SIMULATIONS OF LOCALIZED DISSIPATIVE STRUCTURES IN EXCITABLE MEDIA BY AN ENSEMBLE OF BROWNIAN WALKERS*

Marcin Kostur[a,b] and Lutz Schimansky-Geier[a]

[a]Institut für Physik,Humboldt-Universität zu Berlin
D-10115 Berlin, Germany
[b]Institute of Physics, University of Silesia
Uniwersytecka 4, 40-007 Katowice, Poland

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The effective method of simulation of stochastic excitable media by en ensemble of Brownian particles is presented. The system studied is a variant of Rinzel–Keller model with global inhibition. The formation, time evolution, and statistical properties of localized structures — spots — are investigated.

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1. Introduction

Beside the great breakthrough in the understanding of the physical side of nature, which has been caused at the beginning of XX century by the development of Quantum Mechanics and Relativity Theory, the notion of self-organization in non-equilibrium systems has led to the remarkable changes in outlook upon the living nature. The fact that a system can increase its complexity, which was before thought to be a feature of the living *materia*, has also been observed in experiments with non-living objects. Since the first works, structure formation phenomena have attracted much attention from both theoretical as well experimental scientists over.

In the beginning of 50's the Russian chemist Belousov observed temporal oscillations in the concentration of some chemicals during catalytic oxidation of citric acid [1]. This, as it was ahead of its time, was strongly criticized and due to its novelty was not even taken seriously[1]. One had to wait till the

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[1] His manuscript was rejected due to the referee comments "it is impossible". A brief survey of Belousov life and work can be found on Web page http://www.math.chalmers.se/~jacques/kf2na/Historia/Belousev.html

70's, when the new findings of a study in the field of non-equilibrium thermodynamics made by groups of Prigogine and Haken dramatically changed common beliefs on the complexity of systems (see *e.g.* [2,3]). In this time, Belousov's work was continued by A.M. Zabotynsky. He modified the original reaction; his variant was easier to reproduce and the oscillations were visualized by changes of color [4]. Finally, due to his contribution, the existence of chemical oscillations have been accepted in professional circles. Nowadays, the so called Belousov–Zabotynsky (BZ) reaction due to its novel and universal features belongs to one of the most popular chemical reactions, even amongst non-chemists.

If one conducts the BZ reaction in a medium where the diffusion length of reactants is smaller than the size of the reaction volume, spatial patterns appear — chemical waves [5]. There are many types of chemical waves possible, the most frequently investigated are rotating spirals. They have attracted much attention in recent years many different aspects have been studied *e.g.*: the problem of the motion of spiral tip [6], the influence of fluctuations on its motion, [7] and the control of the spiral tip by the means of feedback effects [8,9].

The structure formation is not only limited to the BZ reaction; in principle any nonlinear spatially extended system with *e.g.* excitable type in some regime becomes a medium where dissipative structures can exist. Experimentally, some such systems are know like the catalytic oxidation of CO on Pt(110) [10], and the gas discharge and transport processes in semiconductors [11]. In these systems, however, other factors become significant. Firstly the *global coupling* plays an important role. In the case of catalytic oxidation processes it is due to coupling of different reacting parts of solid phase via partial pressure variation of the surrounding gas phase. Secondly, in contrary to the structures obtained in typical BZ reaction, the structures observed in the above processes are microscopic, hence the influence of *fluctuations* becomes important.

In this paper we will study localized structures which arise in excitable medium with global inhibition — *spots*. Such structures have been investigated theoretically in [12]. It has been shown that spots can be in two regimes: traveling and stationary. The aim of our work will be to investigate how the internal fluctuations influence the behavior the spots. In order to to that we will propose a particle oriented algorithm, which will naturally include random factors. The paper is organized as follows: in the next section we present the system of interest, in the third section we explain the method of simulation used here, in the fourth section the main results are presented.

2. The model system

We will here consider an excitable system which is a variant of Rinzel–Keller model [13] described by following Reaction–Diffusion equations:

$$\begin{aligned} \partial_t u &= k_u \theta(u-a)(v_0 - v_{\text{kopp}} v) - k_{su} u + D_u \nabla^2 u, \\ \partial_t v &= k_v u - k_{sv} v + D_v \nabla^2 v, \end{aligned} \tag{1}$$

where u and v are concentrations of activator and inhibitor correspondingly, k_i are kinetic constants, θ is Heaviside step function, a is an excitability threshold, and D_u, D_v are diffusion constants. Notice that the only nonlinearity is the term containing the step function $\theta(u-a)$. Above system due to its excitable kinetics exhibits such features as: moving excitable fronts, rotating spiral waves etc. In order to obtain the localized solutions we will impose the global inhibition:

$$a = a_0 + \mu \iint u(x,y)dxdy, \tag{2}$$

where μ is global inhibition constant. The stable solution of the system (1) with (2) is the localized excitation, which looks as a piece of spiral with end which are hindered to grow. The value of the coupling strength μ controls its shape (see figure 1). We are interested in the case of large μ — in such a case the spot is well localized.

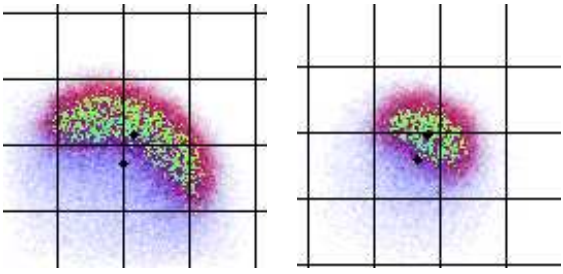

Fig. 1. Spots for small $\mu = 1.2$ (left) and large $\mu = 2.2$ (right); the number of particles is different but the shape changes dramatically.

3. The simulation by an ensemble of Brownian particles

There are several methods of simulating Activator–Inhibitor systems on the microscopic scale. They differ in assumptions, the precision, and the required amount of computational power. Perhaps the most straightforward approach is the numerical simulation of mean field equations with an additional noise term. This, however, does not guarantee that the microscopic origin of fluctuations are sufficiently good reproduced. Nevertheless

the efficiency of such treatment, especially for one dimensional systems, has been commonly used [14]. The next, recently very popular and efficient way of producing spatial structures, are Cellular Automata (CA) [15–18]. The biggest advantage of this approach is its computational efficiency, however pictures of microscopic scale is in this approach relatively rough. In the contrary the most accurate is a direct simulation of individual molecules: Molecular Dynamics. Unfortunately it is computationally the most expensive method. Here we will propose a particle oriented algorithm which due to some approximations is not as precise as MD, however is well reflecting underlying molecular nature of the medium.

We represent each field u and v by an ensemble of Brownian particles which performs a stochastic motion on two dimensional domain as well as are destroyed or born according to deterministic kinetics.

The additional parameter which appears in such approach is the number of particles. It controls the amount of noise in our system: less particles we put in the simulation, more noisy picture we get. In the limit of infinite number of particles we expect the quantitative equivalence with the deterministic model described by the equation (1). We want to introduce the number of particles independently of the mean field properties of the medium. Therefore we will scale the concentration $\hat{u} \equiv N/V$ by the density ρ: $u = \hat{u}/\rho$. The interpretation of ρ if following: it is a number of particles which are on the average in the unit of volume when the dimensionless concentration is $u = 1$. In our simulation the typical values of ρ will vary between 3000–100000.

Let us explain details of the implementation. The diffusion terms $D_u \nabla^2 u$ ($D_v \nabla^2 v$) in (1) are simulated by the Langevin dynamics:

$$\begin{aligned} \dot{x}_i &= \sqrt{2D}\xi_i(t), \\ \dot{y}_i &= \sqrt{2D}\eta_i(t), \end{aligned} \tag{3}$$

where $\xi_i(t)$ and $\eta_i(t)$ are uncorrelated white Gaussian noises.

Linear terms in (1) can be straightforwardly implemented in terms of birth and death processes. The only term in (1) which includes many particles interaction is and can not be simulated in particle picture directly without taking into the account correlation between particles is: $k_u \theta(u-a)(v_0 - v_{\mathrm{koppl}} v)$. In the sake of efficiency we will introduce following approximation. We introduce the rectangular grid with box volume V_{B}. During each time step the number of particles in each box n_i is calculated. Then, having the density ρ we can calculate the local concentration in the box $u_i = n_i/(\rho V_{\mathrm{B}})$. The field of local concentrations is used for evaluation of the nonlinear θ-term in (1). It is done in two steps:

- In each box it is checked if $u_i > a$ ($\theta(u_i - a)$), if so the box is marked as excited.

- Each excited box box produces particles with a rate $\rho V_{\mathrm{B}}(v_0 - v_{\mathrm{koppl}} v)$; new particles are placed within the given box with random position.

The natural time stepping is given by the simulation of the Langevin dynamics (3). The counting of particle on a grid is done once per simulation step.

We have simulated spots using above algorithm with following restrictions concerning characteristic volumes and macroscopic observable — the size of the spot V_s:

- $V_s \ll V_{\mathrm{B}}$; the spot should be much bigger than anisotropy of the medium.

- $V_{\mathrm{B}} \geq V_p$; if the volume of the particle is bigger than the box it means that there are less than one particle per box in excited region. Thus the relative fluctuation of the particles are extremally large. In such a case the spot is usually unstable and we are not interested in such regime.

4. Results

At first let us look at the spot for different parameters values. The basic control on the size of the spot is provided by the global inhibition constant μ. In the figure 1 we have plotted two spots for different values of $\mu = 1.2$ and 2.2. The spot with the smaller feedback is larger and resembles more a piece of spiral whereas the strongly inhibited one is almost round. The medium here has a constant particle density — the number of particles of which the spot is built is proportional then to its area. Hence, one could have used the global inhibition as a control of the transition between microscopic and macroscopic spots. However, as we see in figure 1, not only the size but also the shape of spot is influenced by the change of μ. Therefore in order to isolate features connected with the particle number of the spot, we decided to use the density of the medium ρ. The spots for different ρ have approximately the same shape but differ in the number of particles (see figure 2). In this paper we will consider only the spot with relatively strong global inhibition $\mu \simeq 2.0$ (like in figure 2).

In the contrary to the deterministic case, due to the stochastic character of the simulation the spot never becomes stationary. It changes the shape and the direction of motion permanently. We neglect the fluctuation of the

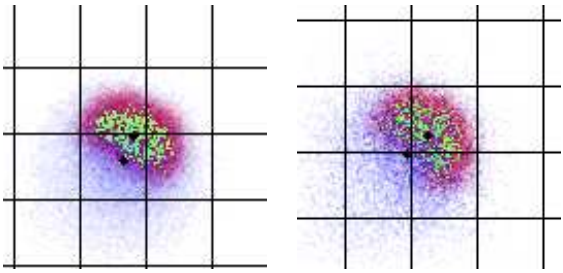

Fig. 2. Spots for small $\rho = 42000$ (left) and large $\rho = 10000$ (right). The number of particles is different without essential change of the shape.

shape and take trace of the center of mass:

$$\vec{x}_u(t) = \frac{1}{U}\int dx\vec{x}u(\vec{x},t), \tag{4}$$

$$\vec{x}_v(t) = \frac{1}{V}\int dx\vec{x}v(\vec{x},t), \tag{5}$$

where $U = \sum u_{ik} = \int u(x)dx$ and $V = \int v(x)dx$. A typical path of $\vec{x}_u$ is depicted in figure 3.

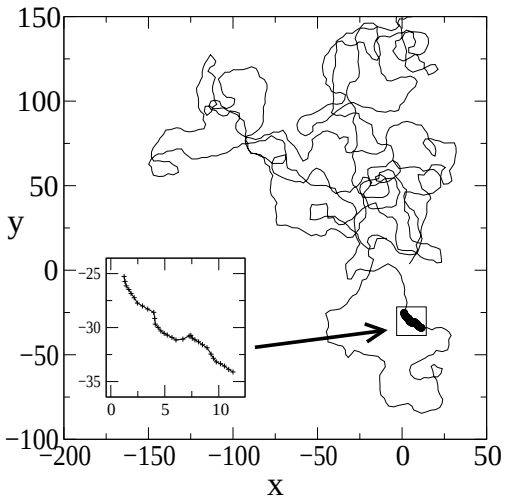

Fig. 3. A typical trajectory for a running spot in presence of fluctuation. In the insert we show magnification, of the trajectory. On the large scale the path looks similar to Brownian particle but on small scale the correlation of the direction of motion are noticeable.

4.1. Transition from ballistic to diffusive motion controlled by internal fluctuations

The trajectory of the spot on short time scale (see figure 3) exhibits features of the ballistic motion (the velocity and direction remain constant). On the other hand on the large time scale the motion seems to be of diffusional type. This has been thoroughly investigated by measuring the displacement of the spot from the initial point and averaging over an ensemble of realizations. In the general case the dependence of mean square displacement of the particle position can be written in the form:

$$\sqrt{\langle \Delta r^2 \rangle} = \sqrt{2D} t^{\alpha}. \tag{6}$$

The exponent α is equal to one for ballistic motion and 1/2 for pure diffusive one. Therefore one could expect a transition from ballistic to diffusive motion for on a certain time-scale. The another appropriate indicator of character of the motion of particle is the correlation function of velocity. At small time-scales one should expect strong correlation of spot's velocity, while for long time intervals the velocity should be uncorrelated.

We have generated an ensemble of long enough trajectories of the spot, then the mean displacement from initial point, the exponent α and finally the correlation function of the velocity $c(t)$ have been calculated. In figure 4 we have plotted for running and stationary spots all above characteristics. Firstly one can notice that the exponent α varies from 1 for small time scales ($t < 100$) to 0.5 for long times ($t > 1000$). Secondly, the time when the correction function vanish coincides with the time of the transition α : $1 \to 0.5$.

The numerical experiment has been repeated for different number of particles; the controlled by the parameter ρ. The number of particles is connected with the amount of noise in the system: smaller value of ρ, larger fluctuations occur in the system. The results are shown in figure 4. One can observe that more noisy running spots undergo the transition into the diffusive motion on shorter time-scale then less noisy ones.

It has been shown in [12] that the steady solution of reaction–diffusion system might be in one of two regimes: steady or moving. The transition between those states can be controlled by the diffusion of inhibitor D_v. We have also studied the influence of macroscopic features of the spot on the transition point. For values of inhibitor diffusion: $D_v = 0.30, 0.20, 0.11$ we have analyzed the trajectory as in the previous case figure 5. The transition point depends significantly on the type of spot. For stationary spots the ballistic motion is changes into diffusive for shorter times.

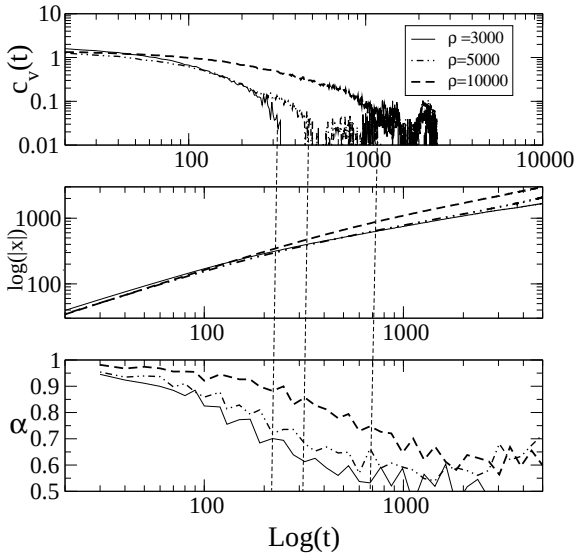

Fig. 4. The comparison of statistical properties for spots with consisting of different number of particles. The spot is in running regime: $D_v = 0.2$. The number of particles is controlled via parameter $\rho = 3000, 5000, 10000$. One can observe that the transition from ballistic into diffusive motion is shifted to smaller times as amount of noise increases (ρ decreases). In the upper plot we have shown the correlation function of velocity $c_v(t)$, in the middle the mean displacement of the spot, and the bottom contains the exponent α (see equation (6)).

4.2. Mean field limit

The important issue is the question whether the particle algorithm can reproduce the mean field description in the limit of large number of particles on correspondingly small grid:

$$\begin{aligned} \rho &\to \infty, \\ V_{\mathrm{B}} &\to 0, \\ \rho V_{\mathrm{B}} &\simeq \text{const.} \gg 1. \end{aligned} \tag{7}$$

We have been able to increase the number of particles to *ca.* 10^6 and number of boxes to *ca.* 10^5. In this case we expect that the properties of the spot are comparable with properties of deterministic spot *i.e.* the solution of the system (1). Because one of the most important parameters of the spot is its velocity, we have compared distribution function of velocities of the stochastic spot with the numerically obtained value of velocity of deterministic spot. In figure 6 we have plotted the velocity distribution for three spot build by increasing number of particles and deterministic velocity for the same macroscopic parameters. We see that the algorithm reproduces solution of RDS system when the number of boxes within one spot and number of particles which compose one spot are large.

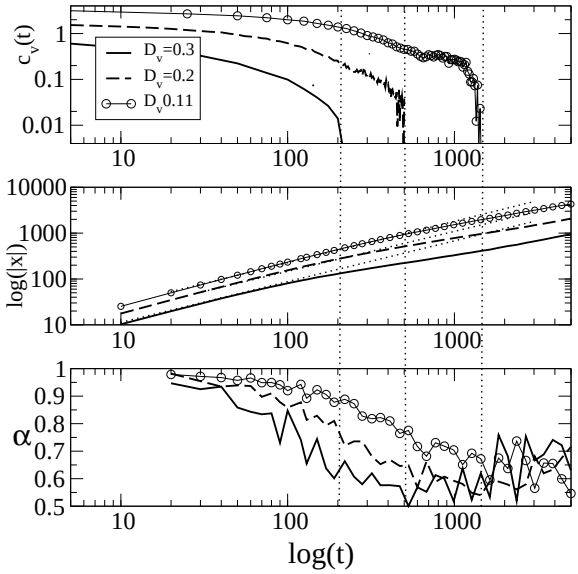

Fig. 5. The comparison of statistical properties for spots with different velocities controlled via diffusion constant of inhibitor D_v. The spot consists of relatively small number of particles: $\rho = 5000$. The upper plot shows exponent α, middle correlation function of velocity $c(t)$, and the last shows mean displacement. The straight lines show approximately time scales at which the transition from ballistic into diffusive motion occurs. In the upper plot we have shown the correlation function of velocity $c_v(t)$, in the middle the mean displacement of the spot, and the bottom contains the exponent α (see equation (6)).

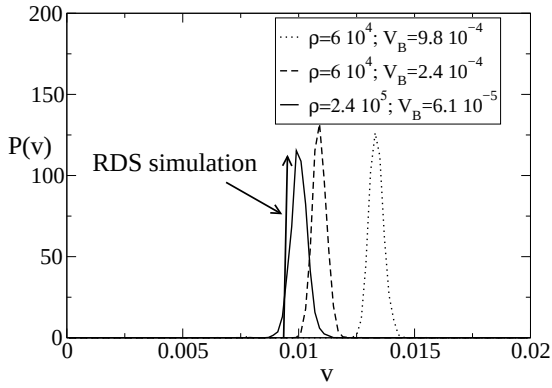

Fig. 6. The radial part of velocity distribution for a spot for different grid sizes (V_{B}) and particle densities (ρ). The velocity approaches the mean field result in the limit (7).

5. Summary

We have presented a way of simulating stochastic excitable media. The main concern was to study the influence of internal fluctuation on the behavior of the dynamics of spot. Using our algorithm we have shown that the spots perform of short and long time-scales two different kinds of motion. On the short time-scale the velocity is strongly correlated and the motion is of ballistic type. The long time-scale is, in turn, dominated by diffusion like motion, which is characterized by vanishing correlations of velocity. Those two time-scales are connected by the transitional region ($0.5 < \alpha < 1$). The time where this transition occurs is strongly influenced by the fluctuations. In general the stronger internal noise shifts the transition toward shorter time-scales.

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