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Pattern formations and optimal packing

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ABSTRACT

Patterns of different symmetries may arise after solution to reaction–diffusion equations. Hexagonal arrays, layers and their perturbations are observed in different models after numerical solution to the corresponding initial-boundary value problems. We demonstrate an intimate connection between pattern formations and optimal random packing on the plane. The main study is based on the following two points. First, the diffusive flux in reaction–diffusion systems is approximated by piecewise linear functions in the framework of structural approximations. This leads to a discrete network approximation of the considered continuous problem. Second, the discrete energy minimization yields optimal random packing of the domains (disks) in the representative cell. Therefore, the general problem of pattern formations based on the reaction–diffusion equations is reduced to the geometric problem of random packing. It is demonstrated that all random packings can be divided onto classes associated with classes of isomorphic graphs obtained from the Delaunay triangulation. The unique optimal solution is constructed in each class of the random packings. If the number of disks per representative cell is finite, the number of classes of isomorphic graphs, hence, the number of optimal packings is also finite.

1. Introduction

The Turing mechanism for reaction–diffusion equations models biological and chemical pattern formations. This approach was widely discussed in literature and supported by many numerical examples (see the recent books [2,4,5] and many works cited therein). Patterns of different symmetries may arise after solution to reaction–diffusion equations. Hexagonal arrays, layers and their perturbations are observed in different models after numerical solution to the corresponding initial-boundary value problems for nonlinear partial differential equations. However, these models do not answer the question, why the most frequently observed patterns are close to the optimal packing structures. Why do the hexagonal array arise? One can see, for instance, that a resulting structure can be the hexagonal array disturbed by pentagon inclusions. Is it related to a model approximation or to an inherent feature of pattern formations?

In the present paper, we try to answer the above questions to demonstrate an intimate connection between pattern formations and optimal random packing on the plane. The main study is based on the following two points. First, the diffusive flux in reaction–diffusion systems is approximated by piecewise linear functions in the framework of structural approximations [3,7]. This leads to a discrete network approximation of the considered continuous problem. Second, the discrete energy minimization yields optimal random packing of the domains in the representative cell. The packed domains are approximated by equal disks. This approach is described in the bulk of the paper.

Packing problems refer to geometrical optimization problems [11]. In the present paper, we consider the optimal packing of disks on the plane in the random statement fitted to the description of pattern formations. Optimal packing in the classic deterministic statement is attained for the hexagonal array when the packing concentration holds $\frac{\pi}{\sqrt{12}}$ [11]. Computer simulations demonstrate that random packing have a lower density and depends on the protocol of the random packing [1].

It is shown in Section 3 that pattern formations lead to the optimal random packing problem in the equivalence classes of graphs obtained by means of the Delaunay triangulation. The justification of such an approach is based on the observation that solution to the physical problem of the optimal diffusion implies solution to the geometrical problem of the packing disks [8]. The unique optimal solution is constructed in each class of the random packings. If the number of disks per representative cell is finite, the number of classes of isomorphic graphs, hence, the number of optimal packings is also finite.

The proposed method to study pattern formations is based on the minimization of the discrete energy for graph structures by analytical and numerical methods within treatment of PDE by

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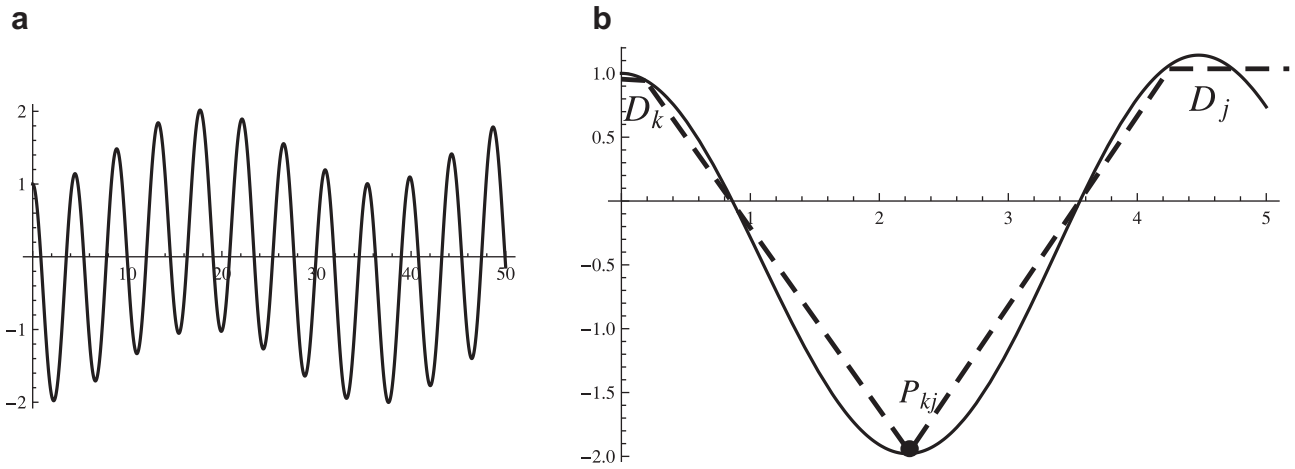

Fig. 1. (a) Dependence of the inhibitor on the spatial variable. (b) Piecewise linear approximation of the inhibitor on a smaller interval (dashed line). The maxima are approximated by segments D_k and D_j (disks in 2D) and the minima by points P_{kj} (segments in 2D).

the structural approximation method. Though PDE are not directly written in the paper, they are implicitly used in estimations of the local flux between local spatial extrema of the inhibitor.

2. Structural approximation

The Turing mechanism can create temporally stable and spatially non-homogeneous structures. In order to present the main idea of the structural approximation we consider 1D Schnakenberg system [5, p. 156]. A typical dependence of the inhibitor on the spatial variable is displayed in Fig. 1a. It is assumed that such a dependence can be approximated by a piecewise linear function as shown in Fig. 1b. The solution of the continuous reaction–diffusion equations is approximated by the discrete diffusion model with the constant diffusion fluxes (derivatives of the linear approximations) between the extrema of the potential.

A similar approximation can be extended to multidimensional reaction–diffusion equations [9]. In the present paper, we deal with 2D double periodic structures. Let $\mathbf{e}_1 = (e_1, 0)$ and $\mathbf{e}_2 = (e_{21}, e_{22})$ be the translation vectors of the lattice $\mathcal{Q} = \{l_1\mathbf{e}_1 + l_2\mathbf{e}_2 : \ l_{1,2} \in \mathbb{Z}\}$ where $\mathbb{Z}$ denotes the set of integer numbers. Consider the periodic representative cell

$$Q_0 = \{\mathbf{x} = t_1\mathbf{e}_1 + t_2\mathbf{e}_2\}, \ 0 < t_{1,2} < 1\}.$$

For simplicity, we approximate the places of maximal diffusion potential by equal disks D_i $(i = 1, 2, \dots, N)$ of radius r centered at the set of points $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_N)$ displayed in Fig. 2. The maxima of the diffusion potential are approximated by disks and the minima by lines. Every line segment P_{kj} is perpendicular to the segment $(\mathbf{a}_k, \mathbf{a}_j)$, its length holds $|P_{kj}| = 2r$ and it is divided onto equal parts by $(\mathbf{a}_k, \mathbf{a}_j)$. The described approximations fits for functions of type shown in Fig. 1. Appendix contains a formal general description of the approximations.

It is convenient to introduce new distance (metric) as follows. Two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^2$ are identified if their difference $\mathbf{a} - \mathbf{b} = l_1\mathbf{e}_1 + l_2\mathbf{e}_2$ belongs to the lattice $\mathcal{Q}$. Hence, the classic flat torus topology with the opposite sides welded is introduced on the cell Q_0. The distance $\|\mathbf{a} - \mathbf{b}\|$ between two points $\mathbf{a}, \mathbf{b} \in Q_0$ is introduced as

$$\|\mathbf{a} - \mathbf{b}\| := \min_{l_1, l_2 \in \mathbb{Z}} |\mathbf{a} - \mathbf{b} + l_1\mathbf{e}_1 + l_2\mathbf{e}_2|, \tag{2.1}$$

where the modulus means the Euclidean distance in $\mathbb{R}^2$ between the points $\mathbf{a}$ and $\mathbf{b}$.

Construct the double periodic Voronoi diagram and the Delaunay triangulation corresponding to the set $\mathbf{A}$ on the torus $\mathcal{Q}_0 = \cup_{l_1, l_2 \in \mathbb{Z}}(Q_0 + l_1\mathbf{e}_1 + l_2\mathbf{e}_2)$. The edges of the Delaunay triangulation E correspond to linear approximations of the diffusion flux between disks. The Delauney triangulation of the vertices $\mathbf{A}$ consists of straight lines connecting by pairs points of $\mathbf{A}$ belonging to neighbor Voronoi regions.[1] Let the neighborhood relation between two vertexes be denoted by $\mathbf{a}_j \sim \mathbf{a}_k$ or shortly $j \sim k$. We call the constructed double periodic graph $(\mathbf{A}, E)$ by the Delaunay graph.

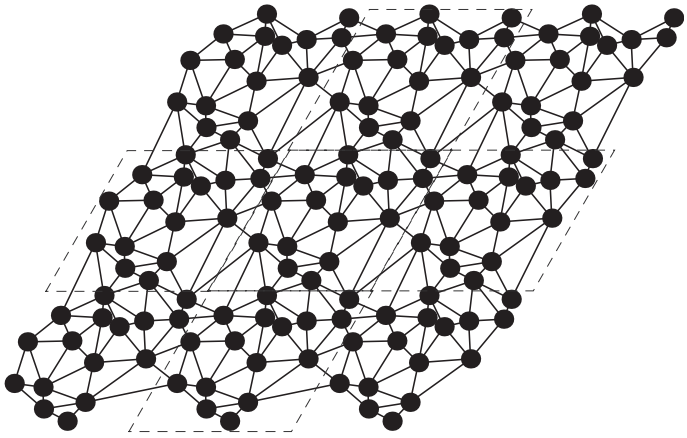

Fig. 2. 2D approximation of the inhibitor. The diffusion potential is approximated by appropriate constants in disks and the diffusion flux between the disks by linear functions along the edges of the Delaunay triangulation.

Two graphs are called isomorphic if they contain the same number of vertices connected in the same way. One of the most important notation of the present paper is the class of graphs $\mathcal{G} = \mathcal{G}_{(\mathbf{A},E)}$ isomorphic to a given graph $(\mathbf{A}, E)$.

Let $\mathbf{u} = (u_1, u_2, \dots, u_N)$ denote the vector whose components are the maximal diffusion potentials in the corresponding disks. The discrete network model for densely packed disks [3,7,10] is based on the fact that the diffusion flux is concentrated in the necks between closely spaced inclusions having different potentials. In our model, closely spaced inclusions means the chain disk–segment–disk $(D_k \leftrightsquigarrow P_{kj} \leftrightsquigarrow D_j)$ displayed in Fig. 1b. For two neighbor

[1] The terms the Delaunay triangulation and graph used in this paper are slightly different from the commonly used notations in degenerate cases. For example, consider a square and its four vertices. The traditional Delaunay triangulation has four sides of the square and one of the diagonals. In our approach, the Delaunay graph has only four sides.