Modeling of self-organization of two-dimensional ordered structures

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Abstract. The problem of the search of biostructures capable to self-organization is quite urgent considering the prospects of application of nanostructured biomaterials as components of composite materials in transplantology and optics as well as “scaffolds” for the synthesis of nanostructured materials based on inorganic particles. The given study focuses on modeling of the growth of structures using the cellular automata with a set of states of the two values (0 and 1), with the value corresponding to the state is determined by the contribution of “the closest neighbor” (by the probability of induction of the state of the next generation in the direction of the interaction) and the geometry of the field is determined by the vector of the direction of the particle and the direction of the interaction.

1. Introduction.
Materials structured “from bottom to top”, from nanometer scale to millimeter one, are perspective to be used in different spheres of human activities – from creation of optically active media to development of extra strong materials. The idea of creation of the chain of machines capable of assembling materials from separate molecules (“billion tiny factories”) which was put out in a lecture by Richard Feynman [1] has not been realized yet. Self-assembling processes are determined by a set of interactions between the elements of the system. To describe the process of self-organization the methods of molecular mechanics and molecular dynamics are commonly used [2]. Previously, we conducted experiments on modeling of self-organization of peptides using sequential molecular docking [3]. The applied methods, though they let us get the results consistent with the experimental data, are quite resource-intensive and do not always allow to quickly make the qualitative description of the system. For rapid qualitative assessment of the ability of the particles to self-organization modeling using cellular automata is possible. For example, work [4] describes the model of the dynamics of oligomerization of prion proteins basing on the theory of cellular automata. Modeling using cellular automata is less resource-intensive in comparison with molecular dynamic modeling. In
contrast with the model based on molecular dynamics, this system can show only the equilibrium or quasi-equilibrium state of the system. The approximation of the game "Life" created by Conway and described by Martin Gardner [5] makes it possible to model only symmetric objects with a very limited range of valences determined by the geometry of a discrete cell of the game field. The probability of the presence of the object in a given cell can take only discrete values - 0 or 1 - and it is determined only by the nearest surrounding of the object. With the help of this model it is possible to describe various biological objects - for example, growth of colonies, however, this approximation is not enough to model physical interactions of the probabilistic nature. Another approach to the description of real interactions of objects is a model created by Ising, which has a probabilistic nature. Further development of the idea led to the creation of the theory of cellular automata, where the cellular automata are considered as a discrete model of real physical and biological processes [6] and the parameters of discrete objects can have different values, including those from continuous sets, depending on the statistically weighted contribution of the closest neighbors of each object in the modeling field.

The given study focuses on modeling of the growth of structures using the cellular automata with a set of states of the two values (0 and 1), with the value corresponding to the state is determined by the contribution of "the closest neighbor" (by the probability of induction of the state of the next generation in the direction of the interaction) and the geometry of the field is determined by the vector of the direction of the particle and the direction of the interaction.

The problem of the search of biostructures capable of self-organization is quite urgent considering the prospects of application of nanostructured biomaterials as components of composite materials in transplantology and optics as well as “scaffolds” for the synthesis of nanostructured materials based on inorganic particles. Modern biotechnological ecologically clean manufacturing technologies make it possible to get practically unlimited number of biomolecules at a low financial cost, and it also lets us talk about the perspective and the urgency of ongoing research.

2. Materials and methods.

Modeling the growth of the structures was performed with the help of the original program (Aggregator2d) which uses the data on the geometry of the interaction of the molecules and the probability of the generation corresponding to the effective energy of the interaction of the particles as the parameters. The result was obtained in the form of the table containing the coordinates of the centers and the vector of the directions of the objects, which was later converted into a graphic two-colored image.

3. Results and discussion.

A discrete model of cellular automata with probabilistic nature of filling of the cells (the growth of the structure) in the field determined by the direction and the nature of the connections between the cells was created. As the model of the growth the model of adherence of the particles with successive generations was chosen taking into consideration the probabilistic nature of the interaction between the active groups on the surface of the particles, and by specifying their location relating to the direction of the axis of the particle the peculiarities of the geometric arrangement of the connections were taken into account. The different nature of the interaction was taken into account by introducing a normalized probability of the formation of the connection.
The algorithm was tested on the model of growth of the linear structures “Fibrils”. Figure 1 shows the example of modeling of the growth of the structure from the geometric analogues of the peptide oligomers. Then with the help of the program the parameters of the interaction were varied. Several specific types of two-dimensional structures were revealed. Figure 2 shows a typical example of the structure of the “Net” type; Figure 3 shows an example of the structure of the same type, which is a typical example of structure remains regular fractals with a complete coverage of the space. Another revealed class of structures was the structures of the “Needle-shaped crystals” type (Figure 4), which are intermediate between the structure of “Fibrils” and “Net” types.

Figure 1. “Fibrils” type structure. example of modeling of the growth of the structure from the geometric analogues of the peptide oligomers.

Figure 2. “Net” type structures.

Figure 3. “Net” type fractal-like structures.
The algorithm used in the research makes it possible to generate structures by changing the rules of the interaction for a single particle. The analysis of the rules of the interaction, which led to the formation of ordered structures, showed that their formation requires the sites of the interaction to be located symmetrically to the axis of the object, and besides, the probability of symmetric interactions were similar in meaning. At the introduction of a small asymmetry in the probability of the interactions the defects similar to defects of crystals appeared in the structures. No objects with an asymmetric interface of the interaction capable of forming ordered extended structures were found during the search. The acquired data are consistent with the data about the prevalence of symmetry in the amino acid sequence of interfaces of protein interactions capable of self-organization into an ordered quaternary structure, previously obtained by the author, and supplement them. The acquired model will be the basis for a three-dimensional model of formation of ordered structures.

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5. References
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