultaneously gain a particle with probability \(\gamma\), if at least \(B\) particles are present at the node, i.e.

\[
n^a(r, k) = \begin{cases} 
\hat{b} & \text{with probability } \gamma \text{ if } n(r, k) \in [B, \hat{b} - 1] \\
n(r, k) & \text{else}.
\end{cases}
\]

(4.27)

Here we are interested in the temporal growth dynamics of particle density and for that reason we neglect the spatial dependence in Eqn. (4.26), i.e.
4.3 Growth processes in lattice–gas cellular automata

\[ f_i(k) \equiv f_i(r, k), \forall r \in \mathcal{L}, \]
and consider the spatially averaged local particle density \( \rho(k) \in [0, 1] \) given by \( \rho(k) := \frac{1}{b} \sum_{i=1}^{b} f_i(k) \). Thus, applying the mean–field assumption (2.15) (p. 34) to Eqn. (4.26) and setting \( B = 1 \) we obtain

\[ \text{Rule (4.22)} \quad \rho(k + 1) = \rho(k) + \gamma \left( 1 - \rho(k) \right) \left( 1 - (1 - \rho(k))^4 \right). \tag{4.28} \]

Of course, this mean–field equation is identical to the one obtained from the cellular automaton growth–Rule (4.9) (Eqn. (4.16), p. 77) due to our specific choice of parameters: For the LGCA we neglect the spatial dependence, assume \( \hat{b} = 5 \) and choose the interaction neighbourhood to be \( \mathcal{N}(r) = \{ r \} \), while for the probabilistic cellular automaton the size of the interaction neighbourhood is \( \nu = 5 \). Hence, in both cases the creation of a new particle depends on the information encoded in a local configuration of ‘size 5’. Note that the design of

\[ \Delta \rho(k)/\rho(k) \]

Figure 4.7: Comparison of relative growth rates; legend: i: mean–field Eqn. (4.28), ii: cellular automaton Rule (4.9) with asyn. movement (\( \tau = 1 \)), iii: LGCA Rule (4.22) (\( \hat{b} = 1 \)), iv: LGCA Rule (4.27) (\( \hat{b} = 1 \)); parameters: \( L = 100 \times 100 \), von Neumann interaction neighbourhood, \( \rho(0) = 0.01, B = 1 \) and \( \gamma = 0.1 \).

LGCA growth rules whose mean–field equations coincide with the mean–field equations of the probabilistic cellular automaton Rules (4.10) and (4.11) is straightforward. As illustrated in Fig. 4.7 mean–field approximation leads to a good prediction of the LGCA growth process combined with a synchronous random walk rule.

As a last example of modelling growth processes in LGCA, we change the point of view from an empty channel to an occupied channel: Each particle at a node \( r \) has an offspring with probability \( \gamma \), but only a maximum number \( \hat{b} - n(r, k) \) of this new particles are placed on the node. Then, the transition
probability is given by

\[
W_i(\eta(r, k) \rightarrow (z_1, \ldots, z_3)|_{z_i = 1}) = \begin{cases} 
0 & \text{if } n(n, k) \in \{0, 5\} \\
\frac{1}{4} \gamma & \text{if } n(n, k) = 1 \\
\frac{1}{3} \gamma^2 + \frac{2}{3} \gamma(1 - \gamma) & \text{if } n(n, k) = 2 \\
1 - ((1 - \gamma)^3 + \frac{3}{2} \gamma(1 - \gamma)^2) & \text{if } n(n, k) = 3 \\
1 - (1 - \gamma)^4 & \text{if } n(n, k) = 4
\end{cases}
\]

\[
= \frac{1}{4} \gamma P(\Psi_1(\eta(r, k) = 1) + \left(\frac{1}{3} \gamma^2 + \frac{2}{3} \gamma(1 - \gamma)\right) P(\Psi_2(\eta(r, k) = 1) \\
+ \left(1 - ((1 - \gamma)^3 + \frac{3}{2} \gamma(1 - \gamma)^2)\right) P(\Psi_3(\eta(r, k) = 1) \\
+ (1 - (1 - \gamma)^4) P(\Psi_4(\eta(r, k) = 1) .
\]

From this, the mean–field equation for the spatially averaged particle density can be derived as

\[
\rho(k + 1) = (1 + \gamma)\rho(k) + 2\gamma^2 \rho(k)^2 + (6\gamma^2 - 2\gamma^3)\rho(k)^3 \\
+ (-12\gamma^2 + 8\gamma^3 - \gamma^4)\rho(k)^4 + (-\gamma + 8\gamma^2 - 6\gamma^3 + \gamma^4)\rho(k)^5 .
\]

This growth process describes an almost exponential growth for low values of \(\rho(k)\), as can be seen from Fig. 4.8(a).

**(a) Temporal dynamics; Almost exponential growth for low densities. The dot indicates the inflection point of the mean–field curve.**

**(b) Relative growth rates**

---

**Figure 4.8:** Lattice–gas growth model according to Eqn. (4.29); **legend:** i: mean–field Eqn. (4.30), ii: simulated growth \((m = 1)\), iii: theoretical exponential growth; **parameters:** \(L = 100 \times 100\), \(\rho(0) = 0.01\) and \(\gamma = 0.1\).
4.4 Summary

This is qualitatively different from the growth models we introduced before: the relative growth rate (Fig. 4.8(b)) is a convex curve while all other relative growth rates are concave curves or decreasing lines (cf. Figs. 4.7, 4.6). In other words, in model (4.29) there is some threshold density below which the particles do almost not interfere with each other while in the other models it is implicitly assumed that the relative growth rate is density-dependent even at lowest densities.

4.4 Summary

In this chapter, we concentrated on spatial particle growth processes based on localised particle reproduction (see p. 71). With the help of various cellular automaton growth rules we demonstrated that the relative growth rate is sensitively dependent on the choice of the local automaton rule. The relative growth rate can not be adequately approximated by mean field theory in probabilistic cellular automata. But if the growth process is combined with an asynchronous or synchronous particle-moving mechanism, then the mean-field approximation is an appropriate tool in order to study the extended growth process, since motion counteracts the upbuilding of correlations. In addition, particle-motion accelerates the growth.

Furthermore, we presented an example of a probabilistic cellular automaton with imposed asynchronous movement, and two different LGCA which all can be described by the same mean-field equation (cf. Fig. 4.7, p. 81). This indicates that cellular automaton models including particle-movement are less sensitive to the particular choice of the automaton interaction rule.

We expect the mean-field approximation to qualitatively grasp the cellular automaton dynamics also for extended particle interaction processes if particle motion is included. In the following chapter examples of two- and three-component interactions based on particle growth and ‘death’ processes are provided to show that such expectations are indeed fulfilled. We put this in the framework of lattice-gas cellular automata, because they are especially useful to model synchronous random particle movement (cf. Sec. 3.4, p. 57). Moreover, corresponding space- and time-dependent difference mean-field equations can be derived, which makes the automaton dynamics accessible not only for temporal but also for spatial pattern formation analysis.
One–component interaction and movement: Growth processes
5 Many interacting and moving components

5.1 Activator–inhibitor interaction

5.1.1 Introduction

1 A concept of pattern formation in biological systems was suggested by Alan Turing in his paper ‘The chemical basis of morphogenesis’ (Turing 1952). He demonstrated therein that a spatially homogeneous stable steady state of a reactive system can lose its stability when diffusive transport is included. The diffusive instability is able to enhance local random fluctuations and as a result a spatially heterogeneous pattern of chemical (morphogen) concentrations may arise from initially homogeneous conditions. The wave lengths of these patterns are functions solely of the values of the diffusion coefficients and the kinetic parameters and not of domain size. In the following we refer to this type of pattern as ‘Turing pattern’. That diffusion, usually considered a stabilising (spatially homogenising) process (Murray 1989), can actually cause instability was a revolutionary concept. An experimental observation of this kind of pattern formation was made in the chlorite–iodide–malonic acid (CIMA) and in the polycrylamide–methylene blue–sulfide–oxygen (PA-MBO) reactions (Castets et al. 1990, Ouyang and Swinney 1991). How far diffusive instability accounts for biological pattern formation is not clear. It was argued by Turing that it can play an important role in morphogenesis (Turing 1952). A review of its role in other biological contexts can be found in Murray (1989).

Turing pattern formation in activator–inhibitor systems was proposed as a model of biological morphogenesis (Gierer and Meinhardt 1972). Such two-component systems are traditionally characterised and studied with the help of appropriately constructed partial differential equations (Gierer and Meinhardt 1972, Murray 1989). However, this characterisation does not provide insight into the microscopic basis of Turing pattern formation. Among others, this problem inspired the development and application of LGCA models for reactive / interactive systems (Kapral et al. 1991, Lawniczak et al. 1991).

\[ \text{http://www.turing.org.uk/turing/ .} \]

\[ \text{http://www.turing.org.uk/turing/ .} \]

\[ ClO_2^- + 4 I^- + 4 H^+ \rightarrow Cl^- + 2 I_2 + 2 H_2O, \quad MA + I_2 \rightarrow IMA + I^- \]
Many interacting and moving components

Hasslacher et al. 1993). Turing patterns observed in LGCA simulations were analysed by means of linear stability analysis of LGCA partial differential equations (Lawniczak et al. 1991, Hasslacher et al. 1993). In addition, cellular automata models mimicking activator–inhibitor interactions were suggested, e.g. as models of vertebrate coat markings or shell pattern formation (Young 1984, Markus and Schepers 1994). Analysis of those automata is based on computer simulations.

In this work, we focus on linear stability analysis of a cellular automaton with activator–inhibitor–like interactions. We study pattern formation in a two–component cellular automaton formulated in terms of LGCA terminology. Particles which can symbolise organisms or cells are created or destroyed at the nodes of the lattice. In addition, particle movement resembles a random walk. This is one of the elements that distinguishes our LGCA from deterministic and probabilistic cellular automaton models. Furthermore, the LGCA rules have been inspired by local interactions of the components in systems capable of Turing pattern formation. The considered rules can be viewed as caricature of local activator–inhibitor interactions and could for example serve as a gross simplification of predator–prey interactions.

Here, our emphasis is on linear stability analysis of discrete space and time automaton mean–field (Boltzmann) equations. Particularly, a critical wave length and a 'Turing condition' for the onset of pattern formation are derived. Since the mean–field description is not exact it is also important to understand how well it can predict and characterise Turing patterns observed in LGCA simulations.

5.1.2 Turing pattern formation in macroscopic reaction–diffusion systems

The objective of this subsection is to outline some important mathematical aspects for the appearance of Turing structures in macroscopic reaction–diffusion systems of two components\(^4\). Originally, Turing studied a "mathematically convenient, though biologically unusual system"\(^5\). He considered a one–dimensional ring of cells \((r = 1, \ldots, L)\) each of which contains various morphogens. In particular, he studied two morphogens whose concentrations are given by \(a_r\) and \(b_r\), \(r = 1, \ldots, L\), and whose dynamics within each identical cell is described by a system of coupled differential equations of the form

\[
\begin{align*}
\partial_t a_r &= F(a_r, b_r) + D_a \left( (a_{r+1} - a_r) + (a_r - a_{r-1}) \right) \\
\partial_t b_r &= G(a_r, b_r) + D_b \left( (b_{r+1} - b_r) + (b_r - b_{r-1}) \right)
\end{align*}
\]

\(^4\)There exists an extensive literature on the problem of Turing pattern formation; for example Murray (1989), Engelhardt (1994) and Maini (1999) give good reviews.

\(^5\)citation from Turing (1952)
where $D_a$ and $D_b$ are ‘cell–to–cell’ diffusion constants. Later on systems defined in continuous space which are mathematically described by partial differential equations are examined. A one-dimensional reaction–diffusion model defined on a line of length $l$, i.e. $x \in [0,l]$, is

$$\begin{align*}
\partial_t a &= F(a,b) + D_a \partial^2 x a \\
\partial_t b &= G(a,b) + D_b \partial^2 x b.
\end{align*}$$

(5.2)

In order to develop a pattern or structure due to an instability of the homogeneous equilibrium, which is triggered by random disturbances, both systems (5.1) and (5.2) have to fulfill the following two ‘Turing conditions’ simultaneously (e.g. Murray 1989, Engelhardt 1994):

1. The system has a **spatially uniform stationary state** $(\bar{a}, \bar{b})$, i.e.

$$F(\bar{a}, \bar{b}) = G(\bar{a}, \bar{b}) = 0,$$

which is **stable**, i.e. the signs of the elements for the Jacobian matrix are

$$J = \begin{pmatrix} \frac{\partial F}{\partial a} & \frac{\partial F}{\partial b} \\ \frac{\partial G}{\partial a} & \frac{\partial G}{\partial b} \end{pmatrix} \xrightarrow{\text{signs}} \left\{ \begin{array}{ll}
\text{‘real activator–inhibitor model’}^6: & \\
( + - ) & \text{or} & ( - + ) , \\
( + - ) & \text{or} & ( - + ) . \\
\text{‘activator–substrate depleted model’}^7: & \\
( + + ) & \text{or} & ( - - ) , \\
( - - ) & \text{or} & ( + + ) .
\end{array} \right\}$$

(5.3)

In other words, for two–component systems, one component has to be autocatalytic and the other one to be self–inhibiting. Furthermore, the cross–activations or –inhibitions need to be of opposite sign, i.e. if one activates the other, the other component has to inhibit the first (or vice–versa). The notion of ‘activator–inhibitor model’ refers to systems in which one component activates itself and the other, while the second component inhibits itself and the first. ‘Activator–substrate depleted models’ are characterised by either component promoting increase in the second component and decrease in the first. The two alternatives in the structure of the Jacobian for each category result from the identification of the self-activating and self-inhibiting components.

2. In addition, Turing instabilities can occur only if the diffusion coefficients of the two components differ significantly, i.e. $|D_a - D_b| \gg 0$. To be

---

^6 e.g. Lengyel–Epstein model, Gérard–Meinhardt model (Engelhardt 1994)

^7 e.g. Selkov model, Brusselator, Schnakenberg model (Engelhardt 1994); another terminology is ‘positive–feedback system’. 

---
more precise, with $a$ being the autocatalytic component in the system (5.2) then the critical diffusion ratio is given by (Engelhardt 1994)

\[
\frac{D_b}{D_a} \geq \frac{(\text{det} \mathbf{J} - \partial_b F \partial_a G) + 2\sqrt{-\partial_b F \partial_a G \text{det} \mathbf{J}}}{(\partial_b F)^2} > 1 \quad (5.4)
\]

\[
det \mathbf{J} := \partial_a F \partial_b G - \partial_b F \partial_a G .
\]

If the system (5.2) is defined in one spatial dimension with system length $l$ satisfying periodic boundary conditions, unstable modes according to wave number

\[
q = \frac{l}{2\pi} \tilde{q}
\]

are determined from the so-called dispersion relation given by

\[
\lambda^2 - \lambda \left( (\partial_a F + \partial_b G) - \tilde{q}^2(D_a + D_b) \right) + \text{det} \mathbf{J} = 0 , \quad \tilde{q}^4 (D_b \partial_a F + D_a \partial_b G) + \tilde{q}^4 D_a D_b = 0 , \quad (5.5)
\]

where those $\tilde{q}$ are relevant for which the largest root $\lambda(\tilde{q}) > 0$. The dispersion relation can be derived with the help of the Fourier transformation of system (5.2). The fastest growing mode is found to have the wave number $q_*$ given by

\[
q_* = \frac{l}{2\pi} \tilde{q}_* \quad \text{where} \quad \tilde{q}_*^4 = \frac{\text{det} \mathbf{J}}{D_a D_b} . \quad (5.6)
\]

Note that in a finite domain situation wave numbers $q_*$ are discrete and so $q_*$ may not be an allowed wave number. In this case the integer number closest to the analytically determined $q_*$ characterises the resulting patterns (Murray 1989).

Under these restrictions $a$ and $b$ concentrations develop steady state heterogeneous spatial patterns at the onset of instability with an intrinsic wave length $2\pi/\tilde{q}_* = l/q_*$, that is, the wave length depends only on the kinetic parameters and diffusion coefficients but not on the geometrical length of the system domain (cf. Eqn. (5.6)). In ‘real activator–inhibitor models’ (cf. Fig. 5.1) high concentrations of both components are found in the same spatial region (they are in phase) while patterns resulting from ‘activator–substrate depleted models’ are out of phase, i.e. the concentration of one component is high where the concentration of the other is low.

### 5.1.3 Definition of the automaton rules

The model system consists of two moving and interacting ‘species’ $\sigma$, $\sigma \in \{A, I\}$, the activator species A and the inhibitor species I. Particles $X_\sigma$ of each
5.1 Activator–inhibitor interaction

![Diagram of activator and inhibitor](image)

(a) Schematic representation of the 'real activator–inhibitor' interaction according to (5.3).

(b) Basic types of two-dimensional Turing patterns in activator concentration depending on different parameter values of a continuous 'real activator–inhibitor model'.

Figure 5.1: Turing pattern formation in a 'real activator–inhibitor model'.

species move on its own one-dimensional periodic lattice \( L_0 \subset \mathbb{Z} \). Later on we will extend the model also to two-dimensional lattices. We assume that \( L_0 \) and \( L_\ell \) possess an identical labeling of nodes and the number of nodes is equal to \( L \). Then, for convenience, we identify both lattices and denote them by \( L \).

Each node \( r \in L \) can host up to three particles, i.e. \( b = 3 \), of each species \( \sigma \) which are distributed in different velocity channels \((r, c_i)\), \( 1 \leq i \leq 3 \), with at most one particle of a given species per channel (Fig. 5.2). Two velocity channels correspond to nearest neighbour directions, i.e. \( c_1 = 1 \) and \( c_2 = -1 \), the third is a rest channel, \( c_3 = 0 \). Hence, the global automaton configuration \( s(k) \in S \) at discrete time \( k \) is described locally at each node \( r \) by

\[
\eta(r, k) = \left( \eta_{A,1}(r, k), \eta_{A,2}(r, k), \eta_{A,3}(r, k), \eta_{I,1}(r, k), \eta_{I,2}(r, k), \eta_{I,3}(r, k) \right)
\]

with Boolean components \( \eta_{\sigma,i}(r, k) \) (cf. Fig. 5.2). \( \eta_{\sigma,i}(r, k) = 1 \) represents the presence and \( \eta_{\sigma,i}(r, k) = 0 \) the absence of a particle of species \( \sigma \) at time \( k \) in the channel \((r, c_i)\).

The number of particles of species \( \sigma \) at node \( r \) at time \( k \) is given by

\[
n_{\sigma}(r, k) = \sum_{i=1}^{3} \eta_{\sigma,i}(r, k).
\]

Automaton dynamics arises from repetitive applications of reactive and diffusive 'interactions' applied simultaneously at all lattice nodes at each discrete
Many interacting and moving components

$\mathcal{L}$

$\mathcal{L}_A$

$\mathcal{L}_I$

Figure 5.2: Possible one-dimensional lattice ($\tilde{b} = 3$) configuration for a two-component model; local node configurations: $\eta_A(r) = (1, 1, 0), \eta_I(r) = (0, 1, 0)$ and hence $\eta(r) = (1, 1, 0, 0, 1, 0)$.

time step. First a reactive interaction step is performed during which particles $X_\sigma$ of each species $\sigma$ are destroyed or created according to a stochastic rule. Next, in a diffusion step particles $X_\sigma$ perform a random walk on their own lattices, independently from the other species (cf. Sec. 3.4, p. 57).

The reactive interaction rule (R) is designed to capture the main characteristics of activator–inhibitor system dynamics as it is shown in Fig. 5.1(a) on page 89. The model contains also a particle-motion process and for the sake of simplicity, the interaction neighbourhood will be restricted to the node itself, i.e. $\mathcal{N}_2(r) = \{r\}$. Next, we define sequences of node- and time-independent identically distributed Bernoulli type random variables $\{\zeta_c(r, k) : r \in \mathcal{L}, k \in \mathbb{N}\}$ and $\{\zeta_d(r, k) : r \in \mathcal{L}, k \in \mathbb{N}\}$ which govern the creation and destruction of particles, such that

$$p_c := P(\zeta_c(r, k) = 1) \quad \text{and} \quad p_d := P(\zeta_d(r, k) = 1) . \quad (5.7)$$

Then, the number of particles $X_\sigma$ at a node $r$ at time $k$ after the reactive interaction step R took place, $n_\sigma^R(r, k)$, is defined as

$$n_\sigma^R(r, k) = \begin{cases} 
\tilde{b} \quad \text{with prob. } p_c \text{ if } n_A(r, k) + n_I(r, k) \geq 0 \\
0 \quad \text{with prob. } p_d \text{ if } 0 \leq n_A(r, k) + n_I(r, k) < \tilde{b} \\
n_\sigma(r, k) \quad \text{otherwise}
\end{cases} \quad (5.8)
$$

for each $\sigma \in \{A, I\}$. Rule (5.8) part (i) states that the activator $A$ autocatalytically activates its own production and that of the inhibitor $I$. Note that the activator $A$ in the absence of the inhibitor $I$ performs a 'growth process' which corresponds to the growth Rule (4.27) (cf. p. 80) studied earlier with the corresponding parameters $B = 1$ and $\gamma = p_c$. In turn, the dynamics of the inhibitor $I$ is determined by its own degradation and by suppression of activator growth $A$ (5.8)(ii). Figure 5.3 illustrates this rule. Since Rule (5.8) depends only on the number of particles of each species at a node, we use the previously defined indicator functions $\Psi_\sigma(\eta(r, k))$ (cf. p. 80) to derive a
5.1 Activator–inhibitor interaction

\[ n_A(r, k) = 2 \quad n^R_A(r, k) = 3 \quad n_A(r, k) = 2 \quad n^R_A(r, k) = 0 \]

\[ n_I(r, k) = 1 \quad n^R_I(r, k) = 3 \quad n_I(r, k) = 3 \quad n^R_I(r, k) = 0 \]

Figure 5.3: Examples of node configurations for Rule (5.8).

A microscopic description of the model. Then, with \( \Psi := (\Psi_0, \Psi_1, \Psi_2, \Psi_3) \) the action of the reactive interaction operator \( R \) can be written as

\[
\eta^R_{\sigma,i}(r, k) = R^R_{\sigma,i}(\eta(r, k)) = \Psi(\eta_A(r, k)) M_{\sigma}(\eta_{\sigma,i}(r, k)) \Psi^T(\eta_I(r, k)),
\]

with the \( 4 \times 4 \) ‘interaction matrices’ \( M_\sigma \). Each matrix \( M_\sigma \) has a non–zero entry if an interaction takes place, depending on the \( n_A(r, k) \) and \( n_I(r, k) \) relationship. They are defined as

\[
M_A(\eta_{\sigma,i}(r, k)) := \begin{pmatrix} 0 & 0 & 0 & 0 \\ \alpha_c & 0 & \alpha_d & \alpha_d \\ \alpha_c & \alpha_c & 0 & \alpha_d \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad M_I(\eta_{\sigma,i}(r, k)) := \begin{pmatrix} 0 & \alpha_d & \alpha_d & \alpha_d \\ \alpha_c & 0 & \alpha_d & \alpha_d \\ \alpha_c & \alpha_c & 0 & \alpha_d \\ \alpha_c & \alpha_c & \alpha_c & 0 \end{pmatrix},
\]

with \( \alpha_c := \zeta_c(r, k) (1 - \eta_{\sigma,i}(r, k)) \) and \( \alpha_d := -\zeta_d(r, k) \eta_{\sigma,i}(r, k) \).

Note that the complete vector of ‘counting functions’ \( \Psi \) is derived in Appendix B.1.

Parameters for the random walk of each particle \( X_\sigma \) are a set of statistically
and time–independent Boolean random variables \( \xi_{\sigma,j}(r, k), j = 1, \ldots, 6 \), which govern the shuffling of the node configuration for each species \( \sigma \in \{ A, I \} \) (cf. Sec. 3.4, p. 57) and with probability distribution

\[
P(\xi_{\sigma,j}(r, k) = 1) := p_{\sigma,j}, \quad P(\xi_{\sigma,j}(r, k) = 0) = 1 - p_{\sigma,j}.
\]

For isotropy reasons, in the following we investigate only the ‘unbiased case’ \( p_{\sigma,j} = \frac{1}{6} \). The microdynamics for each species can be described by

\[
\eta^R_{\sigma,i}(r, k) = R^R_{i}(\eta_{\sigma}(r, k)) = \sum_{j=1}^{6} \xi_{\sigma,j}(r, k) \sum_{l=1}^{3} \eta_{\sigma,l}(r, k) a^j_{l,i},
\]

where \( a^j_{l,i} \) is a matrix element of the permutation matrix \( A_j \in A_3 \) (cf. example given on page 58).
Hence, the spatio–temporal evolution of the automaton dynamics can be expressed by the following system of nonlinear microdynamical difference–equations. If at time $k+1$ the state of a channel $(r + m_{\sigma} c_i, c_i)_{\sigma}$ is described by $\eta_{\sigma, i}(r + m_{\sigma} c_i, k + 1)$, then

$$
\eta_{\sigma, i}(r + m_{\sigma} c_i, k + 1) - \eta_{\sigma, i}(r, k) = \mathcal{R}_i \left( \mathbf{R}_\sigma^\mathbf{n} (\eta_{\sigma}^\mathbf{n}(r, k)) \right) - \eta_{\sigma, i}(r, k) = \mathcal{C}_{\sigma, i}(\eta(r, k)) ,
$$

(5.12)

for $m_{\sigma} \in \mathbb{N}$, $\sigma \in \{A, I\}$ and $i \in \{1, 2, 3\}$.

Simulations of the described automaton dynamics, starting from a random distribution of particles $X_{\sigma, \sigma} \in \{A, I\}$, exhibit formation of patterns for appropriately chosen parameters $p_c, p_d, m_A$ and $m_I$. Examples are shown in Fig. 5.4. In the following section we analyse the formation of these patterns. Furthermore, we investigate the LGCA model with respect to the concept of diffusion–induced pattern formation in analogue to the Turing conditions (cf. p. 87) for contintous systems.

Figure 5.4: Space–time plots of activator–inhibitor LGCA simulations; dark colours indicate regions of high activator concentration. **Parameters:** One-dimensional lattice with $L = 100$ nodes and periodic boundaries, random initial conditions, $k \in \{0, \ldots, 100\}$. 
5.1 Activator–inhibitor interaction

Lattice–Boltzmann equation and its uniform steady states

In order to gain more insight into pattern formation in the automaton, we derive the space– and time–discrete lattice–Boltzmann equation from the microdynamical Eqn. (5.12) and perform a linear stability analysis of this mean–field equation (cf. Subsec. 2.3.2, p. 40). Recall that the lattice–Boltzmann equation is derived by taking the expected value of both sides of Eqn. (5.12) (cf. Eqn. (2.19), p. 36) under the mean–field approximation, in which all correlations between occupation numbers \( \eta_{\sigma,i}(r,k) \) are neglected. Then with the help of Eqn. (3.18) (cf. p. 61) we get

\[
\begin{align*}
    f_{\sigma,i}(r + m_\sigma c_i, k + 1) - f_{\sigma,i}(r, k) &= E \left( R_{\sigma}^k (\eta_{\sigma}^k(r,k)) - \eta_{\sigma,i}(r,k) \right) \\
    &= \frac{1}{3} \sum_{i=1}^{3} E(\eta_{\sigma,i}^k(r,k)) - f_{\sigma,i}(r,k) \\
    &= \tilde{\mathcal{C}}_{\sigma,i}(f(r, k)),
\end{align*}
\]

where

\[
f(r, k) = (f_{A,1}(r, k), f_{A,2}(r, k), f_{A,3}(r, k), f_{I,1}(r, k), f_{I,2}(r, k), f_{I,3}(r, k))
\]

\[
= (f_j(r,k))_{j=1}^6 \in [0,1]^6.
\]

Note that \( \tilde{\mathcal{C}}_{\sigma,i}(f(r, k)) \) is a function depending on the reaction parameters \( p_c \) and \( p_d \). The expanded form of \( E(\eta_{\sigma,i}^k(r,k)) \) is given in Appendix B.1.

The first step in the analysis of pattern formation is the evaluation of the spatially uniform steady states of the lattice–Boltzmann equation. These states are determined by

\[
f_{\sigma,i}(r + m_\sigma c_i, k + 1) = f_{\sigma,i}(r, k), \quad \forall r \in \mathcal{L}, \forall k \in \mathbb{N} \\
\Rightarrow \quad \tilde{\mathcal{C}}_{\sigma,i}(\tilde{f}) = 0,
\]

for \( \sigma \in \{A,I\} \) and \( i = 1, \ldots, 3 \). Hence, assuming that

\[
f_{A,1}(r, k) = \tilde{f}_{A,1} = f_{A,2}(r, k) = \tilde{f}_{A,2} = f_{A,3}(r, k) = \tilde{f}_{A,3} =: \tilde{f}_A, \\
f_{I,1}(r, k) = \tilde{f}_{I,1} = f_{I,2}(r, k) = \tilde{f}_{I,2} = f_{I,3}(r, k) = \tilde{f}_{I,3} =: \tilde{f}_I,
\]

finding the solutions of Eqn. (5.14) corresponds to solving the equations

\[
-3(-1 + \tilde{f}_A)\tilde{f}_A \left( (-1 + \tilde{f}_I)^2 (2 - 2\tilde{f}_I + \tilde{f}_A(-1 + 4\tilde{f}_I)) p_c \\ + \tilde{f}_I^2 (-3 + \tilde{f}_A(3 - 4\tilde{f}_I) + 2\tilde{f}_I) p_d \right) = 0,
\]

and

\[
-3 \left[ \tilde{f}_I p_d + 3 \tilde{f}_A(-1 + \tilde{f}_I)^2((-1 + \tilde{f}_I) p_c - \tilde{f}_I p_d) \right. \\
- 3\tilde{f}_I^2 (1 - 4\tilde{f}_I + 3\tilde{f}_I^2)((-1 + \tilde{f}_I) p_c - \tilde{f}_I p_d) \\
+ \tilde{f}_A^2 (1 - 6\tilde{f}_I + 6\tilde{f}_I^2)((-1 + \tilde{f}_I) p_c - \tilde{f}_I p_d) \left. \right] = 0.
\]
Many interacting and moving components

Solutions \((\vec{f}_A, \vec{f}_I)\) of Eqns. (5.15) and (5.16) are given by

\[ (\vec{f}_A, \vec{f}_I) \in \{(0, 0), (a_1, a_2), (1, 1)\} , \]

where

\[ (a_1, a_2) = (0.5, 0.5) \text{ whenever } p_c = p_d = p , \]

and for \(p_c \neq p_d\) the solution \((a_1, a_2)\) is a function of the reactive probabilities \(p_c\) and \(p_d\), which can be found numerically as illustrated in Fig. 5.5.

\[ \begin{align*}
\text{Figure 5.5: Spatially uniform steady states } \left( \vec{f}_A, \vec{f}_I \right) \text{ for different values of the reaction probabilities } (p_c, p_d) \in \{0.1, 0.2, \ldots, 0.9, 1\}^2.
\end{align*} \]

Derivation of the Boltzmann propagator

In the next step, the stability of these steady states with respect to spatially homogeneous and heterogeneous fluctuations \(\delta f_{\sigma, i}(r, k) := f_{\sigma, i} - \overline{f}_{\sigma, i}\) is determined. Following the linear stability analysis described in Subsec. 2.3.2 (p. 40), as a result of the linearisation and Fourier transformation we obtain equations (cf. Eqn. (2.32), p. 42) for the growth of each Fourier mode with wave number \(q\), i.e. \(F_{\sigma, i}(q, k) = \sum_{r \in \mathcal{L}} \delta f_{\sigma, i}(r, k)e^{-i \frac{2\pi}{L} q \cdot r}\), as

\[ F(q, k) = \Gamma(q)^k F(q, 0) , \]

with

\[ F^T(q, k) = (F_{A, 1}(r, k), F_{A, 2}(r, k), F_{A, 3}(r, k), F_{I, 1}(r, k), F_{I, 2}(r, k), F_{I, 3}(r, k)) \]

\[ = (F_j(r, k))_{j=1}^6 , \]

and where the Boltzmann propagator (2.31) (cf. p. 42) for this model is given by

\[ \Gamma(q) = T \left\{ I + \Omega^0 \right\} , \quad q = 0, \ldots, L - 1 , \]
with \( T = \text{diag} \left( e^{-1} \frac{d}{q^m A}, e^{1} \frac{d}{q^m A}, 1, e^{-1} \frac{d}{q^m I}, e^{1} \frac{d}{q^m I}, 1 \right) \),

\[
\mathbf{Q}^0 = \begin{pmatrix}
\frac{\partial Q_A}{\partial f_1} & \cdots & \frac{\partial Q_A}{\partial f_L} \\
\vdots & \ddots & \vdots \\
\frac{\partial Q_I}{\partial f_1} & \cdots & \frac{\partial Q_I}{\partial f_L}
\end{pmatrix}
\quad \text{and} \quad
\mathbf{I} + \mathbf{Q}^0 = \begin{pmatrix}
\omega_1 & \cdots & \omega_1 & \omega_2 & \cdots & \omega_2 \\
\vdots & \ddots & \vdots \\
\omega_1 & \cdots & \omega_1 & \omega_2 & \cdots & \omega_2 \\
\omega_3 & \cdots & \omega_3 & \omega_4 & \cdots & \omega_4 \\
\vdots & \ddots & \vdots \\
\omega_3 & \cdots & \omega_3 & \omega_4 & \cdots & \omega_4
\end{pmatrix},
\]

where \( \mathbf{f} = (f_A, f_A, f_A, f_i, f_i, f_i) \).

The matrix elements \( \omega_i \), \( i = 1, \ldots, 4 \), are terms depending on \( p_c, p_d, f_A \) and \( f_i \). They are given in Appendix B.2 by Eqn. (B.2.4).

The spectrum of the Boltzmann propagator can be obtained as

\[
\Lambda_{\Gamma(q)} = \{ \lambda_1(q), \lambda_2(q), 0 \},
\]

where \( 0 \) has a multiplicity of 4 and

\[
\lambda_{1,2}(q) = \frac{1}{2} \left( \omega_1 u_A(q) + \omega_4 u_i(q) \right) \pm \sqrt{4 \left( \omega_2 \omega_3 - \omega_1 \omega_4 \right) u_A(q) u_i(q) + \left( \omega_1 u_A(q) + \omega_4 u_i(q) \right)^2}
\]

with \( u_{\sigma}(q) := 1 + 2 \cos \left( \frac{2\pi}{L} q m_{\sigma} \right) \), \( \sigma \in \{ A, I \} \), \( q \in \{ 0, \ldots, L \} \).

Furthermore, \( \Gamma(q) \) is diagonalisable, since the dimension of the eigenspace of eigenvalue \( 0 \) is \( 6 - \text{rank} (\Gamma(q)) = 4 \). Hence, the complete solution of system (5.18) for each wave number \( q = 0, \ldots, L - 1 \), is given by (cf. Eqns. (2.34), (2.35), p. 43)

\[
F_{\sigma,i}(q,k) = d_1(q) v_{1i}^\sigma(q) \lambda_1(q)^k + d_2(q) v_{2i}^\sigma(q) \lambda_2(q)^k,
\]

for \( i = 1, 2, 3 \), \( \sigma \in \{ A, I \} \) and with eigenvectors \( v_i(q) = (v_{i1}^A(q), \ldots, v_{i6}^A(q)) = (v_{ij}(q))_{j=1}^6 \), for \( l = 1, \ldots, 6 \). The constants \( d_1(q) \) and \( d_2(q) \) are specified by the initial condition

\[
\sum_{l=1}^6 d_l(q) v_{lj}(q) = \sum_{r=0}^{L-1} e^{i \frac{2\pi}{L} q \sigma} \delta f_j(r, 0).
\]

Recall that spatially inhomogeneous structures are determined by undamped modes according to wave numbers \( q \in Q^c \) (cf. def. p. 43). In the following, we decompose this set of critical wave numbers in \( Q^+ \cup Q^- \subset Q^c \), where

\[
Q^+ := \{ q \in \{ 0, \ldots, L - 1 \} : \lambda(q) > 1 \land |\lambda(q)| \equiv \mu(q) \}
\]
\[ Q^- := \{ q \in \{0, \ldots, L - 1 \} : \lambda(q) < -1 \land |\lambda(q)| = \mu(q) \} . \]

Furthermore, let \( q_* \) be the dominant critical wave number for which the spectral radius is maximal, i.e. \( \mu(q_*) = \max_{q \in Q^-} \mu(q) \). Since the corresponding mode \( F(q_*, k) \) grows fastest, linear stability analysis predicts a spatial pattern with a dominant wave length of \( L/q_* \).

**Spatially homogeneous perturbations**

The stability of the spatially uniform steady states \( (\bar{f}_A, \bar{f}_I) \) with respect to spatially homogeneous fluctuations is determined by studying the problem for \( q = 0 \), since \( \sum_{r \in \mathcal{L}} \delta f_{\sigma,i}(r,0) = F_{\sigma,i}(0,0) \). In this case the eigenvalues \( \lambda_{1,2} \) simplify to

\[
\lambda_{1,2}(0) = \frac{3}{2} \left( \omega_1 + \omega_4 \pm \sqrt{4 \omega_2 \omega_3 + (\omega_1 - \omega_4)^2} \right) .
\]

(5.22)

For the trivial steady states \((0,0)\) and \((1,1)\) these eigenvalues become

\[
\lambda_1(0) = 1 + 2p_c \quad \text{and} \quad \lambda_2(0) = 1 - p_d \quad \text{for} \quad (\bar{f}_A, \bar{f}_I) = (0,0) ,
\]

and

\[
\lambda_1(0) = 1 + 2p_d \quad \text{and} \quad \lambda_2(0) = 1 - p_c \quad \text{for} \quad (\bar{f}_A, \bar{f}_I) = (1,1) .
\]

Clearly, the spectral radius is always larger than one, i.e. \( \mu(0) = \lambda_1(0) > 1 \). Therefore, the homogeneous steady states \((0,0)\) and \((1,1)\) are **unstable** with respect to spatially homogeneous perturbations. Hence, spatial diffusion-induced pattern formation close to these homogeneous steady states is not possible since the first Turing condition (see p. 87) is not satisfied.

Now we investigate the stability of the nontrivial steady state \((a_1, a_2)\). If we choose \( p_c = p_d := p \) the eigenvalues (5.22) become

\[
\lambda_1(0) = 1 - \frac{5}{8} p \quad \text{and} \quad \lambda_2(0) = 1 - p .
\]

For other non-equal reaction probabilities \( p_c \) and \( p_d \) the eigenvalues can be found numerically as it is shown in Fig. 5.6.

Thus, for any \( p_c \) and \( p_d \) the spectral radius is given by \( \mu(0) = \lambda_1(0) < 1 \), and hence the stationary state \((a_1, a_2)\) is **stable** with respect to any spatially homogeneous perturbation. In the next subsection we investigate how a difference in the speed parameters \( m_A \) and \( m_I \) can act as a destabilising influence.
5.1 Activator–inhibitor interaction

Figure 5.6: Eigenvalues \((\lambda_1(0), \lambda_2(0))\) for different values of the reaction probabilities \((p_c, p_d) \in \{0.1, 0.2, \ldots, 0.9, 1\}\); the larger dots represent values for which \(p_c = p_d =: p\).

Note that as we consider the spatially homogeneous case here, the expected occupation numbers \(f_{\sigma,i}(r,k)\) are the same for all nodes \(r\) and directions \(c_i\), i.e. \(f_{\sigma,i}(r,k) \equiv f_{\sigma}(k)\). Therefore, the total density \(\rho_{\sigma}(k)\) is given by

\[
\rho_{\sigma}(k) = \frac{1}{3L} \sum_{r=0}^{L-1} \sum_{i=1}^{3} f_{\sigma,i}(r,k) = f_{\sigma}(k).
\]

Figure 5.7 shows trajectories obtained by iterating the lattice–Boltzmann equation (5.13) (cf. p. 93) at a fixed node \(r\) \((m_{\sigma} = 0)\) starting from different initial conditions. The illustrated trajectories confirm the stability results obtained above.
Figure 5.7: Trajectories of the lattice–Boltzmann equation (5.13) (cf. p. 93) for reaction parameters $p_c = p_d = 0.5$ (left), $p_c = 0.9, p_d = 0.1$ (right) and different initial conditions $(f_A(0), f_f(0)) \in \{(0.5, 0.1), (0.1, 0.9)\}$; solid lines refer to Eqn. (5.15), dashed lines refer to Eqn. (5.16), stationary points $(\tilde{f}_A, \tilde{f}_f)$ are $P_1 = (0, 0), P_2 = (a_1, a_2), P_3 = (1, 1)$. 
5.1.4 Pattern formation in one dimension: Analysis and simulations

Since we are interested in explaining the formation of diffusion-induced spatial structures, we investigate the case of spatially heterogeneous fluctuations, i.e., \( q \neq 0 \), for the stationary solution \((a_1, a_2)\), only. Furthermore, primary attention will be given to studying the case \( p_c = p_d = 1 \), and therefore \((a_1, a_2) = (0.5, 0.5)\), because of its ‘better’ analytical tractability. Recall that a significant difference in the diffusion coefficients of a two-component system is a necessary condition for the evolution of Turing patterns (cf. 2. Turing condition, p. 87). In our LGCA model the ‘diffusion coefficients’ of species \( A \) and \( I \) are functions of only the parameters \( m_A \) and \( m_I \). When \( m_A = m_I \), then both components ‘diffuse’ within the same range. When \( m_A < m_I \), then the ‘diffusion coefficient’ of species \( A \) is greater than that of species \( I \), and vice versa.

General comments on simulations All simulations are performed on a periodic lattice with \( L \) nodes and with different random seedings of the initial state such that a channel \((r, c_i)\) is occupied with probability \( P(\eta_{r,i}(r,0) = 1) = 0.5 \), if not stated otherwise. Spatially averaged occupation numbers, \( f^*(k) = (f_{A,i}^*, \ldots, f_{I,i}^*) \) with \( f_{\sigma,i}^*(k) := 1/L \sum_{r=0}^{L-1} \eta_{\sigma,i}(r,k) \), are determined from simulations. They show if the system has reached on average the steady state \((\bar{f}_A, \bar{f}_I) = (0.5, 0.5)\). Furthermore, with \( q^* \) we denote wave numbers which are found in simulation plots.

We begin with the case when both species move on their lattice with the same speed, i.e., when \( m_A = m_I \). From Eqn. (5.20) we obtain with \( p_c = p_d = 1 \) that for each wave number \( q \)

\[
\lambda_1(q) = \frac{1}{3} u_A(q) \left( 1 - \frac{5}{8} p \right) \quad \text{and} \quad \lambda_2(q) = \frac{1}{3} u_A(q) \left( 1 - p \right),
\]

where \( u_A(q) = u_I(q) \). Hence, the spectral radius is given by

\[
\mu(q) \equiv |\lambda_1(q)| = \frac{1}{3} |u_A(q)||\left( 1 - \frac{5}{8} p \right)| \leq \frac{1}{3} < 1,
\]

which implies that all modes \( F(q, k) \) are damped, and local fluctuations \( \delta f_{\sigma,i}(r, k) \) decay to zero when time \( k \to \infty \). Consequently, the spatially homogeneous steady state \((\bar{f}_A, \bar{f}_I) = (0.5, 0.5)\) is stable when diffusive transport is present and spatially inhomogeneous structure does not emerge. This coincides with the simulation results shown in Fig. 5.8.

Next we study the effects of unequal diffusion coefficients on the stability of the steady state \((\bar{f}_A, \bar{f}_I) = (0.5, 0.5)\). Linear stability analysis and simulations show that stationary patterns can emerge in both cases, i.e., when \( m_A < m_I \) and \( m_A > m_I \). This is in contrast with the traditional Turing-type pattern formation scenario in which patterns can emerge only in one case of these


Figure 5.8: Evolution of activator concentration in space and time for equal diffusion coefficients; **parameters**: \( m_A = m_I = 1, \ p_c = p_d =: p, \ L = 100, \ k = 0, \ldots, 100. \)

inequalities but not the other. The second Turing condition (cf. p. 87) requires that the diffusion coefficient ratio \( D_b/D_a > 1 \) which means that component \( b \) must diffuse faster than the component \( a \).

**The deterministic case**: \( p_c = p_d =: p = 1 \)

Let us first look at the automaton dynamics when the reactive interactions are **deterministic**, i.e. \( p_c = p_d =: p = 1 \). In this case the Boltzmann propagator (5.19) has only one non-zero eigenvalue, i.e. by Eqn. (5.20)

\[
\lambda_1(q) = \frac{3}{8} u_A(q) - \frac{1}{4} u_I(q) \quad \text{and} \quad \lambda_2(q) = 0, \tag{5.23}
\]

where \( u_{\sigma(q)} = 1 + 2 \cos\left(\frac{2\pi}{L} q m_{\sigma}\right), \ q \in \{0, \ldots, L\}. \)

From this, the sets of critical wave numbers \( Q^+ \) and \( Q^- \) can easily be determined for fixed speed parameters \( m_A \) and \( m_I \). Some examples are shown in Fig. 5.9. Note that since \( \lambda_1(q) \) is a sinusoidal function it is sufficient to consider \( q \in \{0, \ldots, \left\lfloor \frac{L}{2}\right\rfloor\}.^8 \)

Hence, if particles of species \( I \) move faster than those of the species \( A \), i.e., if we choose \( m_I > 2 > m_A = 1 \), then the stationary solution \( \left( \bar{f}_A, \bar{f}_I \right) = (0.5, 0.5) \) becomes unstable for non-zero ‘small’ wave numbers \( q \leq 16 \) if \( L = 100 \) (cf. Fig. 5.9(a)). Moreover, the dominant wave numbers \( q_* \in Q^+ \) are well

\[ ^8 \left\lfloor y \right\rfloor \text{ denotes the smallest integer greater than or equal to } y \in \mathbb{R}. \]
5.1 Activator–inhibitor interaction

(a) $q \in Q^+ : \lambda_1(q) > 1$, $m_A = 1$
(b) $q \in Q^- : \lambda_1(q) < -1$, $m_A = 1$

(c) $q \in Q^+ : \lambda_1(q) > 1$, $m_I = 1$
(d) $q \in Q^- : \lambda_1(q) < -1$, $m_I = 1$

Figure 5.9: Critical wave numbers $q$ for which $\mu(q) \equiv |\lambda_1(q)| > 1$; the dots represent the dominant critical wave numbers $q_*$. Parameters: $L = 100$, $p_c = p_d = p = 1$.

approximated by\(^9\)

$$q_* \approx \left[ \frac{L}{2m_I} \right] \quad \text{for} \quad m_A = 1, m_I > 2,$$

(5.24)

because the derivative of $\lambda_1(q)$ (5.23) with respect to $q$ evaluated at this value is almost zero for sufficient large lattices, i.e.

$$\left. \partial_q \lambda_1(q) \right|_{q = \frac{L}{2m_I}} = -\frac{3\pi}{2L} \sin\left( \frac{\pi}{m_I} \right) = \left( -6\pi^2 m_I + 4\pi^2 m_I^3 \right) \frac{1}{L^3} + \mathcal{O}\left( \frac{1}{L^7} \right).$$

As an example, space–time plots of two automaton simulations are given in Fig. 5.10 for $(m_A, m_I) \in \{(1,4), (1,7)\}$. The wave numbers $q^*$ seen in the plots correspond to the predicted dominant wave numbers $q_*$ shown in Fig. 5.9(a).

\(^9\)[[y]] denotes the integer closest to $y \in \mathbb{R}$.
The wave length of the pattern in the case $(m_A, m_I) = (1, 7)$ gained from linear stability analysis is $L/7 \approx 14.29$, where we assumed $L = 100$. The simulation shown in Fig. 5.10(a) confirms this prediction. The observed wave length is approximatively 15. If we take a different lattice size, i.e. $L = 30$, the selected wave number according to the spectral radius and simulation is $q \approx 2$. Therefore, the wave length of approximately 15 does not change, i.e. it depends on the reaction rates and speed parameters, only. Figure 5.11 shows pattern evolution if there is no influence of the boundaries in the beginning of the simulation. The simulation was started with one single particle in the middle of the domain, i.e. $\eta_{A,1}(50, 0) = 1$ and $\eta_{\sigma,i}(r, 0) = 0$ for all $\sigma \in \{A, I\}, i = 1, 2, 3$ and $r \neq 50$.

Hence, from linear stability analysis ‘Turing-type’ structures are predicted to
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evolve for parameters $m_l > 2 > m_A = 1$ and $p_c = p_d =: p = 1$.

A pattern, in which two spatial wave lengths are simultaneously visible is
exhibited in Fig. 5.4(f) on page 92, where we took $m_A = 3$ and $m_l = 11$. In
this case, $Q^+$ contains wave numbers of very different magnitude, from which
$q_1 = 4$ and $q_2 = 32$ are local extrema of the corresponding eigenvalue $\lambda_1(q)$,
as can be confirmed in Fig. 5.12. Although $q_2 = 32 = q^*$ is the dominant

\[
\lambda_1(q)
\]

![Figure 5.12: Eigenvalue $\lambda_1(q)$ given by Eqn. (5.23) for $m_A = 3, m_l = 11$ and
L = 100.](image)

critical wave number, the mode corresponding to a wave number of $q_1 = 4$ is
also visible.

If we allow species $A$ to move faster than species $I$, i.e. $m_A > m_l$, then
according to linear stability analysis the critical dominant wave numbers are
$q^* \in Q^+$ and of ‘large’ magnitude ($q \geq 30$ if $L = 100$), corresponding to wave
lengths of less than 4, if $L = 100$ (cf. Fig. 5.9(c)). A space-time pattern from
a simulation run is shown in Fig. 5.13.

![Figure 5.13: Evolution of activator concentration in space and time if $m_A >
m_l = 1$; parameters: $m_A = 7, m_l = 1, p_c = p_d =: p$, $L = 100$, $k =
0, \ldots, 100$.](image)
Checkerboard structures

Another type of pattern evolves if the eigenvalue (5.23) has a dominant instability at minus one, i.e. $q_* \in Q^-$. This situation arises for example in the case $(m_A, m_I) = (1, 2)$, where the mode according to wave number $q = L/2$, i.e. wave length 2 if $L = 100$, grows fastest (cf. Fig. 5.9(b)). Since this mode grows with an oscillating sign of period two, a checkerboard-like structure develops, as it is shown in Fig. 5.14.

![Checkerboard structures](image)

(a) $q' = 50$

$f'(100) = (0.5, 0.46, 0.49, 0.5, 0.48, 0.47)$

(b) Checkerboard pattern: magnified small area of the left figure.

Figure 5.14: Evolution of activator concentration in space and time if the instability $\lambda_1(q) < -1$ is dominant, i.e. $q_* \in Q^-$; **parameters**: $m_A = 1, m_I = 2$, $p_c = p_d =: p = 1$, $L = 100$, $k = 0, \ldots, 100$.

Influence of initial conditions

We have demonstrated that the evolving pattern in a simulation has the wave length of the fastest growing mode, i.e. the mode corresponding to the dominant wave number $q_*$. But this is not true in general, since the unstable mode selection also depends on the initial distribution of particles\(^{10}\). In general, any arbitrary random initial distribution consists of many modes superimposed on one another. The decisive role of initial conditions is illustrated in the following, using the parameters $(m_A, m_I) = (1, 4)$, $L = 100$ and $p = 1$. For this parameter set, the dominant critical wave number is $q_* = 12$ (cf. Fig. 5.9(a), p. 101) and $\lambda_1(12) \approx 1.16778$. But, for the wave number $q = 50$, i.e. short wave lengths, which is also critical, we find $\lambda_1(50) = -1.125$. Hence, mode $F(12, k)$ grows only slightly faster than mode $F(50, k)$. Nevertheless, as it is shown in Fig. 5.15 in almost 95% of 500 simulations, started with different

\(^{10}\)as it is the case in continuous reaction–diffusion systems (Murray 1989)
random initial conditions, modes corresponding to high critical wave numbers determine the pattern, finally\textsuperscript{11}. A typical space–time plot for this situation is given in Fig. 5.4(e) on page 92. It can be seen, that the initially growing mode \( F(12, k) \), which leads to stripes, becomes ‘suppressed’ by \( F(50, k) \), which leads to a checkerboard–like pattern.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.4.png}
\caption{Statistics of 500 LGCA simulations: Fraction of simulations with dominant critical wave numbers \( q^* \) at each time step \( k \) starting from different random initial conditions; \textbf{parameters}: \( m_A = 1, m_I = 4, p_c = p_d =: p = 1, L = 100 \) and \( P(\eta_{\sigma,i}(r, 0) = 1) = 0.5 \) for each \( \sigma \in \{A, I\}, i = 1, 2, 3. \)
}
\end{figure}

A different picture arises if we start with a randomly perturbed initial condition which has a wave number of \( q = 12 \). Then, as illustrated in Fig. 5.16, \( F(12, k) \) (stripes) dominates the pattern in almost 96\% of 500 simulation runs.

Effects, as described above, result from an \textbf{interaction} of modes. This can \textbf{not} be captured by a linear theory where it is assumed that perturbations are ‘small’, implying an independent growth or decay of each of the various modes. Perturbations may soon grow so strongly that the simplifying linearisation is

\textsuperscript{11}For Fig. 5.15 simulation data are transformed into Fourier space as \( G(q, k) := \left( \sum_{r=0}^{99} e^{i \phi^r} q^r(r, k) \right)^2 \), where \( q^r \) denotes the mass at each node. At each time step the wave number \( q \neq 0 \) with maximal \( G(q, k) \) is extracted.
no longer appropriate. Hence, in order to take mode interaction processes into account, a nonlinear analysis of the Boltzmann equation (5.13) would have to be carried out. Segel (1984) gives a good introductory overview about the qualitative features of mode–amplitude equations for nonlinear behaviour, devoted to pattern formation in macroscopic reaction–diffusion systems\(^\text{12}\).

The role of fluctuations: \( p_c = p_d =: p < 1 \)

Our objective here is to investigate the case of probabilistic reactive interactions, i.e. \( p_c = p_d =: p < 1 \). The non-trivial eigenvalues (5.20) (p. 95) of the Boltzmann propagator for this parameters are given by Eqn. (B.2.6) in Appendix B.2. All space-time patterns, introduced so far, emerging from growing modes corresponding to critical wave numbers \( q \in Q^+ \cup Q^- \), are conceivable, i.e.

\[
\begin{align*}
q \in Q^+ & \quad \text{and } q \text{ is 'small'} & \text{(stripes, e.g. Fig. 5.4(b), p. 92),} \\
q \in Q^+ & \quad \text{and } q \text{ is 'large'} & \text{(very small narrow stripes, e.g. Fig. 5.4(f), p. 92), and} \\
q \in Q^- & \quad \text{for any magnitude of } q & \text{(checkerboard pattern, e.g. Fig. 5.4(e), p. 92).}
\end{align*}
\]

Although linear stability analysis yields a very good insight into the automaton dynamics, there are situations in which local fluctuations still play an important role. Especially, if the value of the spectral radius is less but close to 1 in automaton simulations, a dominant wave length is present, which contrasts the results of linear stability analysis. We discuss this phenomenon for parameters \((m_A, m_I) = (1, 7)\) and \( L = 100 \). We calculate from Eqn. (B.2.6) (p. 151)

\(^{12}\text{Haken and Olbrich (1978) and Mikhailov (1994) are recommended as well.}\)
the threshold value of the bifurcation parameter $\hat{p}$, for which the spectral radius $\mu(q)$ becomes unstable, i.e.

$$\forall p < \hat{p} : \quad \mu(q)|_p < 1 \quad \forall q \in \{0, \ldots, \left\lfloor \frac{L}{2} \right\rfloor\}$$

and

$$\exists \tilde{q} \in \{0, \ldots, \left\lfloor \frac{L}{2} \right\rfloor\} : \quad \mu(\tilde{q})|_{\hat{p}} = 1 .$$

We find $\hat{p} \approx 0.46593$ and $\tilde{q} = 5$ as indicated in Fig. 5.17.

Figure 5.17: Spectral radius $\mu(q)$ for different values of $p$; the curve in between $p = 0.24$ and $p = 0.25$ belongs to the critical reaction parameter $\hat{p} \approx 0.246593$. **Parameters**: $m_A = 1$, $m_I = 7$ and $L = 100$.

Hence, linear stability analysis predicts that no pattern evolves if $p < \hat{p}$. Simulation results are different! We performed 500 simulation runs with a reactive interaction probability of $p = 0.1 < \hat{p}$ and identical random initial conditions. From this we find that in about 35% of all simulations the mode corresponding to the wave number $q = 3$ is dominating, and in almost 90% of the simulations modes corresponding to one of the wave numbers $q \in \{2, \ldots, 5\}$ determine the pattern. These results are presented in Fig. 5.18.
Figure 5.18: Statistics of 500 LGCA simulations: Fraction of simulations with dominant critical wave numbers $q^*$ at each time step $k$ starting from the same random initial conditions; parameters: $m_A = 1$, $m_I = 7$, $p_c = p_d =: p = 0.1$ and $L = 100$. 
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In comparison, a simulation of the deterministic nonlinear Boltzmann equation (5.13) (cf. p. 93), started with the same initial condition that we chose for the LGCA simulations, shows (cf. Fig. 5.19(a)) that all modes with non-zero wave numbers disappear, i.e. all perturbations vanish. On the other hand, a simulation for a reaction parameter \( p = 0.25 > \hat{p} \) shows the theoretically expected wave number \( q = 5 \) (cf. Figs. 5.17 and 5.19(b)). In this case the dynamics of the nonlinear Boltzmann equation is well captured by linear stability theory.

![Graphs showing evolution of activator mass \( g_A^s(r,k) \) in space and for different times in a simulation of the (deterministic) Boltzmann equation (5.13) (cf. p. 93) with random initial conditions; small dashed line: \( k = 10 \), medium dashed line: \( k = 100 \), solid line: \( k = 1000 \); parameters: \( m_A = 1, m_I = 7, L = 100 \) and \( \hat{p} \approx 0.246593 \).](image)

(a) \( p = 0.1 < \hat{p} \)

The system has reached the spatially homogeneous equilibrium at time \( k = 1000 \).

(b) \( p = 0.25 > \hat{p} \)

The system has reached a spatially inhomogeneous structure with wave number \( q^* = 5 \) at time \( k = 1000 \).

Figure 5.19: Evolution of activator mass \( g_A^s(r,k) \) in space and for different times in a simulation of the (deterministic) Boltzmann equation (5.13) (cf. p. 93) with random initial conditions; small dashed line: \( k = 10 \), medium dashed line: \( k = 100 \), solid line: \( k = 1000 \); parameters: \( m_A = 1, m_I = 7, L = 100 \) and \( \hat{p} \approx 0.246593 \).

Hence, spatial pattern formation in LGCA simulations is supported by microscopic fluctuations which lead to continuous perturbations over a wide range of spatial wave lengths.
5.1.5 Derivation and analysis of a macroscopic description of the LGCA

In this section we show that in appropriate space and time scaling the lattice–Boltzmann equation (5.13) (cf. p. 93) can be reduced to LGCA macroscopic partial differential equations (PDE). In order to derive these equations we assume that the LGCA dynamics takes place on a lattice \( \mathcal{L} = \mathcal{L}_\epsilon \) with periodic boundary conditions, and that \( \mathcal{L}_\epsilon \) has \( |\mathcal{L}_\epsilon| = L = l/\epsilon \) nodes in order to cover the interval \([0,l]\), where \( \epsilon \in \mathbb{R}^+ \) is a small parameter. On each lattice \( \mathcal{L}_\epsilon \) we impose an initial concentration profile of particles as follows. We assume that the initial distribution \( \xi_0 = \xi_{0,\epsilon} \) is a product distribution, such that

\[
E(\eta_{\sigma,i}(r,0)) = g_{\sigma,i}(\epsilon r), \quad \sigma \in \{A,I\}, \quad i = 1,2,3,
\]

where \( g_{\sigma,i}(x) \) are non-negative periodic smooth functions independent of \( \epsilon \) and bounded by one on the interval \( x \in [0,l] \). Since the microscopic space variable \( r \) has been scaled by \( \epsilon \) to obtain finite velocities in the LGCA model we must also scale time. Hence, the microscopic lattice–node \( r \in \mathcal{L}_\epsilon \) and time \( k \in \mathbb{N} \) correspond to the macroscopic variables \( x \) and \( t \), such that

\[
x = r \epsilon \in [0,l], \quad t = k \delta \in \mathbb{R}^+, \quad \epsilon, \delta \in \mathbb{R}^+.
\]

Additionally, we assume that for each lattice \( \mathcal{L}_\epsilon \) the reaction probabilities \( p_c \) and \( p_d \) scale by \( h(\epsilon, \delta) \). This means that the probability of creation or destruction of particles in a short time interval of duration \( \delta \) in a small space interval of length of order \( \epsilon \) is approximately \( h(\epsilon, \delta) p_c \) and \( h(\epsilon, \delta) p_d \), respectively. Note that \( h(\epsilon, \delta) \) has to be decreasing with the arguments to obtain finite reaction rates in the macroscopic regime. Since the described LGCA model does not represent a discretisation of any macroscopic system, we can choose the relation between \( \delta \) and \( \epsilon \) in a suitable way later on.

Under the discussed scaling the lattice–Boltzmann equation (5.13) (cf. p. 93) become the continuous space– and time–finite difference equations

\[
\begin{align*}
  f_{\sigma,1}(x + m_\sigma \epsilon, t + \delta) - f_{\sigma,1}(x, t) &= h(\epsilon, \delta) \hat{C}_{\sigma,1}(f(x, t)) , \quad (5.25) \\
  f_{\sigma,2}(x - m_\sigma \epsilon, t + \delta) - f_{\sigma,2}(x, t) &= h(\epsilon, \delta) \hat{C}_{\sigma,2}(f(x, t)) , \quad (5.26) \\
  f_{\sigma,3}(x, t + \delta) - f_{\sigma,3}(x, t) &= h(\epsilon, \delta) \hat{C}_{\sigma,3}(f(x, t)) . \quad (5.27)
\end{align*}
\]

The Taylor expansion of Eqns. (5.25), (5.26) and (5.28) in powers of \( \epsilon \) and \( \delta \)

\[13\] The following derivation of the LGCA reaction–diffusion equations follows the lines of the theory described in Deutsch (1999); see also Chopard and Droz (1998)
5.1 Activator–inhibitor interaction

up to second order yields

\[
\begin{align*}
\delta \partial_t f_{\sigma,1} &+ \frac{\delta^2}{2} \partial_{tt} f_{\sigma,1} + m_\sigma \epsilon \partial_x f_{\sigma,1} + \frac{m_\sigma^2 \epsilon^2}{2} \partial_{xx} f_{\sigma,1} + m_\sigma \epsilon \delta \partial_{tx} f_{\sigma,1} \\
& + \mathcal{O}(\delta^2 \epsilon) + \mathcal{O}(\delta \epsilon^2) = h(\epsilon, \delta) \hat{\mathcal{C}}_{\sigma,1}(\mathbf{f}) , \\
\delta \partial_t f_{\sigma,2} &+ \frac{\delta^2}{2} \partial_{tt} f_{\sigma,2} - m_\sigma \epsilon \partial_x f_{\sigma,2} + \frac{m_\sigma^2 \epsilon^2}{2} \partial_{xx} f_{\sigma,2} - m_\sigma \epsilon \delta \partial_{tx} f_{\sigma,2} \\
& + \mathcal{O}(\delta^2 \epsilon) + \mathcal{O}(\delta \epsilon^2) = h(\epsilon, \delta) \hat{\mathcal{C}}_{\sigma,2}(\mathbf{f}) , \\
\delta \partial_t f_{\sigma,3} &+ \frac{\delta^2}{2} \partial_{tt} f_{\sigma,3} + \mathcal{O}(\delta^3) = h(\epsilon, \delta) \hat{\mathcal{C}}_{\sigma,3}(\mathbf{f}) ,
\end{align*}
\]

(5.28)

(5.29)

(5.30)

where \( f_{\sigma,i} = f_{\sigma,i}(x, t) \). Let \( J_{\sigma}(x, t) := m_{\sigma}(f_{\sigma,1}(x, t) - f_{\sigma,2}(x, t)) \) be the flux and \( \varrho_\sigma(x, t) := f_{\sigma,1}(x, t) + f_{\sigma,2}(x, t) + f_{\sigma,3}(x, t) \) be the local mass of particles of component \( \sigma \in \{ A, I \} \), then from Eqns. (5.28–5.30) we get

\[
\begin{align*}
\delta \partial_t \varrho_\sigma + \frac{\delta^2}{2} \partial_{tt} \varrho_\sigma + \epsilon \partial_x J_{\sigma} + \frac{m_\sigma^2 \epsilon^2}{2} \partial_{xx} \varrho_\sigma + \epsilon \delta \partial_{tx} J_{\sigma} \\
+ \mathcal{O}(\delta^2 \epsilon) + \mathcal{O}(\delta \epsilon^2) + \mathcal{O}(\delta^3) = h(\epsilon, \delta) \sum_{i=1}^{3} \hat{\mathcal{C}}_{\sigma,i}(\mathbf{f}) ,
\end{align*}
\]

(5.31)

\[
\frac{\delta}{m_\sigma} \partial_{tx} J_{\sigma} + \frac{\delta^2}{2 m_\sigma} \partial_{tt} J_{\sigma} + m_\sigma \epsilon \partial_x \varrho_\sigma + \frac{m_\sigma^2 \epsilon^2}{2} \partial_{xx} J_{\sigma} + m_\sigma \epsilon \delta \partial_{tx} \varrho_\sigma \\
+ \mathcal{O}(\delta^2 \epsilon) + \mathcal{O}(\delta \epsilon^2) = h(\epsilon, \delta) \left( \partial_t \hat{\mathcal{C}}_{\sigma,1}(\mathbf{f}) - \partial_t \hat{\mathcal{C}}_{\sigma,2}(\mathbf{f}) \right) ,
\]

(5.32)

where we used that \( \partial_x \varrho_\sigma = \partial_x (f_{\sigma,1} + f_{\sigma,2}) + \partial_x f_{\sigma,3} = \partial_x (f_{\sigma,1} + f_{\sigma,2}) \). Solving Eqn. (5.32) for \( \partial_{tx} J_{\sigma} \) and substituting into Eqn. (5.31) yields after rearranging terms

\[
\partial_t \varrho_\sigma = \frac{h(\epsilon, \delta)}{\delta} \sum_{i=1}^{3} \hat{\mathcal{C}}_{\sigma,i}(\mathbf{f}) + \frac{m_\sigma^2 \epsilon^2}{2 \delta} \partial_{xx} \varrho_\sigma \\
- \frac{h(\epsilon, \delta)}{\delta} m_\sigma \epsilon \left( \partial_t \hat{\mathcal{C}}_{\sigma,1}(\mathbf{f}) - \partial_t \hat{\mathcal{C}}_{\sigma,2}(\mathbf{f}) \right) - \frac{\delta}{2} \partial_{tt} \varrho_\sigma \\
- \frac{\epsilon}{\delta} \partial_x J_{\sigma} + \frac{m_\sigma^2 \epsilon^3}{2 \delta} \partial_{xx} J_{\sigma} + m_\sigma^2 \epsilon^2 \partial_{tx} \varrho_\sigma \\
- \mathcal{O}(\delta^2 \epsilon) - \mathcal{O}(\delta \epsilon^2) - \mathcal{O}(\delta^3) + \mathcal{O}(\delta^2 \epsilon^2) + \mathcal{O}(\delta \epsilon^3) .
\]

(5.33)

Hence, in the ‘diffusion limit’, i.e. if

\[
\delta \to 0, \epsilon \to 0 \quad \text{and} \quad \lim_{\delta \to 0} \frac{\epsilon^2}{\delta} = \text{const} := a ,
\]
and with appropriate scalings of the reaction rates, e.g.

\[ h(\epsilon, \delta) = \hat{a} \delta, \quad \hat{a} \in \mathbb{R}^+ , \]

Eqn. (5.33) reduces to

\[ \partial_t \rho_\sigma(x,t) = \hat{a} \sum_{i=1}^{3} \tilde{C}_{\sigma,i}(f(x,t)) + D_\sigma \partial_{xx} \rho_\sigma(x,t) , \quad (5.34) \]

where

\[ D_\sigma := \lim_{\delta \to \delta} \frac{m_\sigma^2 \epsilon^2}{2 \delta} = \frac{1}{2} a m_\sigma^2 \]

is the diffusion coefficient of species \( \sigma \in \{A, I\} \). Since the LGCA dynamics does not emphasize any particular direction, we assume that the number of particles moving to the left, right or rest are equal, i.e. \( f_{\sigma,i}(x,t) = \rho_\sigma(x,t)/3, \quad i = 1, 2, 3 \). Then, the reaction part of Eqn. (5.34) becomes\(^{14}\)

\[ \hat{a} \sum_{i=1}^{3} \tilde{C}_{\sigma,i}(f) = 3 \hat{a} \left( 1 - \frac{\rho_A}{3} \right) \frac{\rho_A}{3} \left( 1 - \frac{\rho_I}{3} \right)^2 \left( 2 \left( 1 - \frac{\rho_I}{3} \right) \right) - \frac{\rho_A}{3} \left( 1 - \frac{\rho_I}{3} \right) p_c \]

\[ - \left( \frac{\rho_I}{3} \right)^2 \left( 3 \left( 1 - \frac{\rho_A}{3} \right) - 2 \frac{\rho_I}{3} \left( 1 - 2 \frac{\rho_A}{3} \right) \right) p_d \]

\[ =: H_A (\rho_A, \rho_I) \]

and

\[ \hat{a} \sum_{i=1}^{3} \tilde{C}_{I,i}(f) = \hat{a} \left( 1 - \frac{\rho_I}{3} \right) \rho_A \left( 3 \left( 1 - \frac{\rho_I}{3} \right)^2 - \rho_A \left( 1 - \frac{\rho_I}{3} \right) + \frac{\rho_I}{3} \right) \]

\[ + \left( \frac{\rho_A}{3} \right)^2 \left( 1 - 2 \rho_I + 2 \frac{\rho_I}{3} \right) p_c - \hat{a} \left( 1 - \frac{\rho_A}{3} \right) \rho_I \]

\[ \left( 1 + \frac{\rho_A}{3} \left( 2 \rho_I - 2 \frac{\rho_I}{3} \right) + \left( \frac{\rho_A}{3} \right)^2 \left( 1 - 2 \rho_I + 2 \frac{\rho_I}{3} \right) \right) p_d \]

\[ := H_I (\rho_A, \rho_I) , \]

where \( \rho_\sigma = \rho_\sigma(x,t) \).

Hence, we obtain the following system of LGCA reaction–diffusion equations

\(^{14}\)cf. Eqns. (B.1.2) and (B.1.3) in Appendix B.1
5.1 Activator–inhibitor interaction

\[
\begin{align*}
\partial_t q_A(x, t) &= H_A(q_A(x, t), q_I(x, t)) + D_A \partial_{xx} q_A(x, t), \\
\partial_t q_I(x, t) &= H_I(q_A(x, t), q_I(x, t)) + D_I \partial_{xx} q_I(x, t),
\end{align*}
\] (5.37)

where \( q_A(x, t), q_I(x, t) \in [0, 3] \) for all \( x \in [0, l] \) and \( t \in \mathbb{R}^+ \).

Recall that a continuous reaction–diffusion system exhibits diffusion–driven instability if a homogeneous steady state is stable to small spatially homogeneous perturbations in the absence of diffusion but becomes unstable to small spatial perturbations when diffusion is present (cf. Subsec. 5.1.2, p. 86).

Next, we investigate if Turing pattern can be observed in LGCA macroscopic Eqn. (5.37). Again, for the sake of simplicity in the mathematical derivations, primary attention will be given to the special case of reaction parameters

\[ p_c = p_d =: p \in [0, 1]. \]

Following the steps given in Subsec. 5.1.2 (cf. p. 87), first we determine the stability of spatially uniform stationary states \((\bar{q}_A, \bar{q}_I)\), given by

\[
H_A(q_A, q_I) = 0 \quad \land \quad H_I(q_A, q_I) = 0
\]

\[
\implies (\bar{q}_A, \bar{q}_I) \in \left\{(0, 0), \left(\frac{3}{2}, \frac{3}{2}\right), (3, 3)\right\}.
\]

The Jacobian matrix evaluated at the nontrivial steady state \((\bar{q}_A, \bar{q}_I) = \left(\frac{3}{2}, \frac{3}{2}\right)\) becomes

\[
J = \begin{pmatrix}
\partial_A H_A & \partial_I H_A \\
\partial_A H_I & \partial_I H_I
\end{pmatrix}
\]

\[
= \hat{\alpha} p \begin{pmatrix}
\frac{1}{8} & -\frac{3}{4} \\
\frac{9}{8} & -\frac{7}{4}
\end{pmatrix}, \quad \hat{\alpha}, p > 0,
\] (5.38)

where \( \partial_{\sigma} H_{A/I} \) denotes the partial derivative of \( H_{A/I} \) with respect to \( \sigma \). Hence, according to the signs of \( J \), the system (5.37) can be identified as a ‘real activator–inhibitor model’ (cf. (5.3), p. 87) and therefore \((\bar{q}_A, \bar{q}_I) = \left(\frac{3}{2}, \frac{3}{2}\right)\) is stable with respect to spatially homogeneous perturbations.

Next, we determine the critical diffusion ratio \( D^c \) given by Eqn. (5.4) (cf. p. 88)

\[
\frac{D_I}{D_A} > D^c \coloneqq \frac{\left| \det J - \partial_I H_A \partial_A H_I \right| + 2\sqrt{\partial_I H_A \partial_A H_I \det J}}{\left(\partial_A H_A\right)^2}
\] (5.39)

\[
\approx 186.952,
\]

where \( \det J : = \partial_A H_A \partial_I H_I - \partial_I H_A \partial_A H_I \), and the dominant critical wave number \( q^* \) which is given by (cf. Eqn. (5.6), p. 88) is

\[
q^* = \frac{l}{2\pi \hat{q}^*} = \frac{l}{2\pi} \sqrt{\frac{0.625 \hat{\alpha}^2 p^2}{D_A D_I}}.
\] (5.40)
Therefore, only if the diffusion ratio $D_l/D_A$ is larger than $D^c$, it is possible to destabilize the system (5.37) and we can find (a finite range) of wave numbers which are linearly unstable. Depending on the size $l$ of the spatial domain, the allowable discrete wave numbers $q_*$ can be determined. In the example illustrated in Fig. 5.20 only one mode becomes unstable, i.e. the mode corresponding to the wave number $q_* = 3$.

![Graph](image)

Figure 5.20: Plot of the largest root $\lambda$ of the dispersion relation (5.5) (cf. p. 88) for the LGCA reaction–diffusion system (5.37); parameters: $p = 1, \hat{a} = 0.5, D_A = 0.25, D_l = 56.25$ and $l = 58.058$.

**Comparison of lattice–Boltzmann and PDE LGCA systems**

As demonstrated in Subsec. 5.1.4 (cf. p. 100), the LGCA lattice–Boltzmann model exhibits Turing-type patterns for $m_l > 2 > m_A = 1$. Hence, with $m_A = 1$ we get

$$D_A = \frac{1}{2} a, \quad \text{and} \quad D_l = \frac{1}{2} a m_l^2 = D_A m_l^2,$$

and the inequality for the ratio of diffusion coefficients (5.39) becomes

$$m_l^2 > 186.952 \quad \Rightarrow \quad m_l > 13.673\ldots.$$

An expression for the dominant critical wave number $q_*$ (Eqn. (5.40)) in terms of the speed parameter $m_l$ is obtained as

$$q_* = \frac{l}{2 \pi} \sqrt{\frac{2.5 \hat{a}^2 p^2}{a^2 m_l^2}} = \epsilon \frac{L}{2 \pi} \sqrt{\frac{2.5 \hat{a}^2 p^2}{a^2 m_l^2}}. \quad (5.41)$$

Therefore, with the parameters $p$, $m_l$ and $L$ we can compute the dominant critical wave number $q_*$ of the LGCA lattice–Boltzmann equation (cf. Eqn. (5.20), p. 95). Then, given the reactive scaling $\hat{a}$, expression (5.41) determines the corresponding space-scaling for the macroscopic reaction–diffusion system (5.37) in terms of $\epsilon$, or in turn, fixing the macroscopic system length $l$ the reactive scaling $\hat{a}$ can be specified.
Example: As an example we choose the following parameters

\[ p = 1, \ m_A = 1, m_I = 15, \ L = 100, \ a = \lim_{\varepsilon \to 0} \frac{\varepsilon^2}{\delta} = 0.5, \ \hat{a} = 0.5 \]

and get

\[ D_A = 0.25, \ D_I = 56.25, \quad \frac{D_I}{D_A} = 225 > 186.952 = D^c. \]

From Fig. 5.9(a) (cf. p. 101) we obtain the dominant critical wave number of the LGCA lattice–Boltzmann system as

\[ q_* = 3, \]

and therefore this system corresponds to the continuous reaction–diffusion system (5.37) (cf. p. 113) with a system length of

\[ l = q_* 2\pi \sqrt{\frac{a^2 m_I^2}{2.5 \hat{a}^2 p^2}} \approx 58.058 \]

and a spatial and temporal scaling of

\[ \varepsilon = \frac{l}{L} \approx 0.581, \quad \delta \approx \frac{\varepsilon^2}{\hat{a}} \approx 0.674. \]

The largest root of the dispersion relation for this example is shown in Fig. 5.20. Furthermore, Fig. 5.21 illustrates the numerical solution\(^{15}\) of the continuous reaction–diffusion system (5.37) (cf. p. 113) with a system length of \( l = 58.058 \) started from random initial conditions. The emerging wave length of \( q^* = 3 \) is consistent with our theoretical expectations.

In summary, Turing instabilities of the continuous LGCA reaction–diffusion system (5.37) can occur if the diffusion coefficients fulfill the inequality (5.39). If the system is viewed as an approximation of the LGCA lattice–Boltzmann model (cf. Eqn. (5.13), p. 93), then Turing instabilities are possible for the speed parameters \( m_I \geq 14 \) if \( m_A = 1 \), and hence for the corresponding diffusion coefficients \( D_A = 1/2 a \) and \( D_I = D_A m_I^2 \). In contrast, the LGCA lattice–Boltzmann model shows Turing pattern already for speed parameters \( m_I \geq 3 \) if \( m_A = 1 \). Furthermore, we derived an appropriate spatial and temporal scaling relation between both models in the ‘Turing regime’, i.e. for \( m_I \geq 14 \).

\(^{15}\)The C-program for the numerical solution of system (5.37) (cf. p. 113) has been kindly provided by the students N. Graf, U. Krause and C. Meyer, University of Osnabrück.
model. In particular, the spectrum of the reaction–diffusion model comprises always at most one group of unstable modes, because it is determined by the parabolic dispersion relation (cf. Eqn. (5.5), p. 88). Contrary, the spectrum of the lattice–Boltzmann model may involve many different groups of unstable modes (cf. Fig. 5.9, p. 101), depending mainly on the speed parameters \( m_A \) and \( m_I \). This results from the imposed particle–motion process, which leads to a spectral radius dependence on sums and products of waves with different frequencies (cf. Eqn. (5.20), p. 95).

### 5.1.6 Pattern formation in two dimensions

Our objective here is to investigate Turing pattern formation in two spatial dimensions. What kind of patterns do evolve, and which influence does the lattice geometry have on pattern formation? In this section, we give answers to these questions for the LGCA activator–inhibitor model - with the help of linear stability analysis. Since the mathematical procedure for the derivation of the microscopic LGCA description, the corresponding lattice–Boltzmann equation and of the linear stability analysis is very similar to the one–dimensional case, we do not go into details here.

It is straightforward to extend the activator–inhibitor interaction LGCA model defined in Subsec. 5.1.3 (cf. p. 88) to two–dimensional lattices: The nearest neighbourhood template \( \mathcal{N}_b \) for the \textbf{square lattice} \( (b = 4) \) is given by

\[
\mathcal{N}_4 = \{(1,0), (0,1), (-1,0), (0,-1)\}
\]
and for the \textbf{hexagonal lattice} \((b = 6)\)

\[
\mathcal{N}_b = \left\{(1,0), \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right), (-1,0), \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right), \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)\right\}.
\]

For both systems we introduce one rest particle, i.e. \(\beta = 1\). Hence, particles \(X_\sigma\) of each species \(\sigma \in \{A, I\}\) are distributed in different velocity channels \((r, c_i)\) as illustrated in Fig. 5.22, where

\[c_i \in \mathcal{N}_b, \quad i = 1, \ldots, b\] and \(c_b = (0,0), \tilde{b} = b + 1\).

Then, the node configuration \(\eta(r,k)\) at node \(r = (r_1, r_2) \in \mathcal{L}\) will be described as

\[
\eta(r,k) = (\eta_{A,1}(r,k), \ldots, \eta_{A,b}(r,k), \eta_{I,1}(r,k), \ldots, \eta_{I,\tilde{b}}(r,k)) = (\eta_A(r,k), \eta_I(r,k)) \in \{0,1\}^{2\tilde{b}}.
\]

(a) square lattice \((b = 4)\)
\[
\eta_\sigma(r,k) = (1,0,1,0,0)
\]

(b) hexagonal lattice \((b = 6)\)
\[
\eta_\sigma(r,k) = (1,0,1,0,0,1)
\]

Figure 5.22: Channels of node \(r\) in two-dimensional lattices with one rest channel; grey-filled circles denote the presence of a particle \(X_\sigma\) in that channel.

We assume that \(|\mathcal{L}| = L_1 \cdot L_2 = L^2\). With an interaction neighbourhood of \(\mathcal{N}_b'(r) = \{r\}\) and reaction parameters \(p_c\) and \(p_d\) defined as in Eqn. (5.7) (cf. p. 90) we obtain the following reactive interaction rule\(^{16}\) \((R)\)

\[
\begin{array}{l}
\tilde{b}
\end{array}
\begin{array}{c}
\text{with prob. } p_c \text{ if } n_A(r,k) > n_I(r,k) \geq 0
\end{array}
\begin{array}{c}
\text{with prob. } p_d \text{ if } 0 \leq n_A(r,k) < n_I(r,k)
\end{array}
\begin{array}{c}
\text{otherwise}
\end{array}
\]

\[
n_\sigma^b(r,k) = \begin{cases} 
\tilde{b} & \text{with prob. } p_c \text{ if } n_A(r,k) > n_I(r,k) \geq 0 \\
0 & \text{with prob. } p_d \text{ if } 0 \leq n_A(r,k) < n_I(r,k) \\
n_\sigma(r,k) & \text{otherwise}
\end{cases}
\]

\(^{16}\text{Note that the formulation and interpretation of this rule corresponds to the reactive interaction rule defined in (5.8) on page 90.}\)
for each $\sigma \in \{A, I\}$, where the number of particles $X_\sigma$ at node $r$ at time $k$ is given by

$$n_\sigma(r, k) = \sum_{i=1}^{b} \eta_{\sigma,i}(r, k).$$

The microdynamical description for the two-dimensional LGCA models and the derivation of the lattice–Boltzmann equation follow along the lines of Subsec. 5.1.3 (cf. p. 88). Then, the lattice–Boltzmann equation is given by an equation of the form

$$f_{\sigma,i}(r + m_\sigma e_i, k + 1) - f_{\sigma,i}(r, k) = \frac{1}{b} \sum_{l=1}^{b} E(\eta_{\sigma,l}(r, k)) - f_{\sigma,i}(r, k) = \hat{C}_{\sigma,i}(f(r, k)), \quad (5.43)$$

where

$$f(r, k) = (f_{A,1}(r, k), \ldots, f_{A,b}(r, k), f_{I,1}(r, k), \ldots, f_{I,b}(r, k)) = (f_j(r, k))_{j=1}^{2b} \in [0,1]^{2b}.$$  

For both systems, we find that the spatially uniform steady states $(\bar{f}_A, \bar{f}_I)$, which are solutions of $\hat{C}_{\sigma,i}(f(r, k)) = 0$, are given by

$$(\bar{f}_A, \bar{f}_I) = \{(0,0), (a_1,a_2), (1,1)\}, \quad (5.44)$$

where $(a_1, a_2)$ depends on the model and reaction parameters, and will be determined later on. As in the one-dimensional case, the stationary states $(0,0)$ and $(1,1)$ are unstable and $(a_1, a_2)$ is stable with respect to spatially homogeneous perturbations. As a result of the linearisation of Eqn. (5.43) around $(\bar{f}_A, \bar{f}_I) = (a_1, a_2)$ and Fourier transformation we obtain the Boltzmann propagator (2.31) (cf. p. 42)

$$\Gamma(q) = T \{I + \Omega^0\}, \quad q = (q_1, q_2) \quad \text{with} \quad q_1, q_2 = 0, \ldots, L - 1, \quad (5.45)$$

where

$$T = diag(e^{-i\frac{2\pi}{L}(c_1 \cdot q)} m_A, \ldots, e^{-i\frac{2\pi}{L}(c_\ell \cdot q)} m_A, e^{-i\frac{2\pi}{L}(c_1 \cdot q)} m_I, \ldots, e^{-i\frac{2\pi}{L}(c_\ell \cdot q)} m_I)$$
and\textsuperscript{17} \[ I + \Omega^0 = \begin{pmatrix} \omega_1 & \ldots & \omega_1 & \omega_2 & \ldots & \omega_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \omega_1 & \ldots & \omega_1 & \omega_2 & \ldots & \omega_2 \\ \omega_2 & \ldots & \omega_2 & \omega_3 & \ldots & \omega_3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \omega_2 & \ldots & \omega_2 & \omega_3 & \ldots & \omega_3 \end{pmatrix} \in \mathbb{R}^{2\tilde{b} \times 2\tilde{b}}. \]

The spectrum of the Boltzmann propagator (5.45) is given by \[ \Lambda_{\Gamma(q)} = \{ \lambda_1(q), \lambda_2(q), 0 \} , \]
where 0 has a multiplicity of $2\tilde{b} - 2$ and

\[ \lambda_{1,2}(q) = \frac{1}{2} \left( \omega_1 u_A(q) + \omega_4 u_I(q) + \sqrt{4(\omega_2 \omega_3 - \omega_1 \omega_4) u_A(q) u_I(q) + (\omega_1 u_A(q) + \omega_4 u_I(q))^2} \right) \] \quad (5.46)

with \[ u_\sigma(q) := 1 + \sum_{j=1}^{\tilde{b}} e^{-\frac{2\pi}{(c_j q)} m_\sigma}, \quad \sigma \in \{A, I\}, \quad q = (q_1, q_2) \text{ and } q_1, q_2 = 0, \ldots, L - 1. \]

For both models, $\Gamma(q)$ is diagonalisable and therefore the temporal growth of modes $F_{\sigma,i}(q,k)$ is solely determined by the dominant eigenvalue.

In two-dimensional systems, groups of unstable modes with identical absolute value of the wave number $|q| = q$ simultaneously start to grow. Therefore, according to linear theory, any superposition of these modes determines the dynamics of the system\textsuperscript{18} i.e. according to Eqn. 2.37 (p. 43)

\[ \delta f_{\sigma,i}(r,k) \sim \sum_{q \in Q^c} e^{-\frac{2\pi}{q} r} F_{\sigma,i}(q,k) , \] \quad (5.47)

where $Q^c$ is the set of critical wave numbers.

The following analysis will be restricted to two sets of reaction parameters:

(i) $p_c = p_d = 1$ and (ii) $p_c = 0.9$, $p_d = 0.1$.

With these reaction parameters ‘typical patterns’ evolving from the LGCA dynamics are captured. Furthermore, we take $m_A = 1$, $m_I = 11$ and $L_1 = L_2 = L = 100$.

\textsuperscript{17} The matrix elements $\omega_i$, $i = 1, \ldots, 4$, are different terms for the square and hexagonal lattice model depending on the reaction parameters.

\textsuperscript{18} For further reading see Mikhailov (1994)
Many interacting and moving components

The square lattice model

The stationary states \((\vec{f}_A, \vec{f}_I) = (a_1, a_2)\) of our LGCA model on a square lattice are given by

(i) \(p_c = p_d = 1\) : \[a_1 = a_2 = 0.5 \quad \text{and} \quad a_1 = a_2 \approx 0.473, \quad a_2 \approx 0.727, \]

and the corresponding dominant eigenvalues \(\lambda_1\) (cf. Eqn. (5.46), p. 119) are shown in Fig. 5.23. In order to stress the instability–dependence on the wave number magnitude (cf. Eqn. (5.47)), the wave numbers are represented in polar coordinate form in Figs. 5.23(a) and 5.23(c), i.e.

\[ q = (q_1, q_2) \quad \text{with} \quad q_1 = |q| \cos(\phi), \quad q_2 = |q| \sin(\phi). \]

In the first case (i), very distinguished collections of critical wave numbers according to various directions \(\phi\) exist (cf. Fig. 5.23(a)). The spectral radius \(\mu(q) = |\lambda_1([q], \phi)|\) is maximal for wave numbers associated with the diagonal directions, i.e. \(\phi_d \in \{45^\circ, 135^\circ\}\), and a magnitude of \(|q| \approx 6.36\). Figure 5.23(b) shows that discrete wave numbers \((q_1, q_2)\) of the fastest growing modes are \(q_* \in \{(4, 5), (5, 4)\}\). Consequently, linear stability analysis predicts a spatial pattern with these wave numbers \(q_*\) and strong anisotropies in diagonal directions. This result is in good agreement with LGCA simulations. Fig. 5.24(a) (p. 122) shows two snapshots of the spatial distribution of activator concentration after 100 time steps. Both simulations were prepared in a spatially uniform initial state at \(k = 0\). Note that the dominant eigenvalue \(\lambda_1\) has also instabilities at \(-1\), i.e. \(Q^- \neq \emptyset\), which explains the existence of local areas of checkerboard patterns in Fig. 5.24(a).

In the second case (ii), as displayed in Fig. 5.23(c), instabilities of \(\lambda_1\) are of much smaller magnitude than in case (i). Furthermore, the patches of critical wave numbers are less distinguished. Dominant critical wave numbers, which refer to the maximal spectral radius \(\mu(q) = |\lambda_1([q], \phi)|\), have a magnitude of \(|q| \approx 5.57\). As can be seen in Fig. 5.23(d) this corresponds to a discrete wave number of \(q_* = (4, 4)\). Hence, as in case (i), modes associated to diagonal directions grow fastest but, in contrast to case (i), the growth is very slow. Furthermore, since the maximum of the spectral radius is not very distinctive, modes corresponding to other wave numbers, e.g. \((2, 5), (3, 5), (5, 2), (5, 3)\) (cf. Fig. 5.23(d)), might appear. But again, the emerging pattern is characterised by a superposition of modes referring to both diagonal directions, as it is shown in Fig. 5.24(b).
5.1 Activator–inhibitor interaction

Figure 5.23: Dominant Eigenvalue $\lambda_1$ (cf. Eqn. (5.46), p. 119) for the square lattice dependent on the wave number $q = (q_1, q_2)$, which is represented in polar coordinate form in (a) and (c); dots in (b) and (d) represent wave numbers $q$, whose magnitude is close to the line. Parameters: $m_A = 1$, $m_I = 11$ and $L_1 = L_2 = L = 100$. 
(a) Two simulations with reaction parameters $p_c = p_d = 1$

(b) Two simulations with reaction parameters $p_c = 0.9, p_d = 0.1$

Figure 5.24: Four simulations: Activator concentration in a two-dimensional **square lattice** after $k = 100$ time steps started from different random initial conditions where $P(\eta_{A,i}(r, k) = 1) = \tilde{f}_A = a_1, P(\eta_{I,i}(r, k) = 1) = \tilde{f}_I = a_2$ for each direction $e_i$; **parameters:** $m_A = 1, m_I = 11, L_1 = L_2 = L = 100$. 
The hexagonal lattice model

The stationary states \((\tilde{f}_A, \tilde{f}_I) = (a_1, a_2)\) for a hexagonal lattice are given by

(i) \(p_c = p_d = 1: \quad a_1 = a_2 = 0.5 \quad \text{and} \quad a_1 \approx 0.505, \ a_2 \approx 0.721\),

and the corresponding dominant eigenvalues \(\lambda_1\) (cf. Eqn. (5.46), p. 119) are shown in Fig. 5.25, where the wave numbers are represented in polar coordinate form in Figs. 5.25(a) and 5.25(c).

**Case (i):** The dominant eigenvalue \(\lambda_1\) for the hexagonal lattice (cf. Figs. 5.25(a,b)), has less isolated patches of critical wave numbers than the corresponding eigenvalue for the square lattice (cf. Fig. 5.23(a,b)). Furthermore, the dominant critical wave numbers are associated with directions \(\phi \in \{0^\circ, 60^\circ, 120^\circ, 180^\circ\}\), rather than with diagonal directions. Hence, the spatial pattern is characterised by a superposition of stripes with \(\phi\) directions. An example of this type of pattern is shown in Fig. 5.26(a) (p. 125).

**Case (ii):** From Fig. 5.25(c) it can be seen that the dominant eigenvalue \(\lambda_1\) is nearly isotropic, i.e. \(\lambda_1(\phi, |q|)\) is equal–valued for all directions \(\phi\) associated with the maximal value \(|q| \approx 5.26 =: q\). Hence, all modes related to wave numbers with \(|q| = q\) start to grow simultaneously (cf. Eqn. (5.47), p. 119). As they grow, nonlinear terms neglected during linearisation of the lattice–Boltzmann equations may become important. Then, groups of modes may enhance or suppress the development of themselves and/or other groups. In continuous systems, this process is studied by a nonlinear evolution equation for the amplitudes of unstable modes (Mikhailov 1994). It turns out that a group of three modes \(q^0, q^1\) and \(q^2\) with equal magnitude and whose vectors of wave numbers form an equilateral triangle (cf. Fig. 5.27(a)), i.e.

\[
q^j = (q_1^j, q_2^j) = q \left( \cos \left( \phi + j \frac{2\pi}{3} \right), \sin \left( \phi + j \frac{2\pi}{3} \right) \right), \quad j = 0, 1, 2, \tag{5.48}
\]

enhance one another’s growth. The spatial pattern in continuous systems produced by the superposition of these modes is a collection of spots. Since LGCA simulations show similar patterns (cf. Fig. 5.26(b)), we suspect the mutual selfenhancement property of mode groups corresponding to wave numbers characterised by Eqn. (5.48) to be valid also for the discrete lattice–Boltzmann model. In the linear stage, the portion of the solution determined by this group of modes is given by

\[
\delta f_{\sigma,i}(r,k) \sim A_{\sigma,i}(k) \sum_{j=0}^{2} e^{-1} \frac{2\pi}{3} q^j \cdot r, \tag{5.49}
\]

where we assumed that \(A_{\sigma,i}(k) := F_{\sigma,i}(q^j, k)\) for \(j = 0, 1, 2\). As illustrated in Fig. 5.27(b), the contour line of the real part of the right hand side of Eqn. (5.49) is almost circular.
Figure 5.25: Dominant Eigenvalue $\lambda_1$ (cf. Eqn. (5.46), p. 119) for the hexagonal lattice dependent on the wave number $q = (q_1, q_2)$, which is represented in polar coordinate form in (a) and (c); dots in (b) and (d) represent wave numbers $q$ whose magnitude is close to the line. Parameters: $m_A = 1$, $m_l = 11$ and $L_1 = L_2 = L = 100$. 

(a) $p_c = p_d = 1$

(b) $p_c = p_d = 1$ line: $|q| \approx 5.95$

(c) $p_c = 0.9$, $p_d = 0.1$

(d) $p_c = 0.9$, $p_d = 0.1$ line: $|q| \approx 5.26$
5.1 Activator–inhibitor interaction

Figure 5.26: Two simulations: Activator concentration in a two dimensional hexagonal lattice after $k = 100$ time steps started from different random initial conditions where $P(\eta_A(i, r, k) = 1) = \tilde{f}_A = a_1, P(\eta_I,i(r, k) = 1) = \tilde{f}_I = a_2$ for each direction $c_i$; parameters: $m_A = 1, m_I = 11$ and $L_1 = L_2 = L = 100$.

Figure 5.27: Groups of unstable modes associated with wave numbers which form an equilateral triangle (a) and the induced spatial pattern (b).

In this subsection we showed, that in two–dimensional systems the Turing pattern variety is enlarged. Depending on the reaction parameters $p_c$ and $p_d$ striped or spot–like pattern evolve. We illustrated that the lattice geometry has a strong influence on the evolving pattern, and that this phenomenon is correctly predicted by mean–field analysis. On a square lattice the pattern shows anisotropies in diagonal directions (cf. Fig. 5.24) which are not present on a hexagonal lattice (cf. Fig. 5.26). A similar pattern–dependence on the underlying lattice has been observed and analysed by Bussemaker (1996), who introduced a LGCA model of random walkers that interact through nearest neighbour attraction. On the other hand, a LGCA model of ‘swarming’
(Deutsch 1996, Basseemaker et al. 1997) shows the formation of streets, which are very similar for the square and hexagonal lattice. This type of pattern results from the formation of ‘orientational order’ by the particles. The corresponding spectrum has a maximum at wave number $q = (0,0)$ which prevents spatial anisotropies to manifest as strongly as in LGCA models with non-zero maxima indicating spatial frequencies in the patterns (Deutsch 1999). A related situation is found for the spectrum of a LGCA model for excitable media which we introduce in the next section (5.2).
5.2 Spirals and excitable media

5.2.1 Introduction

The subject of this subsection is the spatio–temporal dynamics of spiral waves. Spiral waves have been found to be a relevant pattern in a variety of physical, biological and chemical systems. For example, Hassell et al. (1991; see also Comins et al. 1992) introduced a spatial model for host–parasitoid interactions which exhibits formation of spiral waves. Furthermore, plankton population spiral waves have been observed in the ocean on a kilometer scale (Wyatt 1973), and modelled, e.g., by Medvinskii et al. (2000) who used Pascual–Scheffer’s model of phytoplankton–zooplankton interactions with randomly moving fish. The best known examples of chemical systems are the Belousov–Zhabotinsky reaction (Zhabotinsky and Zaikin 1970, Winfree 1972) and the chemical signalling system of the cellular slime mold Dictyostelium discoideum (Newell 1983).

Some of these examples can be represented as ‘excitable’ systems. The concept of excitable media was introduced in 1946 by Wiener and Rosenblueth (1946) in order to explain heart arrhythmias caused by spiral waves. They invented the notations of refractory, excitable and excited states. The defining characteristics of excitable systems are: (i) starting at a stable equilibrium (resting state) a stimulus above a certain threshold generates (ii) a burst of activity (excited state) followed by (iii) a refractory period (recovery state). The behaviour of a typical trajectory in an excitable system is summarised in Fig. 5.28. Due to the activity initiated by a supercritical perturbation travelling excitation waves of various geometries occur, including ring and spiral waves (Winfree 1987). Excitable media can be characterised by a two–component

![Diagram](image)

Figure 5.28: The behaviour of a typical trajectory in an excitable system (Greenberg et al. 1978).
system of nonlinear partial differential equations of the type
\[
\begin{align*}
\partial_a &= \frac{1}{\tau} F(a, b) + D_a \nabla^2 a, \\
\partial_b &= G(a, b) + D_b \nabla^2 b,
\end{align*}
\]
(5.50)
where \(\nabla^2\) is the Laplacian operator and \(D_a\) and \(D_b\) are diffusion coefficients, for which \(D_a \neq 0\) and \(D_b\) may be 0 (Murray 1989). \(\tau\) is a small positive constant (0 < \(\tau\) \ll 1), which determines the different time scales for the faster component \(a\) (‘excitation’ variable) and the slower component \(b\) (‘recovery’ variable) which typically exist in excitable media. While \(G\) can be a monotonic or even linear function, \(F\) has to be a nonlinear function with a sigmoidal shape. The relevant information about the nullclines \(F(a, b) = 0\) and \(G(a, b) = 0\) is summarised in Fig. 5.29. The intersection point \(S\) of the two nullclines defines

![Diagram](image)

**Figure 5.29:** Typical schematic nullclines of excitable kinetics; the rest state \(S\) is excitable for perturbations larger than threshold \(D\) and a trajectory occurs during which \(a\) increases rapidly \((DA)\), causing a slower and temporary increase in \(b\) \((AB)\), followed by a rapid extinction of \(a\) \((BC)\) and a slow decrease of \(b\) back to the rest state \((CS)\).

the steady state which is a unique asymptotically stable resting state of the medium. Small perturbations from this resting state to a value \(a\) to the left of point \(D\) are immediately damped out, but large perturbations to a value \(a\) to the right of point \(D\) trigger a long excursion before returning to the resting state \(S\). The time for \(a\) to change from its value at \(S\) \((B)\) to that of \(A\) \((C)\) is relatively fast compared to the time for a change from \(A\) \((C)\) to \(B\) \((S)\). The diffusive transport in Eqn. (5.50) reinforces and excites (neighbouring) states which are close to the equilibrium.

Cellular automaton models of excitable media attempt to reduce an excitable medium to its simplest possible form as it is shown in Fig. 5.28 (Ermentrout and Edelstein-Keshet 1993). A very ‘simple’ deterministic cellular automaton model with ‘excited’, ‘refractory’ and ‘resting’ states was suggested by Greenberg et al. (1978). In its simplest form, the evolution of the cells in a two-dimensional square lattice is characterised by the following rule: A ‘resting’ cell \((s(r) = 0)\) becomes ‘excited’ \((s(r) = 2)\) if at least one of its neighbours
is 'excited', otherwise it remains 'resting'; an 'excited' cell becomes 'recovering' 
\((s(r) = 1)\) and a 'recovering' cell becomes 'resting' in the next time step, i.e.

\[
s(r, k + 1) = R(s_{N(r)}(k)) = \begin{cases} 
0 & \text{if } s(r, k) = 1 \text{ or } \forall \hat{r} \in \mathcal{N}_4^r(r): s(\hat{r}, k) \neq 2 \\
1 & \text{if } s(r, k) = 2 \\
2 & \text{if } s(r, k) = 0 \land \exists \hat{r} \in \mathcal{N}_4^r(r): s(\hat{r}, k) = 2
\end{cases},
\]

where the interaction neighbourhood template \(\mathcal{N}_4^r\) is taken to be the von Neumann neighbourhood. Figure 5.30 shows the evolution of a spiral wave generated with this rule.

![Evolution of the Greenberg–Hastings cellular automaton](image)

Figure 5.30: Evolution of the Greenberg–Hastings cellular automaton for times 
k = 0, \ldots, 10 in a lattice with 21 x 21 cells; white – resting cell \((s(r) = 0)\),
grey – recovering cell \((s(r) = 1)\), black – excited cell \((s(r) = 2)\).

This approach was extended later on, for example, by Markus and Hess (1990),
Gerhardt et al. (1990) and Fast and Efimov (1991). Problems of these
 discrete models are related to curvature effects\(^{20}\), lack of dispersion\(^{21}\), spatial
 anisotropy and computational complexity. Another type of cellular automaton
 model is derived by a finite-difference approximation of the partial differential
 equation model for excitable media given by Eqn. (5.50) (Weimar et al. 1992).

In the following we introduce a LGCA interaction–diffusion model, based on
 the concept summarised in Fig. 5.28, which exhibits ring and spiral waves in a
two-dimensional space. Snapshots of simulations (cf. Fig. 5.33, p. 132) show
very 'natural' spiral waves. Furthermore, we show that a crucial difference
between our LGCA model and the corresponding lattice–Boltzmann model
exists: although the LGCA model mimics an excitable medium the lattice–
Boltzmann model does not!

---

\(^{19}\) For further reading Kapral et al. (1991) and Schönfisch (1993) are recommended.

\(^{20}\) The propagation speed depends on the curvature of the wavefront.

\(^{21}\) A wavefront lacks dispersion if it can propagate only into resting medium but not into
partially recovered medium.
5.2.2 Definition of the automaton rules

The LGCA consists of three components \( \sigma \in \{A, B, C\} \), of which \( A \) represents an excitation variable which can be excited \( (\eta_{A,i} = 1) \) or unexcited \( (\eta_{A,i} = 0) \), whereas \( B \) and \( C \) are viewed as ‘information carrier’ which control the duration of excitation of \( A \). The system is defined on a two-dimensional square \( (b = 4) \) lattice \( \mathcal{L}_\sigma = \mathcal{L} = \mathcal{L}_1 \times \mathcal{L}_2 \) with \( L_1 = L_2 = L \) nodes in each space direction. Particles \( X_\sigma \) are distributed in four velocity channels \( (r, c_i)_\sigma \), \( i = 1, \ldots, 4 \), and one rest channel \( (r, c_5)_\sigma \), and the interaction–neighbourhood for each species \( \sigma \) is taken as \( \mathcal{N}_{\sigma}^{1}(r) = \{r\} \). Hence, the node configuration becomes

\[
\eta(r, k) = (\eta_A(r, k), \eta_B(r, k), \eta_C(r, k)) \in \{0, 1\}^{15}
\]

with

\[
\eta_{\sigma}(r, k) = (\eta_{\sigma,1}(r, k), \ldots, \eta_{\sigma,5}(r, k)) \quad \sigma \in \{A, B, C\}.
\]

The automaton interaction rule consists of two subrules: a reactive interaction rule \( (R) \) and the local shuffling rule for an isotropic random walk \( (M) \), which we introduced before (cf. Sec. 3.4, p. 57). The reactive interaction rule \( (R) \) specifies the creation or destruction of particles \( X_\sigma \) in each channel \( (r, c_i)_\sigma \) and solely depends on the states in that channel \( (r, c_i)_\sigma \), i.e.

\[
\eta_{\sigma,i}^R(r, k) = R_{\sigma,i}^R(\eta_{A,i}(r, k), \eta_{B,i}(r, k), \eta_{C,i}(r, k)).
\]

Let \( h(\theta, \eta_A) \) be a threshold function with the threshold value \( \theta \in \{0, \ldots, 5\} \) defined as

\[
h(\theta, \eta_A) := \sum_{i=0}^{5} \Psi_i(\eta_A) = \begin{cases} 1 & \text{if } \sum_{i=0}^{5} \eta_{A,i} \geq \theta \smallskip \end{cases},
\]

with the previously defined counting functions \( \Psi_i \) (cf. p. 80). Furthermore, let \( \{\zeta(r, k) : r \in \mathcal{L}, k \in \mathbb{N}\} \) be a sequence of node– and time-independent identically distributed Bernoulli type random variables, such that \( \mathbb{P}(\zeta(r, k) = 1) = 1/2 \). Then, the interaction rule is described by the following equations

\[
\begin{align*}
R_{A,i}^R &= \eta_{A,i} + \bar{\eta}_{A,i} \bar{\eta}_{B,i} \bar{\eta}_{C,i} h(\theta_1, \eta_A) + \bar{\eta}_{A,i} (\eta_{B,i} \bar{\eta}_{C,i} + \bar{\eta}_{B,i} \eta_{C,i}) h(\theta_3, \eta_A) \\
&\quad - \eta_{A,i} \eta_{B,i} \eta_{C,i} - \eta_{A,i} (\eta_{B,i} \bar{\eta}_{C,i} + \bar{\eta}_{B,i} \eta_{C,i}) h(\theta_2, 1 - \eta_A),
\end{align*}
\]

\[
\begin{align*}
R_{B,i}^R &= \eta_{B,i} + \zeta \bar{\eta}_{B,i} \bar{\eta}_{A,i} \bar{\eta}_{C,i} - \eta_{B,i} \eta_{A,i} \eta_{C,i} (1 - h(\theta_2, 1 - \eta_A)) \\
&\quad - \zeta \bar{\eta}_{B,i} \bar{\eta}_{A,i} \bar{\eta}_{C,i} - \eta_{B,i} \bar{\eta}_{A,i} \bar{\eta}_{C,i} (1 - h(\theta_3, \eta_A)),
\end{align*}
\]

\[
\begin{align*}
R_{C,i}^R &= \eta_{C,i} + \zeta \bar{\eta}_{C,i} \bar{\eta}_{A,i} \bar{\eta}_{B,i} + \bar{\eta}_{C,i} \eta_{A,i} \eta_{B,i} (1 - h(\theta_2, 1 - \eta_A)) \\
&\quad - \zeta \bar{\eta}_{C,i} \bar{\eta}_{A,i} \eta_{B,i} - \eta_{C,i} \bar{\eta}_{A,i} \bar{\eta}_{B,i} (1 - h(\theta_3, \eta_A)),
\end{align*}
\]

where we dropped the node and time dependence and used the shortcuts \( \bar{\eta}_{\sigma,i} := (1 - \eta_{\sigma,i}) \) and \( 1 - \eta_A = (1 - \eta_{A,1}, \ldots, 1 - \eta_{A,5}) \). The threshold values \( \theta_1 \) and \( \theta_3 \) define the minimum number of particles of species \( A \) at node
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$r$, which are necessary to activate ($\eta_{A,i} = 1$) new $X_A$ particles; $\theta_2$ gives the minimum number of deactivated ($\eta_{A,i} = 0$) $X_A$ particles on the node which is needed to deactivate an activated $X_A$ particle. These rules are summarised in Fig. 5.31. Note that the reactive interaction rule $R$ is symmetrical with respect to the components $B$ and $C$.

\[ [\eta_{A,i} \mid \eta_{B,i} \mid \eta_{C,i}] = [0 \mid 0 \mid 0] \quad h(\theta_1, \eta_A) \quad [1 \mid 0 \mid 0] \]

Figure 5.31: Schematic representation of the reactive interaction rule $R$ with threshold variables $\theta_1, \theta_2$ and $\theta_3$. The sequences represent all possible configurations of \([ \eta_{A,i}(r,k) \mid \eta_{B,i}(r,k) \mid \eta_{C,i}(r,k) \]). For instance, a transition from \([1 \mid 0 \mid 1]\) to \([0 \mid 0 \mid 1]\) is only possible, if the total number of free channels of species $A$ exceeds $\theta_2$, i.e. if $h(\theta_2, 1 - \eta_A) = 1$; a transition from \([1 \mid 0 \mid 0]\) to \([1 \mid 0 \mid 1]\) occurs with probability $1/2$.

The stable equilibrium state at node $r$ according to this reactive interaction rule is given by $\eta(r) = (0, \ldots, 0)$. Any stimulus of this state with respect to the components $B$ or $C$ leads back to the equilibrium state in one time step, if $\theta_1, \theta_2, \theta_3 > 0$. An example of a trajectory initiated by a stimulus with respect to component $A$ and threshold values $\theta_1 = 1, \theta_2 = \theta_3 = 3$ is illustrated in Fig. 5.32. With these threshold parameters the local interaction rule defines an **excitable system**. In the following, examples are based on these parameters, i.e. $\theta_1 = 1, \theta_2 = \theta_3 = 3$.

The complete spatio–temporal evolution of the automaton dynamics for reactive interaction, shuffling and propagation $(P \circ M \circ R)$ is described by the following microdynamical difference–equation

\[ \eta_{\sigma,i}(r + m_\sigma e_i, k + 1) - \eta_{\sigma,i}(r, k) = R^\sigma_i (\eta^\sigma_i(r, k)) - \eta_{\sigma,i}(r, k) \quad (5.51) \]

for $m_\sigma \in \mathbb{N}, \sigma \in \{A, B, C\}$ and $i \in \{1, \ldots, 5\}$. This LGCA model leads to a ‘spiral-shaped’ concentration profile of component $A$ in the lattice, as it is shown in Fig. 5.33. The simulation was started with a single seed in the center of the lattice, with threshold parameters $\theta_1 = 1, \theta_2 = \theta_3 = 3$ and speed parameters $m_A = m_B = m_C = 1$. 
Figure 5.32: Example of a possible trajectory resulting from the application of the reactive interaction rule $R$ with threshold parameters $\theta_1 = 1$, $\theta_2 = 3$; $
abla(r, k) = (\eta_A(r, k), \eta_B(r, k), \eta_C(r, k))$.

Figure 5.33: Snapshot of concentration of component $A$ in a two-dimensional square lattice with periodic boundary conditions, started from a seed in the center, i.e. $\eta_{A1}(50, 50) = 1$ and $\eta_{\sigma,i}(r, 0) = 0$ else; parameters: $L = 100$, $\theta_1 = 1$, $\theta_2 = \theta_3 = 3$, $m_A = m_B = m_C = 1$. 
5.2 Spirals and excitable media

5.2.3 Lattice–Boltzmann equation and its uniform steady states

Again, we follow along the lines of Subsec. 2.3.2 (cf. p. 40) and derive the lattice–Boltzmann equation from Eqn. (5.51) as

\[ f_{\sigma i}(r + m_{\sigma i}, k + 1) - f_{\sigma i}(r, k) = \frac{1}{5} \sum_{i=1}^{5} E(\eta_{\sigma i}(r, k)) - f_{\sigma i}(r, k) \]

(5.52)

where

\[ f(r, k) = (f_A(r, k), f_B(r, k), f_C(r, k)) = (f_j(r, k))_{j=1}^{15} \in [0, 1]^{15} . \]

Spatially uniform stationary states \((\vec{f}_A, \vec{f}_B, \vec{f}_C)\), where \(\vec{f}_\sigma = f_{\sigma i}\), are solutions of \(\vec{\mathcal{C}}_{\sigma i}(\vec{f}(r, k)) = 0\), and hence for threshold parameters \(\theta_1 = 1\) and \(\theta_2 = \theta_3 = 3\) are evaluated as

\[ (\vec{f}_A, \vec{f}_B, \vec{f}_C) \in \{(0, 0, 0), (a_1, a_2, a_3)\} , \]

where \(a_1 \approx 0.496, a_2 = a_3 \approx 0.492\). (5.53)

In order to compare the dynamics of the LGCA and lattice–Boltzmann model we look at the dynamics of the number of particles \(n_\sigma(r, k) = \sum_{i=1}^{5} \eta_{\sigma i}(r, k)\) and mass \(g_\sigma(r, k) = \sum_{i=1}^{5} f_{\sigma i}(r, k)\) at a node \(r\), when particle motion is excluded, i.e. \(m_\sigma = 0\). The resulting equation for the lattice–Boltzmann model in terms of \(g_\sigma\) is given by

\[ g_\sigma(r, k + 1) = g_\sigma(r, k) + \sum_{i=1}^{5} \vec{\mathcal{C}}_{\sigma i}(\vec{f}) , \]

(5.54)

where the expanded form is given in Appendix C (cf. Eqn. (C.1–C.3), p. 153). Figure 5.34 shows trajectories for both models starting from the initial conditions

\[ \eta(r, 0) \in \{ (1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) , \]

\( (1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) , \)

\( (0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) , \)

\( (1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \} \),

and hence

\[ (n_A(r, 0), (n_B(r, 0) + n_C(r, 0))/2) = (g_A(r, 0), (g_B(r, 0) + g_C(r, 0))/2) \]

\( \in \{(1, 0), (1, 0.5), (2, 0)\} \),

where we set \(f_{\sigma i}(r, 0) = \eta_{\sigma i}(r, 0)\).
Figure 5.34: Trajectories at a node \( r \) of the LGCA (lines) and lattice–Boltzmann (dots) model for different initial conditions, which are marked with circles; the solid line refers to the example given in Fig. 5.32. Although \( S_1 = (0, 0) \) is the stable equilibrium state of the LGCA model, it is an unstable equilibrium state in the lattice–Boltzmann model. \( S_2 = (2.48, 2.46) \) is the second stationary state of the lattice–Boltzmann model. **Parameters:** 
\( \theta_1 = 1, \theta_2 = \theta_3 = 3, m_A = m_B = m_C = 0. \)

The stationary state \( S_1 = (0, 0) \) which is stable in the LGCA model is unstable in the lattice–Boltzmann model.\(^{22}\)

Furthermore, from linear stability analysis with respect to the second stationary state of the lattice–Boltzmann model (Eqn. (5.54)), we obtain that \( S_2 = (2.48, 2.46) \) is also unstable. Hence, the ‘invariant circle’ shown in Fig. 5.34 is a stable attractor. Therefore, in contrast to the LGCA model, the system described by the lattice–Boltzmann equation can be viewed as an oscillatory medium, which consists of self-oscillating elements, coupled with the neighbours (Mikhailov 1994).

However, the dynamics of the LGCA model with particle motion can be captured locally by the lattice–Boltzmann approximation, as it is indicated in Fig. 5.35. The data are taken from a LGCA simulation with a random initial condition corresponding to the stationary state \( S_2 \) at each node. The (small) dots represent averaged values over all nodes \( r \in \{(r_x, r_y) : r_x = 50 \pm 1, r_y = 50 \pm 1\} \) in a lattice with \( 100 \times 100 \) nodes. Hence, in order to derive the period of oscillation, a linear stability analysis of the lattice–Boltzmann equation (5.52) has to be performed.

\(^{22}\)This can be confirmed by a linear stability analysis of Eqn. (5.54).
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Figure 5.35: Trajectories from a simulation run averaged over all nodes \( r \in \{(r_x, r_y) : r_x = 50 \pm 1, r_y = 50 \pm 1 \} \) of the LGCA (small dots) and lattice–Boltzmann (bold dots) model for an initial condition located at \( S_2 = (2.48, 2.46) \). Parameters: \( L = 100, k = 100, \ldots, 2000, \theta_1 = 1, \theta_2 = \theta_3 = 3, m_A = m_B = m_C = 1 \).

5.2.4 Stability analysis of the lattice–Boltzmann equation

As before, the stability of the spatially homogeneous stationary solutions (5.53) \((\bar{f}_A, \bar{f}_B, \bar{f}_C)\) with respect to fluctuations \( \delta f_{\sigma,i}(r, k) = f_{\sigma,i}(r, k) - \bar{f}_A \) is determined by the spectrum of the Boltzmann propagator (2.31) (cf. p. 42). For the parameters \( \theta_1 = 1, \theta_2 = \theta_3 = 3 \) and \( m_A = m_B = m_C = 1 \) the Boltzmann propagator is of the form

\[
\Gamma(q) = T \{ I + \Omega^0 \}, \quad q = (q_1, q_2) \quad \text{with} \quad q_1, q_2 = 0, \ldots, L - 1, \quad (5.55)
\]

where

\[
T = \text{diag} \left( e^{-1 \frac{\Omega}{m_A}} (c_1, q) m_A, \ldots, e^{-1 \frac{\Omega}{m_A}} (c_5, q) m_A, \\
      e^{-1 \frac{\Omega}{m_B}} (c_1, q) m_B, \ldots, e^{-1 \frac{\Omega}{m_B}} (c_5, q) m_B, \\
      e^{-1 \frac{\Omega}{m_C}} (c_1, q) m_C, \ldots, e^{-1 \frac{\Omega}{m_C}} (c_5, q) m_C \right)
\]
and
\[
I + \Omega^0 = \begin{pmatrix}
\omega_1 & \omega_1 & \omega_2 & \omega_2 & \omega_2 & \omega_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\omega_1 & \omega_1 & \omega_2 & \omega_2 & \omega_2 & \omega_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\omega_3 & \omega_3 & \omega_4 & \omega_4 & \omega_5 & \omega_5 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\omega_3 & \omega_3 & \omega_5 & \omega_5 & \omega_4 & \omega_4 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\omega_3 & \omega_3 & \omega_5 & \omega_5 & \omega_4 & \omega_4 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\omega_3 & \omega_3 & \omega_5 & \omega_5 & \omega_4 & \omega_4 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{pmatrix} \in \mathbb{R}^{3 \times 3 \times 5}.
\]

The spectrum of the Boltzmann propagator (5.55) is given by
\[\Lambda_{\Gamma(q)} = \{\lambda_1(q), \lambda_2(q), \lambda_3(q), 0\},\]
where 0 has a multiplicity of 12 and
\[
\lambda_{1,2}(q) = \frac{1}{2} u(q) \left(\omega_1 + \omega_4 + \omega_5 \pm \sqrt{8\omega_2 \omega_3 + (\omega_4 + \omega_5 - \omega_1)^2}\right),
\lambda_3(q) = (\omega_4 - \omega_5) u(q)
\]
with \(u(q) := 1 + \sum_{j=1}^b e^{-\frac{\pi j}{L} q \cdot q} - 1 + 2 \left(\cos\left(\frac{\pi}{L} q_1\right) + \cos\left(\frac{2\pi}{L} q_2\right)\right) \in [-3, 5].\)
To be more specific, the eigenvalues with respect to each stationary state are given by:
\[
(f_A, f_B, f_C) = (0, 0, 0) : \quad \lambda_1(q) = u(q), \quad \lambda_2(q) = \lambda_3(q) = 0, \quad (5.56)
\]
\[
(f_A, f_B, f_C) \approx (0.496, 0.492, 0.492) : \quad \lambda_{1,2}(q) \approx (0.152 \pm 0.186 i) u(q), \quad \lambda_3(q) \approx 0.062 u(q). \quad (5.57)
\]

Hence, in both cases the spectral radius \(\mu(q) = |\lambda_1(q)|\) depends on the vectors of wave numbers \(q = (q_1, q_2)\) via \(|u(q)| \in [0, 5]\). In contrast to the two-dimensional ‘activator–inhibitor model’ (cf. Subsec. 5.1.6, p. 121), no special direction is preferred, as illustrated in Fig. 5.36.

In case (5.56) the spectral radius is always a real number and its maximum instability refers to wave numbers with magnitude \(|q| = 0\). In the second case (5.57) the dominant eigenvalue has a non-zero imaginary part. The period of oscillation \(\Delta k\) can be determined from
\[
\lambda_1(q) = e^{\alpha + i \omega} = |\lambda_1(q)| (\cos(\omega) + i \sin(\omega)) \approx 0.152 u(q) + i 0.186 u(q),
\]

\footnote{The matrix elements \(\omega_i, \ i = 1, \ldots, 5\), are different terms for both stationary states \((f_A, f_B, f_C)\) given by (5.53).}
5.2 Spirals and excitable media

\[ \mu(|q|, \phi) \]

(a) \((\tilde{f}_A, \tilde{f}_B, \tilde{f}_C) = (0, 0, 0) \) (cf. case 5.36)

(b) \((\tilde{f}_A, \tilde{f}_B, \tilde{f}_C) \approx (0.496, 0.492, 0.492) \) (cf. case 5.57)

Figure 5.36: Spectral radius \( \mu(q) = |\lambda_1(q)| \) dependent on the wave number \( q = (q_1, q_2) = (|q| \cos(\phi), |q| \sin(\phi)) \) represented in polar coordinate form. Parameters: \( L = 100, \theta_1 = 1, \theta_2 = \theta_3 = 3, m_A = m_B = m_C = 1 \).

where \( \alpha \approx \ln(0.241 |u(q)|) \) and \( \omega \approx \arccos\left(0.632 \frac{|u(q)|}{|q|} \right) \), as

\[
\Delta k = \frac{2\pi}{\omega} \approx \begin{cases} 
7.086 & \text{if } u(q) > 0 \\
2.786 & \text{if } u(q) < 0 
\end{cases}
\]

Hence, oscillations in the density of all components resulting from spatially homogeneous fluctuations, i.e. \( |q| = 0 \), have a period of \( \Delta k \approx 7 \). This result is confirmed in Fig. 5.37, where global and local densities perform regular oscillations with the predicted period.

Figure 5.36(b) shows, that \( Q^c = \{ q = (q_1, q_2) : |q| \leq 15 \} \). Although modes with wave numbers of magnitude \( |q| \) = 0 grow fastest, propagating sound-like modes with ‘speed’ \( \frac{L}{|q|} \Delta k^{-1} \) grow almost as fast for small \( |q| \), since (for \( L = 100 \))

| \( |q| \) | 0 | 1 | 2 | 3 | 4 |
|------------------|------------------|------------------|------------------|------------------|
| \( \mu(0,0) - \mu(|q|,0) \) | 0.0001 | 0.0038 | 0.0086 | 0.0151 |

| \( |q| \) | 5 | 6 | 7 | 8 | 9 |
|------------------|------------------|------------------|------------------|------------------|
| \( \mu(0,0) - \mu(|q|,0) \) | 0.0338 | 0.0458 | 0.0595 | 0.0749 | 0.0919 |

According to the analysis regarding the role of fluctuations in a LGCA model performed in Subsec. 5.1.4 (cf. p. 106 and p. 104), we claim that travelling modes, which are observable in simulations, can be explained by our mean-field stability analysis. Figure 5.33 (see p. 132) shows that the rotation time for all
spirals coincides with the predicted rotation time. The snapshot taken at time $k = 956$ is very similar to the ones taken at times $k+7 = 963$ and $k+14 = 970$. But in order to substantiate these considerations, a detailed statistical analysis of the LGCA model, i.e. of the wave length of spirals in simulations, as well as a nonlinear analysis of the lattice–Boltzmann\footnote{see for example Sepulchre and Babloyantz (1995) (discontinuous media) and Mikhailov (1994) (continuous media).} model has still to be done. As a first step in this direction, a Karhunen–Loève decomposition (Killich et al. 1994) of the spatial patterns of a simulation has been performed\footnote{This has been done by Uwe Börner, MPI for the Physics of Complex Systems, Dresden.}. Preliminary results assert the predicted rotation time of $\Delta k \approx 7$ and indicate a wave number of magnitude 4 or 5.

\section{Summary}

In the first Section (5.1), it has been demonstrated that simple LGCA rules (5.8) (p. 90) for activator–inhibitor system dynamics can lead to a large variety of patterns in one (i.e. cf. Fig. 5.4, p. 92) and two (i.e. cf. Figs. 5.24, p. 122, and 5.26, p. 125) space dimensions, which are controlled by the reaction prob-
abilities $p_c, p_d$ and the speed parameters $m_A$ and $m_I$, respectively.

In particular, it has been shown that the spatial dynamics of the automaton can be captured through the linear stability analysis of the discrete automaton lattice–Boltzmann equations. The linear stability analysis and simulations have been performed for LGCA with periodic boundary conditions. However, other types of boundary conditions can be easily implemented and linear stability analysis extended in a straightforward manner. Equally good predictions can be expected also in these cases. The emergence of Turing patterns has been triggered by spatially heterogeneous perturbations of spatially homogeneous stable steady states. We have demonstrated that Turing patterns do not evolve if activator and inhibitor components have the same ‘diffusivity’, for any choice of reaction probabilities (i.e. cf. Fig. 5.8, p. 100). For certain values of $m_A, m_I$ and $p_c, p_d$ with $m_I > m_A$, we observed formation of stripes (i.e. cf. Fig. 5.10, p. 102), which are characterised by an intrinsic wave length, i.e. it depends only on the ‘diffusivities’ and reaction probabilities and is independent of the system size $L$.

Artificial behaviour of the LGCA which is not present in continuous Turing systems can be found, if the value of the dominant eigenvalue is less than $-1$. The induced pattern has checkerboard structure (i.e. cf. Fig. 5.13, p. 103). For some $m_A, m_I$–values several different ranges of unstable modes exist and therefore simulations exhibit mixed patterns (i.e. cf. Fig. 5.4(f), p. 92). Also, unstable modes with very large wave numbers lead to artificial patterns, such as stripes of very small wave length (i.e. cf. Fig. 5.13, p. 103), especially for $m_A > m_I = 1$ (cf. Fig. 5.9(c), p. 101).

Although linear stability analysis yields a very good insight into the automaton dynamics, there are situations in which local fluctuations still play an important role. Especially, if the value of the spectral radius is close to 1 in LGCA simulations, a dominant wave length is present, which contrasts the results of linear stability analysis (i.e. cf. Fig. 5.18, p. 108). Furthermore, ‘mode–selection’ with respect to different initial conditions has been illustrated (cf. p. 104).

The discrete lattice–Boltzmann equations form a basis for the derivation of corresponding continuous partial differential equations for the mass of each component (cf. Eqn. (5.37), p. 113). A linear stability analysis of this continuous system leads to a critical diffusion ratio for which it is possible to obtain diffusion–induced instabilities (‘Turing regime’). Moreover, we derived an appropriate reactive, spatial and temporal scaling relation between the system of partial differential equations and the lattice–Boltzmann model in the ‘Turing regime’, i.e. for $m_I \geq 14, m_A = 1$ (cf. Eqn. (5.41), p. 114). One apparent difference between the continuous reaction–diffusion model and the discrete lattice–Boltzmann model is the capability of pattern formation. As pointed out previously, the lattice–Boltzmann model exhibits a variety of patterns for
many different values and relations of the speed parameters \( m_A \) and \( m_I \), resulting from the imposed particle motion process in the LGCA model, and which can be explained by the spectrum shape. In contrast, the parabolic spectrum of the reaction–diffusion model predicts only one special type of pattern in the ‘Turing regime’.

The Turing pattern variety of the LGCA model is enlarged when the rules for activator–inhibitor interaction are extended to two-dimensional square and hexagonal lattices. Again, a linear stability analysis of the corresponding lattice–Boltzmann equations provides a good approach to study the resulting spatial pattern formation in terms of stationarity, wave length and orientation. While on a square lattice strong anisotropies in diagonal directions are visible, they are absent on a hexagonal lattice (cf. Figs. 5.24, p. 122, and 5.26, p. 125).

In Sec. 5.2 we introduced a LGCA model with a three–component interaction which mimicks the behaviour of excitable media. Typical patterns found in simulations are travelling rings and rotating spiral waves (cf. Fig. 5.33, p. 132). The excitability of a medium is characterised by means of the phase space dynamics of the system in the absence of diffusion. In the motion–free case, a mean–field (Boltzmann) approximation of the LGCA model is expected to be inadequate as we demonstrated for growth processes before (see Chap. 4, p. 83). This might explain why the lattice–Boltzmann approximation of the automaton characterises (theoretically) an oscillatory medium while the LGCA rules lead to excitable dynamics without particle motion. On the other hand, with particle motion, the complete LGCA dynamics of the (local and global) density–oscillations (cf. Fig. 5.37, p. 138) can be captured by the spectrum of the linearised Boltzmann equations. It indicates the occurrence of travelling waves isotropically rotating in the medium with a fixed spatial period.
6 Discussion

All deterministic, probabilistic and lattice–gas cellular automata which we present in this work are strategic models, in the sense that the set of rules is chosen ‘as simple as possible’ in order to capture essential interactions in many particle systems. We started with investigating cellular automaton models for the simultaneous independent random motion of many particles. It turned out that the framework of LGCA modelling is most suited for this kind of processes. We showed that the complete dynamics of the LGCA model, i.e. diffusive and artificial behaviour, can be understood by analysis of the corresponding mean–field equations (lattice–Boltzmann equations), which arise under the assumption that any correlations are neglected.

Afterwards, we studied direct particle–particle interactions for growth processes. It is very easy to define probabilistic cellular automaton rules which lead to growing aggregates of one component in two–dimensions. A large variety of different ‘growth’–rules can be found in the literature. The corresponding temporal growth processes sensitively depend on the choice of the local rules. A mean–field approximation becomes only reasonable when growth is combined with local random particle motion, because then correlations arising from the growth interaction step are (partly) destroyed by the motion step. In this case it is straightforward to derive probabilistic cellular automata with random motion and LGCA models which lead to equal mean–field equations for the particle density. But the important difference between probabilistic cellular automata with random motion and LGCA models is that the mean–field approximation of LGCA models leads to time– and space–dependent difference equations while the spatial dependence is lost in the other case!

This spatial dependence of the mean–field approximation of LGCA models was the cornerstone for our further investigations in spatial pattern formation phenomena. We designed LGCA two– and three–component interaction rules which capture the essentials of activator–inhibitor interactions and excitable media, respectively, and analysed the corresponding lattice–Boltzmann equations with regard to the capability of spatial pattern formation. For this, we performed a stability analysis of space– and time–dependent difference equations, and analysed the spectrum of the linearised and Fourier–transformed discrete lattice–Boltzmann equations. It turned out that this method leads to successful predictions of the spatio–temporal LGCA dynamics. Furthermore, we showed the limits of this approach. These arise on the one hand from the nonlinearity of the lattice–Boltzmann equations and on the other hand from the local fluctuations inherent in the LGCA model, which can not be cap-
tured by the deterministic lattice–Boltzmann equations. We demonstrated in the activator–inhibitor LGCA that fluctuations can support spatial pattern formation processes. Moreover, we showed that, without particle motion, the lattice–Boltzmann model corresponding to the LGCA model with excitable dynamics characterises a different medium, namely an oscillatory medium. The reason for this are strong local correlations between particles at a node which are determined by the LGCA rules.

Extended analysis

Especially in the case of the excitable LGCA model, it is a further challenge to study extended approximations which include higher order (on–node) correlations. These approximations can be derived from the Chapman–Kolmogorov description of the cellular automaton. The lattice–Boltzmann equations, on which we focused in this thesis, represent the simplest approximation of the system. They were obtained by describing the states in terms of single particle distribution functions, which represent the probability to find a particle with a given velocity at a given node. With this ansatz, all pair, triplet, and higher order correlations between particles are neglected. Extended approximations may be derived by including two–, three–, etc. particle distribution functions\(^1\).

Furthermore, we demonstrated that the dynamics of our LGCA model for excitable media can not be fully captured by linear stability analysis, which predicts unstable modes with infinite wave length, while the LGCA model exhibits spiral patterns with a certain finite wave length. Hence, it is reasonable to expect better predictions of the LGCA pattern formation dynamics by a nonlinear analysis of the lattice–Boltzmann equations\(^2\) (using renormalisation tools, see e.g. Haken (1978)).

Further applications

We showed exemplarily for the growth process, that it is possible to design LGCA interaction rules which are in mean–field correspondence to probabilistic cellular automata with imposed particle motion. Furthermore, we demonstrated that various pattern formation mechanisms, e.g. stationary and non–stationary patterns with a fixed wave length (cf. Subsec. 2.3.2, p. 43), are predictable by the linear stability analysis of the LGCA lattice–Boltzmann model. Therefore, it might be worth to apply this ansatz to other existing probabilistic cellular automata which exhibit spatial pattern formation. For example, the single–lane car traffic cellular automaton model, which was outlined in Sec. 1.2 (p. 12), shows backward moving start–stop waves (Fig. 6.1). This spatial pattern might be appropriately tractable by means of the corresponding LGCA lattice–Boltzmann equations.

Wilson et al. (1993) investigated a probabilistic cellular automaton for predator–

\(^1\) see also Sec. 2.3.1, p. 36f, and Bussemaker (1995)

\(^2\) in general, the lattice–Boltzmann equations are typically nonlinear
prey interactions with respect to influences of individual mobility on the spatial distribution of individuals (see Sec. 1.2, p. 6). Since this problem is closely related to the two-component activator–inhibitor LGCA model we studied in this thesis, an application and investigation of the LGCA approach seems to be very promising.

**Freedom of scales**

While the purpose of the derivation of time- and space-dependent difference equations from macroscopic partial-differential equation models is to get a numerical scheme for solving these equations, it is of primary interest in LGCA modelling to gain insight into the microscopic dynamics (cf. Fig. 1.2, p. 8). Cellular automata are primarily a topological construct without any imposed space-time scalings. Therefore, one of the apparent differences between the dynamics described by macroscopic and microscopic models (see Chap. 1) is that the latter systems can be easily adjusted to different time scales between the spatially local dynamics and the diffusive interactions. We demonstrated the importance of this argument by comparing the activator–inhibitor lattice–Boltzmann model with an appropriately derived partial differential equation model. Depending on the choice of reactive and diffusive scalings the partial differential equation model turned out to be more restricted in its pattern formation ability than the lattice–Boltzmann model.

An application which incorporates different spatial scales, e.g. of cellular and molecular dynamics, could be devoted to chemotactic interactions, in which microorganisms move preferentially towards or from a relatively high concentration of a certain chemical. Wave-like population movements and aggregation pattern can be observed in cellular slime molds, e.g. *Dictyostelium discoideum* (Segel 1980, Stevens and Schweitzer 1997). We conducted preliminary experiments with a LGCA model which combines local density-dependent cell–cell interactions (Deutsch 1999) with orientation-dependent cell–chemical
interactions, where the diffusing chemical is produced by the cells while the cell population is conserved. Via the diffusing chemical indirect non-local cell-cell interactions develop. The model exhibits aggregation patterns also in the case of neglected local cell–cell interactions, as it is shown in Fig. 6.2. The effects of different parameters, e.g. chemical production rate, chemical decay rate, cell density or ‘diffusivity’ of the chemical, on the aggregation pattern formation can be investigated by means of an analysis of the corresponding LGCA lattice–Boltzmann approximation. Furthermore, results of the LGCA model approach can be compared with other approaches, e.g. the Langevin ansatz (Stevens and Schweitzer 1997).

Figure 6.2: Snapshot of spatial cell distribution of a two-dimensional LGCA model for chemotaxis resulting from cell–chemical interactions, where the purely diffusive chemical is produced by the cells while the cell population is conserved. The simulation was started from a random distribution of cells in the square lattice.

The problem of different spatio-temporal scales is also important in population dynamics, in which the functioning of food chains and webs and their dependence on internal and external conditions are investigated. For example, in marine ecosystems oceanographic processes are coupled to phytoplankton–zooplankton interactions which are again influenced by some fish species. Classical models of phytoplankton patchiness are often described in terms of partial differential equations (Holmes et al. 1994). Here, the cellular automaton approach could be used in order to couple such small–scale continuous plankton processes, occurring in the cells of the lattice, with the larger–scale fish predation. First investigations of a related ansatz have been done by, e.g., Medvinskii et al. (2000).

There are no general methods which allow one to find a cellular automaton rule, or set of rules, which reproduce some set of observations (inverse problem). But based on the variability in the local dynamics, we demonstrated that cellular automaton modelling provides an intuitive and powerful approach to capture essential aspects of complex phenomena on various scales.

3Nonetheless, as Gutowicz (1990c) remarks “there are systems for which one must invoke
more, due to the simple structure and unconditionally numerical stability of cellular automata, a tool is available which is open for multifaceted experiments in various applications. Because of the discrete nature of cellular automata, attention has to be taken to detect and avoid artificial model behaviour. Although there are almost no limitations in designing local rules, strategic LGCA models should be designed for processes involving synchronous particle motion in order to allow an analytical treatment of the cellular automaton (dealing with the inverse problem).

"global controls, continuous states etc. in order to build a convincing and tractable model".
A Mean–field equation for a LGCA growth model

In this appendix we derive the mean–field equations of the following lattice–gas growth model (see Eqn. (4.27), p. 80): All empty channels \((r, c_i)\) simultaneously gain a particle with probability \(\gamma\), if at least \(B < \bar{b} = 5\) particles are present at the node. The transition probability to reach a node–configuration \(z \in \{0, 1\}^5\) given the node–configuration \(\eta(r, k)\) is expressed by

\[
W(\eta(r, k) \rightarrow z) = \begin{cases} 
1 & \text{if } \eta(r, k) = z \in \{(0, 0, 0, 0, 0), (1, 1, 1, 1, 1)\} \\
\gamma & \text{if } n(r, k) \in [B, \bar{b} - 1] \\
1 - \gamma & \text{if } n(r, k) \in [B, \bar{b} - 1] \\
0 & \text{else .}
\end{cases}
\]

(A.1)

Therefore, based on Eqn. (2.17) (cf. p. 35) we obtain the mean–field equation

\[
f_i(r + mc_i, k + 1) = E \left( R^k(\eta^g(r, k)) \right) \]

\[
= \frac{1}{5} \sum_{l=1}^{5} \left[ \sum_{z \in \mathcal{E}} \sum_{\eta \in \mathcal{E}} z_l W(\eta(r, k) \rightarrow z) P(\eta(r, k)) \right] \\
= \frac{1}{5} \sum_{l=1}^{5} \left[ P((1, 1, 1, 1)) + \sum_{\eta_{l_{1}}=1, \eta_{l_{2}}=1} P(\eta(r, k)) \right. \\
+ (1 - \gamma + \gamma) \sum_{\eta_{l_{2}}=1, \eta_{l_{2}}=1} P(\eta(r, k)) \\
+ \gamma \sum_{\eta_{l_{2}}=1, \eta_{l_{2}}=1} P(\eta(r, k)) \left. \right]
\]
Mean–field equation for a LGCA growth model

\[
\begin{align*}
&= \frac{1}{5} \sum_{i=1}^{5} \left[ \sum_{\eta_{l_{i}=1} \in \mathcal{E}} P(\eta(r,k)) \\
&\quad + \gamma \sum_{\eta_{l_{i}=0} \in \mathcal{E}} P(\eta(r,k)) \right] \\
&= \frac{1}{5} \sum_{i=1}^{5} \left[ f_i(r,k) + \gamma E\left( (1 - \eta(r,k)) \cdot \\
&\quad (\Psi_B(\eta(r,k)) + \cdots + \Psi_4(\eta(r,k))) \right) \right],
\end{align*}
\]

where the indicator functions $\Psi_a$ are defined in (4.23) (cf. p. 80).
B Activator–inhibitor interaction

‘Lengthy’ equations, which are relevant for an analytic investigation of the LGCA model with activator–inhibitor interactions introduced in Sec. 5.1 are given in this appendix.

B.1 Complete interaction rule

Recall that the microdynamical Eqn. (5.9) (cf. p. 91) for the one-dimensional two-component lattice-gas model introduced in Subsec. 5.1.2 is given by

\[
\eta_{\sigma,i}^R(r, k) = \mathcal{R}^R(\eta(r, k)) \\
= \Psi(\eta_A(r, k)) M_\sigma(\eta_{\sigma,i}(r, k)) \Psi^T(\eta_i(r, k)).
\]

The vector of counting functions \(\Psi\) is given by

\[
\Psi(\eta_\sigma) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \eta_{\sigma,1} \eta_{\sigma,2} \eta_{\sigma,3} \end{pmatrix},
\]

where we set \(\hat{\eta}_{\sigma,i} := (1 - \eta_{\sigma,i})\) and all terms are evaluated at \((r, k)\).

Taking the expected value of Eqn. (B.1.1), i.e. \(f_{\sigma,i}^R = E(\eta_{\sigma,i}^R(r, k))\), leads

\[
f_{A,i}^R = f_{A,i} + p_c f_{A,i} \left[ (f_{A,j} \bar{f}_{A,1} + f_{A,j} \bar{f}_{A,1} + f_{A,j} \bar{f}_{A,1}) \bar{f}_{1,i} \bar{f}_{1,j} \bar{f}_{1,l} \\
+ f_{A,j} \bar{f}_{A,1} (\bar{f}_{i,i} \bar{f}_{1,j} \bar{f}_{1,l} + \bar{f}_{i,i} \bar{f}_{1,j} \bar{f}_{1,l} + \bar{f}_{i,i} \bar{f}_{1,j} \bar{f}_{1,l}) \\
- p_d f_{A,i} \left[ \bar{f}_{A,j} \bar{f}_{A,1} (\bar{f}_{i,i} \bar{f}_{1,j} \bar{f}_{1,l} + \bar{f}_{i,i} \bar{f}_{1,j} \bar{f}_{1,l} + \bar{f}_{i,i} \bar{f}_{1,j} \bar{f}_{1,l}) \\
+ (\bar{f}_{A,j} \bar{f}_{A,1} + f_{A,j} \bar{f}_{A,1} + f_{A,j} \bar{f}_{A,1}) \bar{f}_{1,i} \bar{f}_{1,j} \bar{f}_{1,l} \right] \right]
\]
and

\[
f_{l,i}^n = f_{l,i} + p_c f_{l,i} \left[ f_{l,j} f_{l,i} (f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l}) + f_{A,i} f_{A,j} f_{A,l} \right] \\
+ f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} \\
+ (f_{l,j} f_{l,i} f_{l,i}) \left[ (f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} \right] \\
+ (f_{l,j} f_{l,i} f_{l,i}) \left[ (f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} + f_{A,i} f_{A,j} f_{A,l} \right]
\]

where we set \( f_{\sigma,i} := (1 - f_{\sigma,i}) \); all terms are evaluated at \((r, k)\) and the indexes \(i, j, l \in \{1, 2, 3\}\) are always chosen to be distinct, i.e. \(i \neq j \neq l\).

### B.2 Linear stability analysis

The matrix elements \(\omega_i, \ i = 1, \ldots, 4\), from the matrix \(I + \Omega^0\) play an important role in the derivation of the Boltzmann propagator (cf. p. 94). They are explicitly given by

\[
\omega_1 = \frac{1}{3} \left( 1 - (f_I - 1)^2 (2 (f_I - 1) + 3 f_A (2 - f_A + 4 (f_A - 1) f_I)) \right) p_c \\
+ f_I^2 \left( 2 f_I - 3 + 3 f_A (4 - 3 f_A + 4 (f_A - 1) f_I) \right) p_d 
\]

\[
\omega_2 = -2 (f_A - 1) f_A (1 - f_I + f_A (2 f_I - 1))((f_I - 1) p_c - f_I p_d), 
\]

\[
\omega_3 = -((f_I - 1)^2 - 2 f_A (f_I - 1) (3 f_I - 1) + f_A^2 (1 + 6 (f_I - 1) f_I)) \\
((f_I - 1) p_c - f_I p_d), 
\]

\[
\omega_4 = \frac{1}{3} \left( 1 - f_A (9 (f_I - 1)^2 - 3 f_A (f_I - 1) (9 f_I - 5) \\
+ f_A^2 (7 + 6 f_I (3 f_I - 4))) p_c - (1 + f_A (3 - 3 f_A \\
+ f_A^2 - 12 (f_A - 1)^2 f_I + 9 (f_A - 1) (2 f_A - 1) f_I) p_d \right). 
\]

For the case \(p_c = p_d =: p\) the spatially homogeneous steady state is given by \((f_A, f_I) = (0.5, 0.5)\) and therefore we obtain

\[
\omega_1 = \frac{1}{24} (8 + p), \quad \omega_2 = -\frac{1}{4} p, \quad \omega_3 = \frac{3}{8} p \quad \text{and} \quad \omega_4 = \frac{1}{12} (4 - 7 p). \quad (B.2.5)
\]
Using this, the eigenvalues given by Eqn. (5.20) (cf. p. 95) become

\[
\lambda_{1,2}(q) = \frac{1}{2} \left( \frac{1}{24} (8 + p) u_A(q) - \frac{1}{4} p u_I(q)\right) \quad \text{(B.2.6)}
\]

\[
\pm \sqrt{\frac{1}{18} (1 - p)(5p - 8) u_A(q) u_I(q) + \left( \frac{1}{24} (8 + p) u_A(q) - \frac{1}{4} p u_I(q) \right)^2}.
\]
C Spirals: complete interaction rule

Recall that the lattice–Boltzmann Eqn. (5.52) (cf. p. 133) for the two–dimensional three–component LGCA model introduced in Sec. 5.2 is given by

\[ f_{\sigma,i}(r + m_{\sigma}c_{i}, k + 1) - f_{\sigma,i}(r, k) = \frac{1}{5} \sum_{i=1}^{5} E(\eta_{\sigma,i}^a(r, k)) - f_{\sigma,i}(r, k) \\
= \mathcal{C}_{\sigma,i}(\mathbf{f}(r, k)). \]

When particle motion is excluded, i.e. \( m_{\sigma} = 0 \), this becomes

\[ g_{\sigma}(r, k + 1) = g_{\sigma}(r, k) + \sum_{i=1}^{5} \mathcal{C}_{\sigma,i}(\mathbf{f}), \]

where

\[
\begin{align*}
\sum_{i=1}^{5} \mathcal{C}_{A,i}(\mathbf{f}) &= \frac{1}{5} g_A \left( g_B (g_C - 5) - 5 (g_C - 4) \right) \\
&- \frac{2}{25} g_A^2 \left( g_B - 5 \right) (g_C - 5) - \frac{2}{125} g_A^3 \left( g_B g_C - 25 \right) \\
&+ \frac{1}{125} g_A^4 \left( -5 + g_B (g_C - 2) - 2 g_C \right) \\
&+ \frac{1}{15625} g_A^5 \left( g_B (25 - 11 g_C) + 25 (1 + g_C) \right),
\end{align*}
\]

\[
\begin{align*}
\sum_{i=1}^{5} \mathcal{C}_{B,i}(\mathbf{f}) &= g_B (0.1 g_C - 1) + g_A \left( 0.5 + 0.1 (g_B - g_C) \right) \\
&- \frac{2}{125} g_A^3 \left( g_B (g_C - 2) - 3 g_C \right) \\
&+ \frac{1}{625} g_A^4 \left( -8 g_C + g_B (3 g_C - 7) \right) \\
&- \frac{3}{15625} g_A^5 \left( -5 g_C + g_B (2 g_C - 5) \right),
\end{align*}
\]
and

$$\sum_{i=1}^{5} \tilde{c}_{C;i}(f) = \varphi_C (0.1 \varphi_B - 1) + \varphi_A (0.5 + 0.1 (\varphi_C - \varphi_B))$$  \hspace{1cm} (C.3)

$$- \frac{2}{125} \varphi_A^3 (\varphi_C (\varphi_B - 2) - 3 \varphi_B)$$

$$+ \frac{1}{625} \varphi_A^4 (-8 \varphi_B + \varphi_C (3 \varphi_B - 7))$$

$$- \frac{3}{15625} \varphi_A^5 (-5 \varphi_B + \varphi_C (2 \varphi_B - 5))$$.
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<td>lattice–gas cellular automaton/automata</td>
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<td>PDE</td>
<td>partial differential equation</td>
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**Symbols**

- \(|\cdot|\) \hspace{1cm} cardinality of a set
- \([y]\) \hspace{1cm} integer closest to \(y \in \mathbb{R}^+\)
- \([y]\) \hspace{1cm} smallest integer greater than or equal to \(y \in \mathbb{R}^+\) \hspace{1cm} 100
- \(y^T\) \hspace{1cm} transpose of the vector \(y\)

**Greek symbols**

- \(\beta \in \mathbb{N}_0\) \hspace{1cm} number of rest (zero–velocity) channels \hspace{1cm} 20
- \(\Gamma(q)\) \hspace{1cm} Boltzmann propagator \hspace{1cm} 42
- \(\delta\) \hspace{1cm} length of temporal unit \hspace{1cm} 48
- \(\epsilon\) \hspace{1cm} length of spatial unit \hspace{1cm} 48
- \(\eta(r) = (\eta_i(r))_{i=1}^b \in \{0, 1\}^b\) \hspace{1cm} node configuration \hspace{1cm} 21
- \(\Lambda_M\) \hspace{1cm} spectrum of the matrix \(M\) \hspace{1cm} 38
- \(\mu\) \hspace{1cm} spectral radius \hspace{1cm} 39
- \(\mu(q)\) \hspace{1cm} spectral radius according to wave number \(q\) \hspace{1cm} 43
- \(\nu = |\mathcal{N}_r^b|\) \hspace{1cm} number of neighbours in the interaction neighbourhood \hspace{1cm} 24
- \(\rho(r, k) \in [0, 1]\) \hspace{1cm} local particle density of node \(r\) at time \(k\) \hspace{1cm} 34
- \(\rho(k) \in [0, 1]\) \hspace{1cm} total particle density in the lattice at time \(k\) \hspace{1cm} 34
- \(\varrho(r, k) \in [0, \bar{b}]\) \hspace{1cm} local mass of node \(r\) at time \(k\) \hspace{1cm} 34
- \(\varrho(k) \in [0, \bar{b}]\) \hspace{1cm} total mass in the lattice at time \(k\) \hspace{1cm} 34
\[ \sigma \in \{1, \ldots, \varsigma\} \quad \text{single component in a model with } \varsigma \text{ components} \]

\[ \Psi_a(\eta(r, k)) \in \{0, 1\} \quad \text{indicator function} \]

**Symbols in alphabetical order**

\[ A_j \in A_b \quad \text{permutation matrix} \]

\[ b \quad \text{coordination number; number of nearest neighbours on the lattice } \mathcal{L} \]

\[ b = b + \beta \quad \text{total number of channels at each node} \]

\[ c_i \in N_b, \ i = 1, \ldots, b \quad \text{nearest neighbourhood connections of the lattice } \mathcal{L} \]

\[ C_i(\mathbf{s}_{\mathcal{N}(r)}(k)) \quad \text{change in occupation numbers} \]

\[ \tilde{C}_i(\mathbf{f}_{\mathcal{N}(r)}(k)) \in [0, 1] \quad \text{change of the average number of particles} \]

\[ \mathcal{E} = \{z^1, \ldots, z^\varepsilon\} \quad \text{(finite) set of elementary states} \]

\[ \mathbf{f}(r) = (f_i(r))_{i=1}^{b} \quad \text{vector of single particle distribution functions; average occupation numbers} \]

\[ \mathbf{f}^\ast(k) \quad \text{vector of spatially averaged occupation numbers in a simulation} \]

\[ \mathbf{F}(q) = (F_i(q))_{i=1}^{b} \quad \text{Fourier-transformed value} \]

\[ I \quad \text{(general) interaction operator} \]

\[ k = 0, 1, 2, \ldots \quad \text{time step} \]

\[ \mathcal{L} \subset \mathbb{R}^d \quad \text{d-dimensional regular lattice} \]

\[ L_i, \ i = 1, \ldots, d \quad \text{number of cells in space direction } i \]

\[ \mathbb{M} \quad \text{shuffling (mixing) operator} \]

\[ n(r) \in \{0, \ldots, \bar{b}\} \quad \text{total number of particles present at node } r \]

\[ N_b \quad \text{neighbourhood template} \]

\[ N_b^t \quad \text{interaction neighbourhood template} \]

\[ \mathcal{P} \quad \text{propagation operator} \]

\[ q \in \{0, \ldots, L\} \quad \text{(discrete) wave number} \]

\[ q^\ast \quad \text{wave number found in a simulation} \]

\[ q_c \in Q_c \quad \text{dominant critical wave number} \]

\[ Q_c \quad \text{sets of critical wave numbers} \]
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<td>$Q^+, Q^-$</td>
<td>sets of critical wave numbers</td>
</tr>
<tr>
<td>$r \in \mathcal{L}$</td>
<td>spatial coordinate, cell, node, site</td>
</tr>
<tr>
<td>$(r, c_i)$</td>
<td>channel with direction $c_i$ at node $r$</td>
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<tr>
<td>$R$</td>
<td>reactive interaction operator</td>
</tr>
<tr>
<td>$\mathcal{R} : \mathcal{E}^\nu \rightarrow \mathcal{E}$</td>
<td>local cellular automaton rule</td>
</tr>
<tr>
<td>$s(r) \in \mathcal{E}$</td>
<td>state value at node $r$</td>
</tr>
<tr>
<td>$s : \mathcal{L} \rightarrow \mathcal{E}$</td>
<td></td>
</tr>
<tr>
<td>$s = \left( s(r_i) \right)_{r_i \in \mathcal{L}} \in \mathcal{S}$</td>
<td>global configuration</td>
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<tr>
<td>$s_M = \left( s(r_i) \right)_{r_i \in M} \quad M \subset \mathcal{L}$</td>
<td>local configuration</td>
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<td>$\mathcal{S} = \mathcal{E}^{\left</td>
<td>\mathcal{L} \right</td>
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<td>$W : \mathcal{E}^\nu \rightarrow [0, 1]$</td>
<td>time-independent transition probability</td>
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<tr>
<td>$X_\sigma$</td>
<td>particle of ‘species’ $\sigma$</td>
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List of symbols
Erklärung

Ich erkläre, daß ich die vorliegende Arbeit selbständig und nur unter Verwen-
dung der angegebenen Literatur und der nachfolgend aufgeführten Hilfsmittel
angefertigt habe.

Osnabrück, den 22. August 2000

Hilfsmittel

Die Simulationsprogramme wurden in der Programmiersprache ‘C’ auf ver-
schiedenen unix-Rechnern entwickelt. Für die graphische Ausgabe wurde
die an der Universität Cornell (USA) entwickelte Simulationsumgebung ‘X-
Windows Stochastic Spatial Simulator’ (s3) verwendet. Das Programm ist frei
zugänglich unter http://gumby.syr.edu/.

Für diesen Text wurde das Textsatzsystem \text{\LaTeX} (auf Basis von \text{\LaTeX} 1.0.6)
verwendet. Alle eingebundenen Bilder, mit Ausnahme des Fotos auf S. 85,
habe ich selbst erstellt. Sie wurden mit \text{\LaTeX}, mit Mathematica 4.0 oder als
in PostScript konvertierte Snapshots des Simulationsprogramms erzeugt.

Es ist geplant, einige in s3 implementierte LGCA-Modelle sowie Mathematica
notebooks unter http://www.usf.uos.de/~sabine/ zur Verfügung zu stellen.
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Danksagung