Interactive Structure Formation with Brownian Particles

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1 Introduction

A key to the widely spread phenomenon of structure formation should be provided by the insight that interactions of simple elements on the microscopic level may result in the emergence of complex features of the system on the macroscopic level. Examples of this intrinsic dynamic process which are tried to be explained within a physical approach, range from coherent pattern formation in physical and chemical systems (cf. eg. HAKEN, 1983, KAI, 1992, MIKHAILOV, 1994), to the behavior of social groups (cf. eg. WEIDLICH, 1991).

The model proposed in this paper is based on Brownian particles. Obviously, simple Brownian motion is not sufficient to originate structures. Therefore, we introduce *active Brownian Particles* which are Brownian particles with the ability to generate a self-consistent field, which in turn influences their further movement and physical and chemical behavior. This non-linear feedback between the particles and the field generated by themselves results in an interactive structure formation process, which, on the macroscopic level in most cases can be described by sets of coupled reaction-diffusion equations.

Recently, Active Walker models have been used to describe pattern formations in complex systems (KAYSER *et al.*, 1992, LAM, POCHY, 1993, SCHWEITZER, SCHIMANSKY-GEIER, 1994, LAM, 1995). The main idea of our approach is to solve the LANGEVIN equations for an ensemble of active Brownian particles instead of the related nonlinear partial differential equations (PDE). In some cases where only small particle numbers govern the structure formation, like in gas discharges (WILLEBRANDT *et al.*, 1991), on catalytic surfaces (ROSÉ *et al.*, 1994), in cell membranes (FROMMHERZ, ZEILER, 1994), or during cell migration (SCHIENBEIN, GRULER, 1993), the continuous limit becomes questionable and PDE's are not able to describe the behavior of the system. Thus a stochastic approach to structure formation is needed which considers fluctuations in the system.

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In order to demonstrate the applicability of our approach, we investigate different examples of structure formation processes in reaction diffusion systems, and also discuss a simple algorithm of network and trail formation, based on local nondirect interactions of the active Brownian particles.

2   Equations for the Active Brownian Particles

Due to LANGEVIN the equation of motion for a Brownian particle is given by the stochastic differential equations:

$$\frac{dr}{dt} = v \quad ; \quad \frac{dv}{dt} = -\gamma v + \sqrt{2\,\varepsilon\,\gamma} \quad \xi(t) \tag{1}$$

Here $r(t)$ is the position of the particle at time t, which moves for example on a surface S ($r \in \mathbb{R}^2$). $v(t)$ is the velocity permanently changed by impacts of some surrounding liquid which is modelled by the random function $\xi(t)$ and γ is the friction coefficient. In order to obtain diffusion $\xi(t)$ should be Gaussian white noise with

$$< \xi(t) >= 0 \quad ; \quad < \xi(t)\xi(t') >= \delta(t - t'). \tag{2}$$

Diffusion of the Brownian particle is observed in the long-time limit, if $t \gg \gamma^{-1}$ and the intensity ε is related to the macroscopic diffusion coefficient D_n by $\varepsilon = D_n\gamma$.

The purpose of active Brownian particles is the formation of macroscopic structures resulting from collective behaviour of the particles. This can be obtained by some simple assumptions regarding the interaction of the particles. We consider an ensemble of N particles each with a random position $r_i(t)$. N can be changed due to some chemical reactions as discussed later on. Further, we suppose that the N particles are able to generate a macroscopic field $h(r,t)$, which can evolve in space and time due to three processes: (i) production (generation rate q), (ii) decay (rate k_h), (ii) diffusion (coefficient D_h). For the considered field, we therefore obtain a linear evolution law:

$$\frac{\partial}{\partial t}\, h(r,t) = q \sum_{i=1}^{N} \delta(r - r_i(t)) - k_h\, h + D_h\, \Delta h. \tag{3}$$

We note that this equation is a stochastic partial differential equation with

$$n^{micr}(r,t) = \sum_{i=1}^{N} \delta(r - r_i(t)) \tag{4}$$

being the microscopic density of the particles. Assuming a grid with a sufficiently large number of particles in each box, the microscopic density can be transformed into the density $n(r,t)$ of the Brownian particles. In this limit, eq. (3) becomes a linear deterministic equation:

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$$\frac{\partial}{\partial t} h(r,t) = q\, n(r,t) - k_h\, h + D_h\, \Delta h. \tag{5}$$

As a second assumption, a self-consistent feedback between the field and the behaviour of the particles is considered. Depending on the examples of structure formation in reaction-diffusion systems discussed in the following sections, the field $h(r,t)$ will be identified either with a potential field determining the movement of the Brownian particles, or with the local temperature, which determines some chemical reaction rates of the particles. In a third example $h(r,t)$ stands for an inhibitor density, damping the growth of a replicating activator. Below, the first two cases will be specified in some more detail:

(i) The field determines the motion of the particles: The possibly simplest ansatz is that the particles search for the local maxima of the field $h(r,t)$ which they generate during their motion. For this case, the dynamics of the particles reads

$$\frac{dr_i}{dt} = v \quad ; \quad \frac{dv_i}{dt} = -\gamma v_i + \alpha\, \left.\frac{\partial h(r,t)}{\partial r}\right|_{r_i} + \sqrt{2\,\varepsilon\,\gamma}\, \xi_i(t). \tag{6}$$

α indicates the strength of the response to the field $h(r,t)$.

(ii) The field determines chemical reaction rates: We assume that the total number of active Brownian particles is not conserved, but could be changed by an homogeneous influx of particles $N \to N+1$ with a rate ϕ (e.g. by adsorption on the surface due to vapor deposition) and an inhomogeneous outflux $N \to N-1$ with a rate k_n due to the local disappearence of particles (e.g. by desorption processes on the surface or re-evaporation). Since the rates could be functions of the field $h(r,t)$, they are also functions of time and space coordinates.

The dynamics of the particles can be formulated in terms of the grand-canonical N-particle distribution function $P_N(r_1,...,r_N,t)$ which gives the probability to find the N active Brownian particles in the vicinity of $r_1,...,r_N$ on the surface S at time t. Considering chemical reactions, as the birth and death processes described above, the master equation for P_N (FEISTEL, EBELING, 1989) reads in the limit of strong damping $\gamma \to \infty$

$$
\begin{aligned}
\frac{\partial}{\partial t} P_N(r_1,...,r_N,t) = \; & - \; (k_n\, N + \phi\, S)\, P_N(r_1,...,r_N,t) \\
& + \; k_n\,(N+1) \int dr_{N+1}\, P_{N+1}(r_1,...,r_{N+1},t) \\
& + \; \frac{\phi}{N} \sum_{i=1}^{N} P_{N-1}(r_1,...,r_{i-1},r_{i+1},...,r_N,t) \\
& - \; \sum_{i=1}^{N} \left[\nabla_i\, (\mu\, \nabla_i h)\, P_N - D_n\, \Delta_i P_N \right]
\end{aligned}
\tag{7}
$$

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where $\mu = \alpha/\gamma$ is the mobility of the particles and $D_n = \varepsilon/\gamma$ is the spatial diffusion coefficient for the density of the Brownian particles. The first three terms of the right-hand side describe the loss and gain of particles with the coordinates $r_1, ..., r_N$ due to chemical reactions, where k_n and ϕ may depend on the field. The last term describes the change of the probability density due to the motion of the particles on the surface S.

The mean field limit is obtained by introducing the density of the Brownian particles in the grand canonical ensemble:

$$n(r,t) = \sum_{N=1}^{\infty} N \int dr_1...dr_{N-1} \, P_N(r_1, ..., r_{N-1}, r, t) \tag{8}$$

Integrating eq. (7) due to eq. (8) and neglecting higher correlations, we obtain the following reaction-diffusion equation for $n(r,t)$

$$\frac{\partial}{\partial t} n(r,t) = -\nabla \, n \, (\mu \, \nabla h) + D_n \, \Delta n - k_n \, n(r,t) + \phi \, . \tag{9}$$

Based on the explanations above, we want to introduce our simulation algorithm for structure formation in reaction-diffusion systems. The chemical reactions will be considered according to the master equation (eq. 7), i.e. with probability $k_n \Delta t$ a particle is desorbed during the time intervall Δt and with rate ϕ a particle is generated. Eq. (9) indicates that eq. (7) in the mean field limit obeys a reaction diffusion dynamics. However, instead of solving the set of nonlinear partial differential equations for $h(r,t)$ (eq. 5) and $n(r,t)$ (eq. 9) for the mean field limit, we simulate the reaction-diffusion problems by a set of $N(t)$ LANGEVIN equations (eq. 6) and the stochastic partial differential equation (eq. 3), which is integrated on a square lattice using simple standard algorithms for linear PDE.

Let us give some estimate in favour of the proposed algorithm. Usually reaction-diffusion equations are solved by integration on a lattice. Hence, the system of partial differential equations corresponds to a large number of coupled ordinary differential equations. The time step required for the integration, is mainly determined by the nonlinearities of the equations. Considering for example eq. (9), the allowed time step Δt should be less than $(\nabla n(r,t))^{-2}$ if we suppose that $n(r,t)$ and $h(r,t)$ are of the same order. As large gradients comes into play, the time step should be decreased according to the *square* of ∇n. On the other hand, if we solve the corresponding LANGEVIN equations (eq. 6), the gradient appears only in a linear manner and, therefore much larger time steps are allowed for the integration. Hence, a simulation of a large number of particles do not necessarily cause larger simulation times, since in the considered example the equations are in fact linearized.

In the following, we present different examples of pattern formation in reaction- diffusion systems generated by the algorithm proposed above.

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3 Pattern Formation in Reaction-Diffusion Systems Simulated with Active Brownian Particles

3.1 Competition of Spikes

In the first example, $h(r,t)$ is identified with a negative potential of a mechanical force affecting the Brownian particles. This force accelerates the particles to move into the direction of the maxima of $h(r,t)$ (eq. 6), where α is the strength of the response. A similar situation was considered by FROMMHERZ, ZEILER (1994), the results presented here are obtained from SCHWEITZER, SCHIMANSKY-GEIER (1994).

We start our simulations with a homogeneous distribution of Brownian particles. Since chemical reactions are not considered here, the overall particle number is constant. From a bifurcation analysis of the mean field equation one finds the condition for the instability of the homogeneous state n_0, h_0

$$\alpha\, q\, n_0\, /\gamma\, >\, \varepsilon\, (k_h\, +\, \kappa^2\, D_h) \tag{10}$$

where $n_0\, =\, N/S$ and $h_0\, =\, n_0\, q\, /k_h$, S being the surface area, and κ the wave number of a fluctuation. If the influence of the field (α) is large, or if the intensity for the random motion (ε) is small, the Brownian particles quickly form several clusters, which results in a local growth of $h(r,t)$. During a first stage, the spikes of the field grow independently as presented in the time series of Fig. (1). If the production of the field becomes stationary, i.e. the decay with rate k_h compensates the production of the field by the Brownian particles, a transition into a second regime occurs. Here, the different spikes, which have bound the Browninan particles, compete, which leads to a decrease of the number of spikes, as presented in Fig. (2). Asymptotically, a one-peak distribution results.

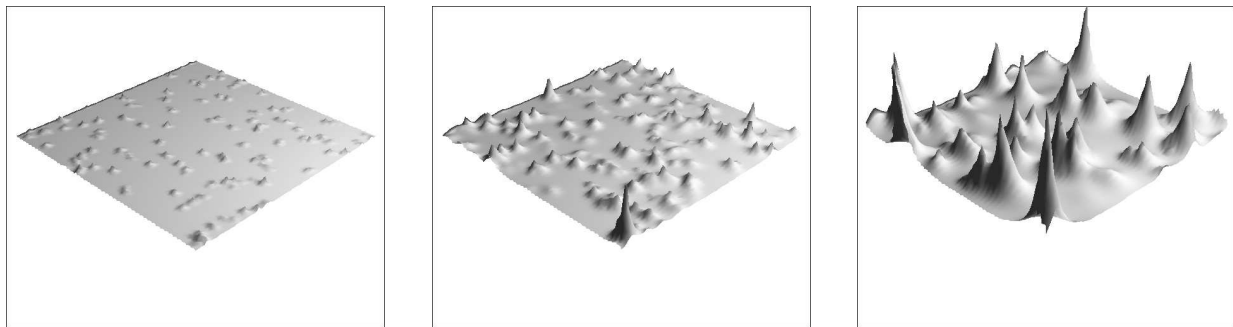
Figure 1: Evolution of $h(r,t)$ generated by $N = 100$ particles during the growth regime. Time in simulation steps: left) $t = 10$, (middle) $t = 100$, (right) $t = 1.000$ (lattice size: $S = 100 \times 100$)

In the example considered, the particles generate a field which forces them to concentrate in its maxima. This, in turn, amplifies the effect of the maxima again and causes a further growth - a
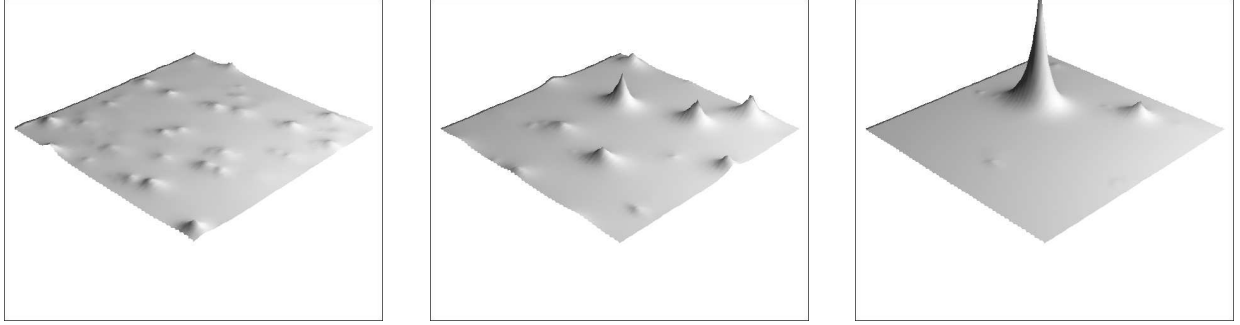
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Figure 2: Evolution of $h(r,t)$ generated by $N = 100$ particles during the competition regime. Time in simulation steps: (left) $t = 1.000$, (middle) $t = 5.000$, (right) $t = 50.000$ (The density scale is 0.1 times the scale of Fig. 1. Hence, the left part of Fig. 2 is the same as the right part of Fig. 1.)

situation which, to some extent, is similar to the gravitational collapse of stars without energy balance. If the growth of the field is bound to a maximum value, h_{max}, a further growth results in a spatial extension of domains with h_{max}, a situation similar to OSTWALD-ripening in phase transitions (SCHIMANSKY *et al.*, 1991).

The selection among the different spikes can be described in terms of a selection equation of the EIGEN-FISHER type (EBELING, FEISTEL, 1986). This can be derived by means of the stationary solution of the FOKKER-PLANCK-equation (eq.(7), neglecting the chemical terms). Using this solution, the dynamics of the field $h(r,t)$ can be rewritten within an adiabatic approximation to obtain the following selection equation (SCHWEITZER, SCHIMANSKY-GEIER, 1994):

$$\frac{dh(r,t)}{dt} = \frac{\gamma\, h_0}{\langle \exp[(\mu/\varepsilon)\, h(r,t)]\rangle_S} h(r,t)$$
$$\times \left\{ \frac{\exp[(\mu/\varepsilon)\, h(r,t)]}{h(r,t)} - \frac{\langle \exp[(\mu/\varepsilon)\, h(r,t)]\rangle_S}{h_0} \right\} + D_h \Delta h(r,t) \qquad (11)$$

where

$$\langle \exp[(\mu/\varepsilon)\, h(r,t)]\rangle_S = \frac{1}{S} \int_S \exp[(\mu/\varepsilon)\, h(r',t)]\, dr' \qquad (12)$$

is similar to the mean "fitness", representing the global selection pressure. The further growth of a spike occurs only as long as

$$\exp[(\mu/\varepsilon)\, h(r,t)]\, b_0 > \langle \exp[(\mu/\varepsilon)\, h(r,t)]\rangle_S\, h(r,t) \qquad (13)$$

holds. Otherwise, the spike will decay again due to the competition process. Provided a suitable neigbourhood, eventually the largest spike will survive, as indicated also by the computer simulations.

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3.2 Coexistence of Spikes

The simple but interesting picture of Sect. 3.1. is changed drastically if we consider chemical reactions of the Brownian particles (SCHIMANSKY-GEIER *et al.*, 1995). Here, we assume the adsorption and desorption of particles, independent on the field $h(r, t)$. Now, chemical reactions control the unlimited growth of the existing spikes and are sources of a permanent formation of new ones. The probability, that a new particle with random position occurs on the surface, is $\phi \Delta t S$, and the probability that an existing particle survives, is $k_n \Delta t$. A bifurcation analysis of the mean field equations proves, that the homogeneous state is instable against periodic fluctuation with wave number

$$\kappa = \sqrt{\frac{q \, n_0 \, \mu \; - \; D_h \, k_h \; - \; D_n \, k_n}{2 \, D_h \, D_n}} \tag{14}$$

if a sufficient large number of particles is present, which means

$$\alpha \, q \, n_0 \, / \gamma \; > \; (\sqrt{D_h \, k_h} \; + \; \sqrt{D_n \, k_n})^2 \tag{15}$$

Here $n_0 = \phi \, / k_n$.

Computer simulations with 8000 particles, presented in Fig. 3 show the coexistence of spikes, which results in a nearly hexagonal pattern. In Fig. 3, the distribution looks still noisy, however indicates already a stationary inhomogeneous pattern. Simulations with larger particle numbers result in very regular patterns, as also discussed in the next section.
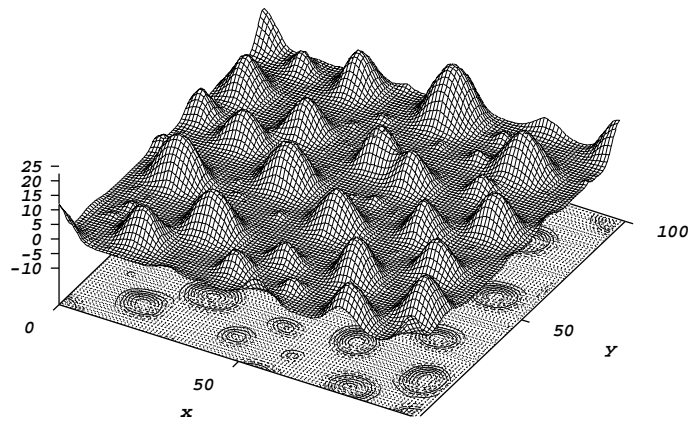

Figure 3: A stationary inhomogeneous field distribution $h(r, t)$. 8000 particles generate the self-consistent field which maxima attract the particles. The coexistence of spikes instead of a collapse to one single spike results from homogeneous adsorption and desorption of particles

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3.3 Formation of LIESEGANG-Like Ring-Distributions

The model introduced in Sect. 3.2. can be generalized by considering that particles, denoted by A are injected at the origin with a constant rate. The particles perform Brownian motion, which results in an inhomogeneous flux induced by the injection procedure. It is assumed that the A-particles react with a second species B, equally distributed on a surface, to form a species C

$$A + B \rightarrow C. \tag{16}$$
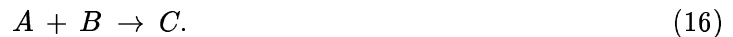
The species B should exist as a finite number of particles at each site of the lattice, which do not move. The C particle resulting from the reaction perform Brownian motion and generate a field $h(r,t)$ which concentrates the particle in its maximum, as already described in Sect. 3.1. Further, the species C is able to precipitate. This situation is known from experiments of LIESEGANG rings (MÜELLER *et al.*, 1982).

As a result of computer simulations, an occurring pattern is shown in Fig. 4. Here, a central cluster is surrounded by two rings of precipitated material, which begin subsequently to decompose into a sequence of clusters. The simulation was performed with 2.000.000 particles, thus the pattern looks much less noisy than in Fig. 3
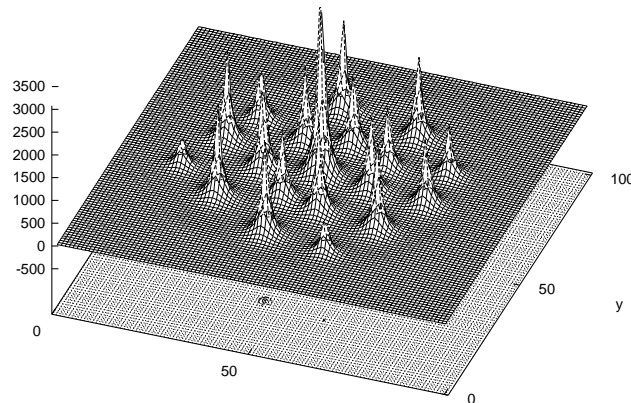

Figure 4: Ring-like distribution of clusters, where a central cluster is surrounded by two rings decomposing into small spikes. The pattern is generated with $2 \cdot 10^6$ particles and reminds on LIESEGANG rings

3.4 Travelling Waves

As ROVINSKY AND MENZINGER (1992) have shown, activator-inhibitor systems with the ability to generate TURING-structures are also able to generate periodic *moving* structures. If the inhibitor

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moves with an overcritical velocity $v_0 > v_0^{crit}$ relative to the activator, a differential flow induced chemical instability occurs. This instability leads to a periodic pattern, resulting from the fast moving inhibitor which violates the local equilibrium.

We have investigated the exothermic reaction of a cross flow reactor (YAKHNIN *et al.*, 1994):

$$A \xrightarrow{k} B + heat \tag{17}$$

with the temperature dependent rate

$$k(T) = k_0 \exp(T / (T_0 + T)) \tag{18}$$

In order to avoid an unlimited increase of B, it is assumed that B permanently flows out with a rate β. Based on the idea of a cross-flow reactor, this depletion is compensated by an inflow of particles A that way that the total number $A + B = C$ should be locally constant. During the computer simulatons, this is simply realized by assuming a second reaction $B \to A$ without heat.

In the system considered, the temperature plays the role of an activator, which increases locally due to the reactions and in turn amplifies the reactions again. With respect to the thermal conduction, the temperature balance reads as follows:

$$\frac{\partial}{\partial t} T = q\, k(T) \sum_{i=1}^{K} \delta(r - r_i(t, s = 1)) - k_T\, T + \chi\, \Delta T. \tag{19}$$

q is the heat released during one reaction, k_T represents the coupling to a thermal bath outside the reactor. Also the microscopic density of the A particles with position $r_i(t, s = 1)$ contributes to the temperature balance. Here, s labels the species of the particle, $s = 1$ stands for A-particles whereas $s = 0$ indicates B-particles, respectively. The corresponding LANGEVIN-equation for the motion of the A and B particles reads in the one-dimensional case as follows:

$$\frac{dr_i(s)}{dt} = v \quad ; \quad \frac{dv_i(s)}{dt} = -\gamma\,(v_i(s) - v_0) + \sqrt{2\,\varepsilon\,\gamma}\, \xi_i(t). \tag{20}$$

In the average, all particles move with velocity v_0 relative to the temperature field $T(r, t)$. Their label s changes according to the chemical reactions: With probability $k(T(r,t))\Delta t$, the transition $s = 1 \to s = 0$ is realized, resulting in a local increase of the temperature. Otherwise $s = 0 \to s = 1$ occurs with probablity $\beta \Delta t$ during the time intervall Δt.

In Fig. 5 we show the occurrence of travelling periodic patterns as a result of computer simulations with $50000\,A$ and B particles, moving according to eq. (20). During every time step, each particle has a certain probability to undergo a chemical reaction, i.e. to change the label s. The temperature distribution corresponds to the field $h(r, t)$, introduced in Sect. 2, and is integrated on a grid during the simulation. The simulation is very stable and fast, and the results are in good agreement with those obtained by YAKHNIN *et al.*, (1994).
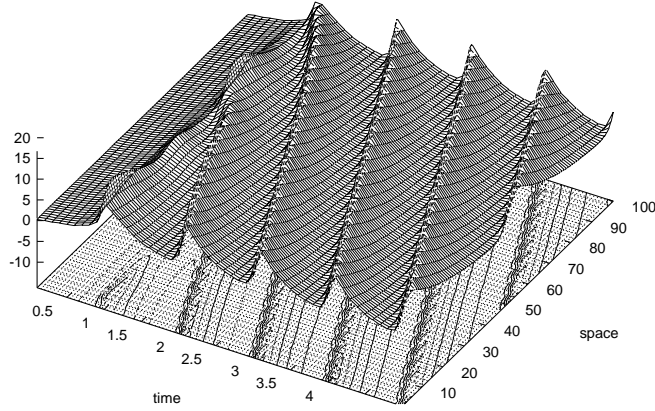
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Figure 5: Space-time plot of traveling periodic structures which occur in the temperature field. The simulation was carried out by 5000 particles.

3.5 Spiral Waves

In a next example, we investigate excitable systems with small particle numbers, which are able to form stable spiral-waves. To simulate this behaviour we use the piece-wise linear RINZL-KELLER-model (MIKHAILOV, 1994)

$$\frac{\partial}{\partial t}\, n(r,t) = -k_n\, n + \Theta[n - a]\,(1 - m) + D_n\, \Delta n \tag{21}$$

$$\frac{\partial}{\partial t}\, m(r,t) = q\, n(r,t) - k_m\, m + D_m\, \Delta m \tag{22}$$

with $\Theta[y]$ being the Heavyside function. n should be the activator. If its concentration locally exceeds the excitation value a, a replication process of the activator starts. Further, the generation of activator is controled by the inhibitor $m(r,t)$ which is generated by the activator with a rate q. The higher the inhibitor concentration, the lower is the replication of n. Additionally, the activator and the inhibitor will decay with a rate k_n and k_m, respectively. Both components can diffuse, however, since the inhibitor influences the actual activator distribution only with some delay q^{-1}, the activator will be able to diffuse into regions where no inhibitor exists yet. As the result, a directed motion of the activator cloud in front of the inhibitor distribution occurs. Considering one spatial dimension, these clouds are pulses of excited regions moving with constant velocity, whereas in two spatial dimensions spirals will be formed.

The activator-inhibitor dynamics described above can be reformulated in terms of the stochastic model, introduced in Sect. 2. Hence, the inhibitor is identified with the field $h(r,t)$, and the activator concentration is replaced by the microscopic density, eq.(4). The motion of both types of particles is modeled by simple Brownian motion, all nonlinear dynamics is given by their chemical behaviour.

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According to the dynamics above, the chemical reactions are simulated as follows: The Brownian particle representing the activator, are permanently desorbed with the probability $k_n \Delta t$ during the time intervall Δt. If the local particle number $N(r,t)$ is above a critical value, N_c, an input of particles different from zero occurs, i.e. the medium is excited at these space co-ordinates. The local value of the input rate depends on the actual inhibitor concentration, $(1 - m(r,t))$. In nonexcited regions the input of particles is zero.

In our computer simulations, we have found waves of excitations as well as single and double spirals. A double spiral starting from an inhomogeneous activator distribution with two open ends is shown in Fig. 6. The well developed structure shown is formed by only about 10^4 particles. An additional advantage of our approach is given by the fact, that the activator dynamics has to be calculated only in regions where particles are present, in contrast to PDE's which often are integrated on the whole lattice.
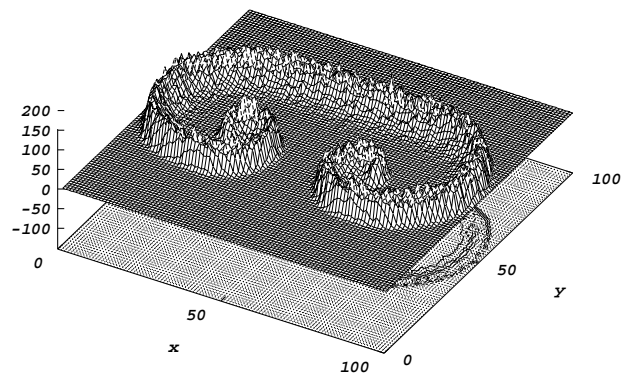

Figure 6: Double spiral of 10^4 activator particles. Initially a target wave with two open ends was considered which evolves to the two rotating spirals

3.6   Travelling Spots

WILLEBRAND *et al.*(1991) and LEE *et al.*(1994) presented experimental results of travelling, interacting and replicating spots, which have been explained as localized moving excitations. Recently, KRISCHER, MIKHAILOV (1994) discussed the complex impact behaviour of these spots. In order to obtain similar structures, we now introduce a global coupling of the excitation value N_c, as an extension of the model discussed in Sect. 3.5.

In our simulations, the exitation value N_c linearly increases with the global number of Brownian particles on the surface. Thus, the spirals are unable to grow up to their normal shape; only their mobility to move with constant velocity in one direction, remains. Fig. 7 shows a moving spot, and Fig. 8 presents one of the possible interactions between spots: Two colliding spots are

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reflected nearly perpendicular to their former motion, which has been also discussed by KRISCHER, MIKHAILOV (1994).
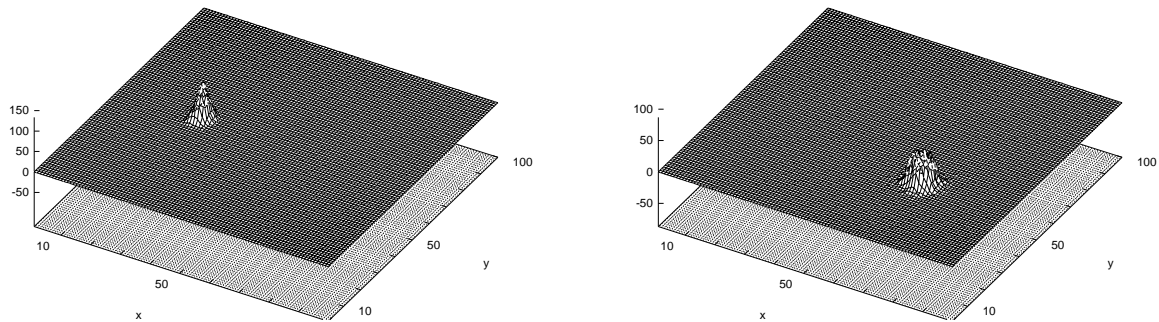
Figure 7: Spot of about 3000 activator particles moving as bounded region of excitation with constant velocity from the left to the right
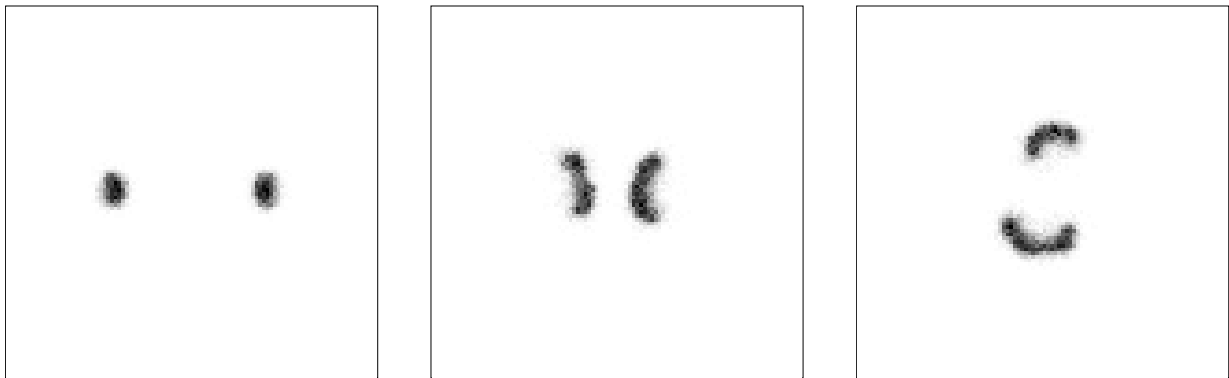
Figure 8: Impact of two travelling spots with reflection perpendicularly to the former motion. Black colour indicates regions of large particle numbers of the activator

Further investigations have shown that the character of the motion of these spots strongly depends on the number of particles forming a spot. For small particle numbers the spots perform nearly Brownian motion whereas for larger particle numbers the motion of the spots becomes more or less ballistic (FRICKE, SCHIMANSKY-GEIER, 1996).

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4 Pattern Formation with Active Brownian Particles Using Internal Degrees of Freedom

4.1 Basic Assumptions

In this chapter, we will simulate patterns which are intrinsically determined by the history of their creation. It means that irreversibility and early symmetry breaks play a considerable role in the determination of the final structure. Those structures are unique due to their evolution, and in order to consider this fact we need a stochastic approach, since the integration of PDE's only gives the average probability of finding a certain structure. As examples we will discuss self-assembling networks and directed trail patterns created by local nondirect interactions of the active Brownian particles.

As proposed by SCHWEITZER AND TILCH, (1996), the model introduced in Sect. 2 can be extended by considering active Brownian particles characterized by an internal degree of freedom (in fact, the example discussed in Sect. 3.4, can be also interpreted that way). This should be expressed by the parameter $\vartheta_i(t)$, which could have one of the following values: $\vartheta = \{0, -1, +1\}$. Initially, $\vartheta_i(t_0) = 0$ yields for every particle.

In the following, we consider a two-dimensional surface, where a number of nodes ($j = 1, ..., z$) are located at the positions r_{nj}. A number of n_+ nodes should be characterized by a positive potential, $V_j = +1$, while $n_- = z - n_+$ nodes have a negative potential, $V_j = -1$. The parameter ϑ_i of the Brownian particles could be changed only, if a particle during its motion hits one of the nodes. Then it takes over the value of the potential of the respecting node, V_j, which means $\vartheta_i = const.$, if $V_j = \vartheta_i$, and $\vartheta_i \to V_j$, if $V_j \neq \vartheta_i$. Further, we assume that the nodes do not have any long-range interaction with the particles, like attractive or repulsive forces. Their effect is restricted to their location, r_{nj}.

As assumed before, the active Brownian particles are able to generate a self-consistent field, which in the considered case, should be a chemical field consisting of two components, A and B. Which of these chemicals will be produced by the particle i, depends on the actual value of the internal parameter, ϑ_i. The production rate, $q_i(\vartheta_i, t)$, is defined as follows:

$$q_i(\vartheta_i, t) = \frac{\vartheta_i}{2}[(1 + \vartheta_i)q_A^0 \exp\{-\beta_A (t - t_{n+})\} - (1 - \vartheta_i)q_B^0 \exp\{-\beta_B (t - t_{n-})\}] \tag{23}$$

q_A^0, q_B^0 are the initial production rates and β_A, β_B are the decay parameters for the production of chemical A or B. Respectively, t_{n+}, t_{n-} are the times, when the particle hits either a node with a positive or a negative potential.

The chemical field generated by the particles is assumed again to obey a recation equation, as given in eq. (3), but diffusion is not considered here ($D_h = 0$). The field should influence the movement of the particles according to the LANGEVIN eq. (6). However, since the chemical field consists of two components A, B, we assume that the internal state of the particles determines which of the components affect the particle's movement:

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$$\vartheta_i = 0 \quad : \quad h(r,t) = 0$$
$$\vartheta_i = +1 \quad : \quad h(r,t) = h_B(r,t)$$
$$\vartheta_i = -1 \quad : \quad h(r,t) = h_A(r,t) \tag{24}$$

Here, $h_A(r,t)$, $h_B(r,t)$ mean the local concentration of the chemicals A and B, respectively.

Summarizing eqs. (23) and (24), our model assumes, that particles with an internal state $\vartheta_i = 0$ do not generate a field and are not affected by the field. Particles with an internal state $\vartheta_i = +1$ contribute to the field by producing component A, while they are affected by the part of the field, which is determined by component B. On the other hand, particles with an internal state $\vartheta_i = -1$ contribute to the field by producing component B and are affected by the part of the field, which is determined by component A.

4.2   Formation of Networks

Based on the model described in Sect. 4.1., the formation of self-assembling networks has been simulated (SCHWEITZER, TILCH, 1996). In the example considered, a set of nodes regularly distributed on a surface, should be linked. The connections have to be established by the active Brownian particles generating a two-component chemical field. In Fig. 9, we can observe the formation of macroscopic structures which resemble path networks to connect the given set of nodes.
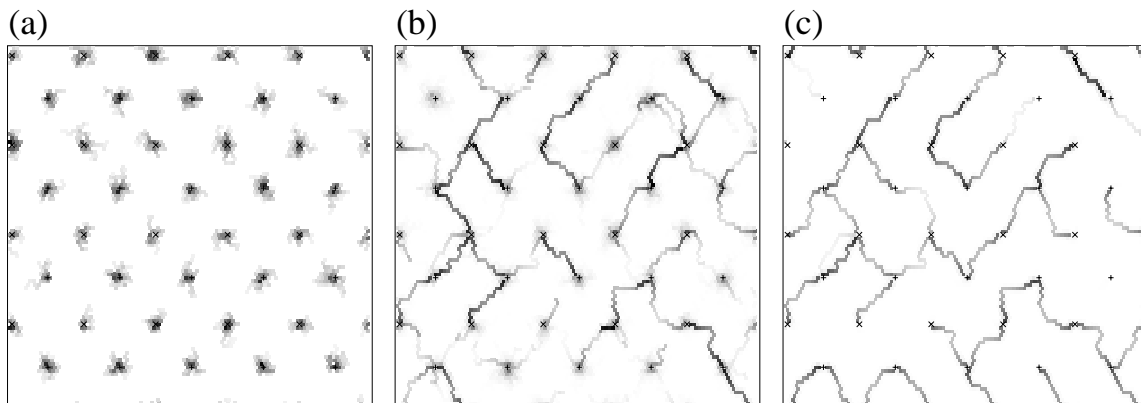

Figure 9: Time series of the evolution of a network after (a) 10 simulation steps, (b) 100 simulation steps, (c) 1000 steps. The network was generated by 5000 particles on a 100×100 lattice with 40 nodes

The network structures obtained are unique due to random forces which influence the formation of the different links in the very beginning. The connections already established, determine the creation of new ones, because of a screening effect which occurs between the different links. Therefore, the

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nodes are not connected in a regular structure. However, as shown in Fig. 9,c, almost all nodes are linked to the network by at least one link. This self-assembling network is created very fast and remains stable after the initial period.

4.3 Formation of Trails

The basic features of interactive structure formation, as provided by the model discussed, have a range of analogies within biological systems, e.g. to chemotactic processes. For example, ants lay a pheromone trail to use it for their orientation (HÖLLDOBLER, WILSON, 1990, CALENBUHR, DENEUBOURG, 1990), or, migrating cells generate a field which guides them during aggregation (SCHIENBEIN, GRULER, 1993).

Here, the model introduced in Sect. 4, is used to describe the formation of directed trails, which appear e.g. in foraging ants. Different from *non-directed* track patters, as obtained by computer simulations of trail-following ants (EDELSTEIN-KESHET, 1994) or of gliding myxobacteria which produce slime tracks commonly used for movement and aggregation (STEVENS, 1990, STEVENS AND SCHWEITZER, 1996), directed trails should link a starting point (e.g. a nest) to a destination point (e.g. a food source).

It has been shown (SCHWEITZER *et al.*, 1996) that characteristic features of trunk trail formation in foraging ants could be simulated by means of active Brownian particles, which do not have the capability of internal storage of information (e.g. of the location of the nest or the food), or of visual navigation (landmark use, route integration). (For simulations of the famous raiding patters of army ants, which are however different from the example considered here, cf. DENEUBOURG *et al.*, 1989.)

In the computer simulations outlined below, we assume on the two-dimensional surface a nest (in the center of the lattice) where the particles are initially concentrated, and an extended food source which is at a larger distance from the nest (at the top/bottom lines of the lattice). Both, the nest and the food sources, *do not attract* the particles by a certain long-range attraction potential, they are just particular sites of a certain size. The particles do not have any information about the location of the nest or the food sources. They only use the local orientation provided by the concentration of that chemical which they are sensitive for and they only make a local decision about the next step.

In addition to the features of the particles described in Sect. 4.1., we introduce some specific assumptions of the model, adapted from biological observations of ants (HÖLLDOBLER, WILSON, 1990). Initially a group of particles, which we call the scouts, leave their nest. Along the way, they drop a trail chemical, denoted by A. If a scout hits a food source by chance, it begins to drop a different chemical, B, indicating the discovery of the food source. But it continues to be sensitive to chemical A, which provides local orientation, and therefore increases the chance that the scout is guided back to the nest.

When a scout that drops chemical B should return to the nest, it recruits a number of particles to move out. The recruits are different from the scouts only in that they are sensitive to chemical B -

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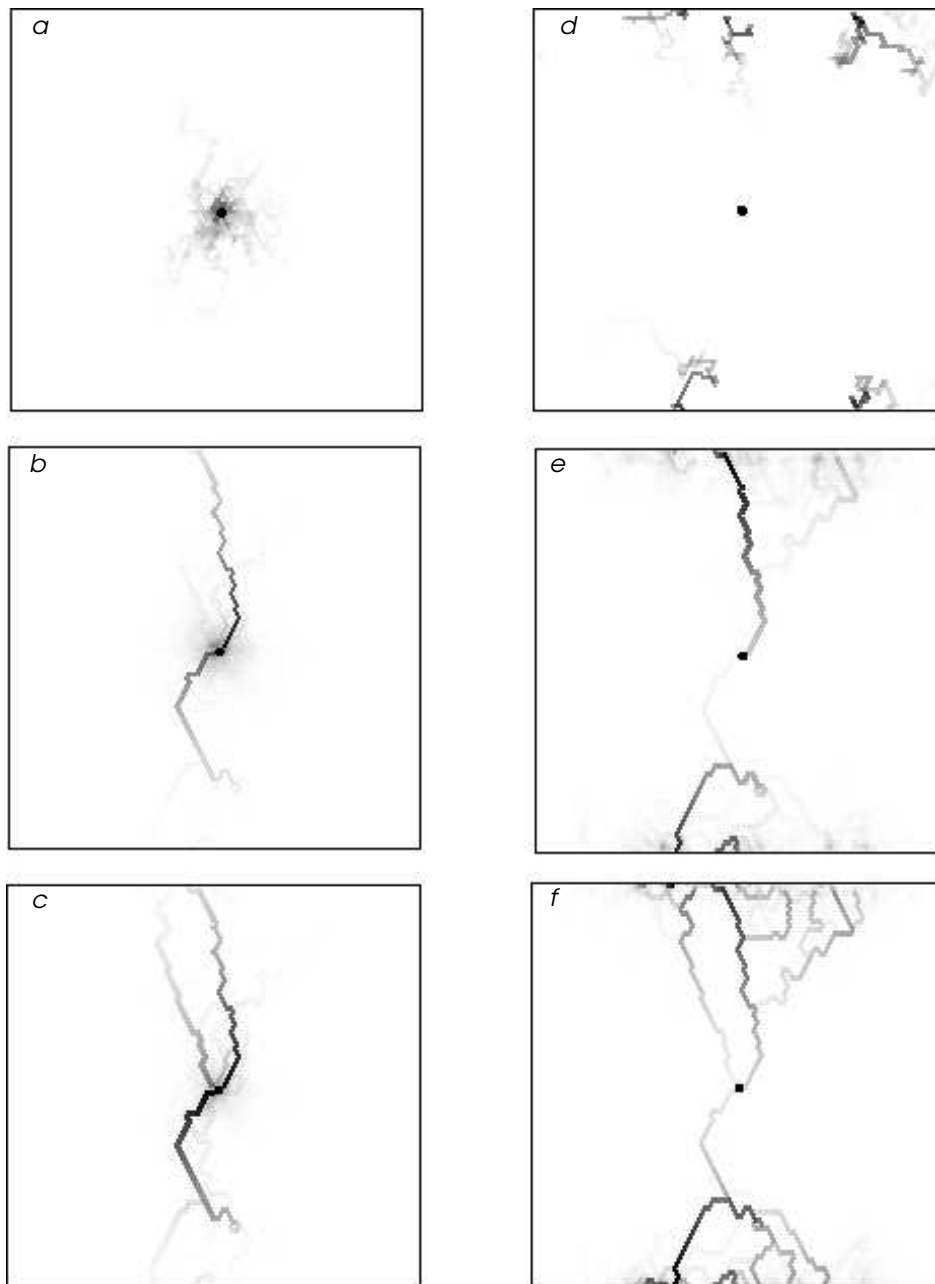Gordon and Breach, London 1997, pp. 101-118

Figure 10: Formation of trails from a nest (middle) to a line of food at the top and the bottom of a lattice. (a-c) show the distribution of chemical A, and (d-f) show the distribution of chemical B, after 1000 steps in (a) and (d), 5000 steps in (b) and (e), and 10000 steps in (c) and (f).(SCHWEITZER *et al.*, 1996)

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and not to A - when they start from the nest, but they also drop chemical A as long as they have not found any food. If a recruit hits a food source, it also begins to drop chemical B and becomes sensitive to chemical A, which should guide it back to the nest where it, indicated by dropping chemical B, can recruit new particles.

In order to increase the mobility of the active particles in cases, where they don't find food, we assume that every particle has an individual sensitivity to respond to the chemical field, which is related to the inverse of the temperature (or to the thermal noise). As long as the particle does not hit a food source, this sensitivity is continuously decreasing, meaning, that the particle more and more ignores the chemical field and thus becomes able to choose also sites not visited so far. However, if the particle does not find any food source after a certain number of steps, it "dies" at a critical low sensitivity and is removed from the system. On the other hand, if the particle hits a food source, this sensitivity is set back to the initial high value and is kept constant to increase the chance that the particle finds its way back along the gradient of the chemical.

Figs. 10 a-f show the time evolution of a trail system which connects a nest and some food sources, in terms of the spatial concentration of the chemicals A (left) and B (right). In the initial period of the simulation, no trail exists between the food and the nest, indicated in the non-overlapping concentration fields of both components. But, after a time lag of desorientation, the emergence of disctinct trunk trails can be clearly observed. A match of the concentration fields for both chemicals A and B for the main trails shows that the particles indeed use the same trunk trails for their movement towards the food sources and back home. The exhaustion of some food clusters and the discovering of new ones in the neighorhood results in a branching of the main trails in the vicinity of the food sources (at the top or bottom of the lattice), leading to dendritic structures. The trail system observed in Figs. 10 c,f remains unchanged in its major parts - the trunk trails, althrough some minor trails in the vicinity of the food sources slightly shift in time - as has been reported also in the biological observations of trunk trail formation in ants (HÖLLDOBLER, MÖGLICH, 1980).

5   Conclusions

It was our purpose to develop an algorithm for interactive structure formation with active Brownian particles, which is applicable to a broad range of different problems. As we have demonstrated, standard patterns known from reaction-diffusion systems could be simulated in a very fast and efficient manner, as well as complex structures, like networks or trail systems.

We want to point out the more general approach of our model, in contrast to the PDE-based description of usual recation-diffusion systems. Our model considers fluctuations which are always present, and is applicable also to problems where only small particle numbers govern the process of structure formation. Moreover, our particle-based approach to structure formation, in a self-consistent way, considers intrinsic effects of self-organized processes, as the non-linear interaction between particles and environment, early symmetry-breaks and the emergence of new qualities, not readily predictable from the basic equations.

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