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Cellular automata simulation on surface triangulation for diffusion processes*

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Abstract. This paper concerns the development of techniques for the cellular automata simulation on triangulation grids on flat and curved surfaces. The possibility of the proposed techniques are shown on examples of the cellular automata simulation of diffusion, front propagation and diffusion-limited aggregation.

1. Introduction

Most cellular automata (CA) models are created for rectangular meshes on the plane [1, 2]. This study aimed at creating and studying cellular automata on various triangulation meshes, which made possible to observe the cellular automata simulation on curved surfaces in 3D space. In addition, this approach allows us to consider CA-simulation on “real” object models having an arbitrary shape, for example, on adaptive unstructured meshes. Also, this method takes into account the geometry of objects. One can pass by without drawing their attention to a wide spread of triangulation meshes and their accessibility with an advent of a laser scanning technology.

2. Cellular automata on triangulation

2.1. Problem definition. The construction of cellular automata on triangulation meshes is associated with several significant advantages of triangulation. Firstly, any surface can be approximated by a mesh of triangles with necessary accuracy. Secondly, the computational complexity of algorithms for partitioning the area into triangles is appreciably less than when using other polygons. Thirdly, there is a widespread tendency to specify objects with triangulation.

This approach makes it possible to construct CA on arbitrary curved surfaces and to observe their evolution directly on the surface. The objectives of this paper are the following:

- to construct methods for CA modeling on triangulation meshes;
- to study the influence of mesh parameters on CA results;

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- to compare CA on triangulation meshes with CA on rectangular meshes;
- to construct CA for diffusion process, diffusion front propagation of substance concentration and diffusion-limited aggregation on triangulation;
- to develop a software package for modeling.

2.2. Basic definitions for the CA modeling on triangulation.

A is an *alphabet* of states, for example, $A_{\mathrm{B}} = \{0, 1\}$ — Boolean alphabet, $A_{\mathrm{R}} = [0, 1]$ — real alphabet.

M is a *naming set*, for example, $M = \{m_i : i = 1, \dots, N\}$.

A pair (a, m) is called the *cell*, where $a \in A$, $m \in M$; a is called the *cell state* (denoted by $a(m)$).

A set of cells $\{(a(m), m) : m \in M\}$ is called the *cellular array.*

Each triangle of a triangulation corresponds to a certain cell. Thus, the whole triangulation corresponds to a cellular array.

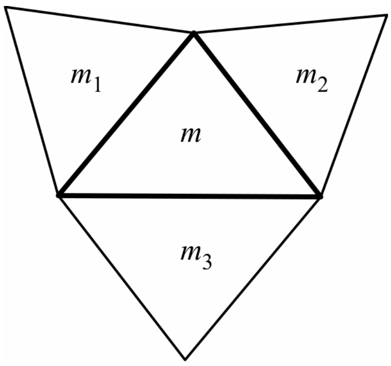

Figure 1. A template $T(m) = \{m_1, m_2, m_3\}$ for the cell m

Template for a cell (a, m) is a set of cell names usually neighboring to the given cell. For example, on triangulation, two cells are neighboring if the corresponding triangles have a common side. Thus, each triangle can have no more than three neighbors (Figure 1).

Transition rule is a function that defines a new state of a cell depending on its current state, states of cells with names from T or any other values, for example, probabilities. This function is the same for all the cells.

Synchronous mode of operation means that transition rules are applied to all cells from a cellular array.

Asynchronous mode of operation means that a cell is randomly chosen from a cellular array and the transition rule being applied to it.

Global iteration is application of transition rules to $|M|$ cells from the cellular array M.

A sequence of cellular arrays, each being obtained as a result of the global iteration to the previous cellular array, is called the *CA-evolution.*

Averaging operation is very often used for CA over Boolean alphabet to obtain real values. It calculates an average value by some neighborhood $T_{\mathrm{av}} \subseteq M$ of a cell:

$$\langle a \rangle = \frac{1}{|T_{\mathrm{av}}|} \sum_{m \in T_{\mathrm{av}}} a(m). \tag{1}$$

Discretization is the inverse operation to averaging—it generates Boolean values from real values:

$$a' = \begin{cases} 1, & r < a, \\ 0, & r \geq a, \end{cases} \tag{2}$$

where $a \in [0, 1]$ and r is a random number from $[0, 1]$.

2.3. Peculiarities of using triangulation in CA. It should be noted that triangles in triangulation may differ in size and are not necessarily equilateral, in contrast to the squares in rectangular meshes. This should be taken into consideration when conducting studies in cellular automata. For example, in asynchronous CA on a rectangular mesh of squares, a random selection of cells on a single iteration has a uniform distribution. To achieve the independence of using a mesh, the choice of a random triangle in triangulation should be based on its area; smaller cells (triangles with a smaller area) change their states faster, thus, the smaller is the space, the more likely this triangle should be chosen as random.

Another aspect that is worth to be highlighted is the closure of borders in rectangular meshes. Because of a simple structure, the borders of a rectangular mesh often close, forming a torus. On triangulation (on the plane), there is no such a possibility, due to the complexity of the area. In this paper, when considering concrete CA models on triangulation, the possibility of closing the borders is ignored. This is because the plane case is usually not interesting, and for curved surfaces in a 3D space, a closed triangulation (without boundary triangles) is often considered. A triangle is the *boundary* one if it has less than three neighbors, otherwise it is the *internal* one.

In addition, a significant role plays the fact that each internal cell of a triangulation has three neighbors, as opposed to four neighbors in a rectangular mesh.

3. Cellular automata diffusion on rectangular meshes

3.1. The basic algorithm of CA-diffusion on rectangular meshes. Diffusion is a process of random walk of particles, which leads to equalization of the concentration in space. In the 2D continuous case with the constant diffusion coefficient d, this process is described by the Laplace equation

$$\frac{\partial u}{\partial t} = d\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right),$$

where $u(x, y, t)$ is concentration of a substance in the Cartesian space with the coordinates x, y at time t.

Classic CA-diffusion models have Boolean alphabet and evolution as a sequence of Boolean arrays. The state of a cell (0 or 1) determines presence or absence of a unit mass, which has no speed. The CA-diffusion on rectangular meshes has already been thoroughly studied [3].

One of CA models of diffusion is the *naive diffusion* [4]. This is the most primitive model of diffusion, which directly reflects the concept of the process as a random walk of particles (cells in state 1) in an attempt to equalize the concentration of a substance in space. In this case, the mode of operation is asynchronous, which corresponds to the nature of the process. The cells neighborhood is its nearest four neighbors. The way of functioning is such that at each iteration a random cell is selected, which changes its value with one of its neighbors, chosen with equal probability. Such a rule shows the implementation of the law of conservation of mass, and random selection of one of the neighbors corresponds to the chaotic motion of particles, according to the definition of the diffusion process.

Another CA model of diffusion is *CA-diffusion with Margolus neighborhood* [4]. For brevity, we call it TM-diffusion of the first letters of the names of its authors, as is customary in Western literature. TM-diffusion is more popular than the naive diffusion, for the two reasons. Firstly, it has the property, which mathematicians call "elegance" that is a combination of simplicity and efficiency. Secondly, there is a rigorous mathematical proof that it approximates the Laplace operator [5]. The cellular array is divided into two subsets, each consisting of blocks containing four cells. The CA functioning occurs in the synchronous mode. Each iteration is divided into two cycles. In the even-numbered cycles, transition rules are applied to the even-numbered blocks, while on the odd—to the odd-numbered blocks. Transition rules are such that the states in a cell block are shifted with equal probability either clockwise or counterclockwise. By reducing the values of probability as well as manipulating with time and space steps, it is possible to simulate the diffusion process with a diffusion coefficient in a wide range [1].

There are two possible ways to verify that CA really simulates the diffusion process: analytical and experimental. The analytical proof exists only for one CA-model, i.e., for TM-diffusion. The experimental proof consists in the CA model execution and comparing the evolution of CA with an equation solution on a certain set of iterations.

3.2. Diffusion front propagation on rectangular meshes. *Front propagation* is a process with a uniform distribution of particles, eventually filling the whole area. The front propagation can be simulated by *cellular automata composition.* This means that a few rules are consistently applied to a cellular array at each iteration. Cellular automata composition reflects well real physical processes, because in most cases, it includes several phenomena [6].

The front propagation of CA is applied in a sequence of rules:

- a global iteration of diffusion is executed;
- the resulting array is averaged according to formula (1);
- a flow is added: in each cell, the concentration u is replaced by the value $0.5u(1-u)$;
- discretization is performed by formula (2).

It should be noted that the flow addition and discretization are operations that do not depend on the type of a mesh, so they can be easily extended to a 3D case on a triangulation mesh.

4. CA-diffusion on triangulation on the plane

4.1. The basic algorithm of CA-diffusion on triangulation on plane. Let us consider a mesh consisting of equilateral triangles. The rules for CA would be similar to the case on a rectangular mesh, but probability of choosing one of the neighbors will be 1/3. Tests of this cellular automaton are carried out over Boolean alphabet. At the initial time, several closely-spaced particles are inserted in the middle of the mesh. In Figure 2, the work of automaton is shown (the plane is of gray color).

As seen from the figure, particles uniformly propagate in all the directions. Thus, there is a visual analogy with a CA on a rectangular mesh (a more formal comparison will be introduced below). This effect was achieved due to the fact that all triangles are identical (equilateral). But since the task is to move beyond limitations of using a mesh, the rules for cellular automaton were selected for any type of a mesh. The neighbor with a smaller side of a triangle is selected likely that with a bigger side. Such a rule was experimentally found:

$$p_i = \frac{1/l_i}{\sum_{j=1}^{3} 1/l_j}. \tag{3}$$

Here p_i is the probability of selecting a neighbor with the length l_i of the corresponding side in the triangle.

As an example, consider CA-diffusion on an unstructured grid (Figure 3). Despite a relatively small number of triangles in triangulation (4129), the diffusion process distributes particles only in the middle of the area for a long time, since the size of triangles in this place is much smaller than that at the edges. But after a sufficiently long time, particles move outside the boundaries of the inner circle with a high density of the mesh.

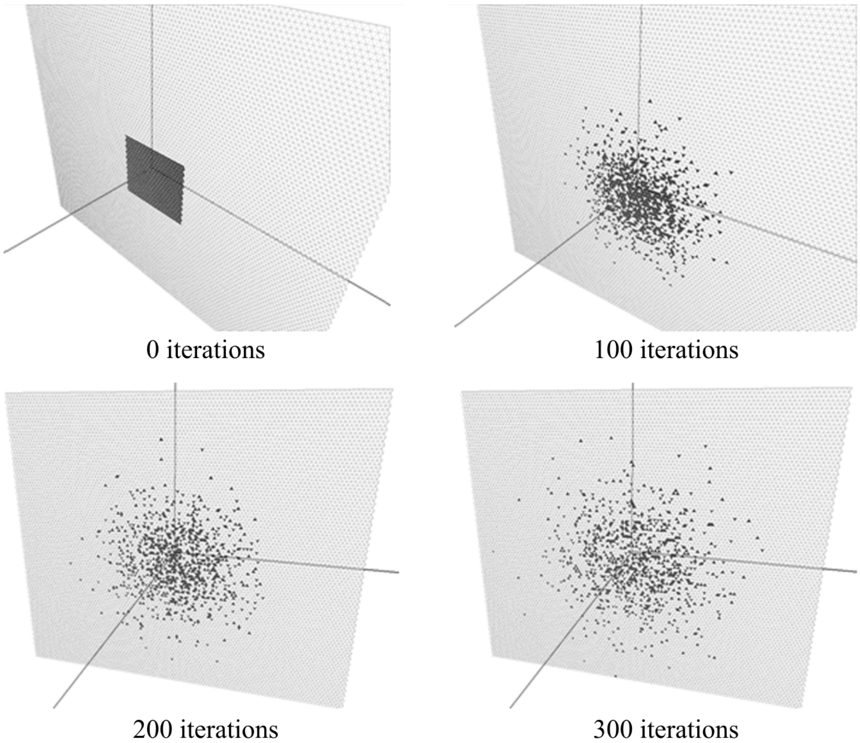

Figure 2. The diffusion process on the equilateral triangles mesh

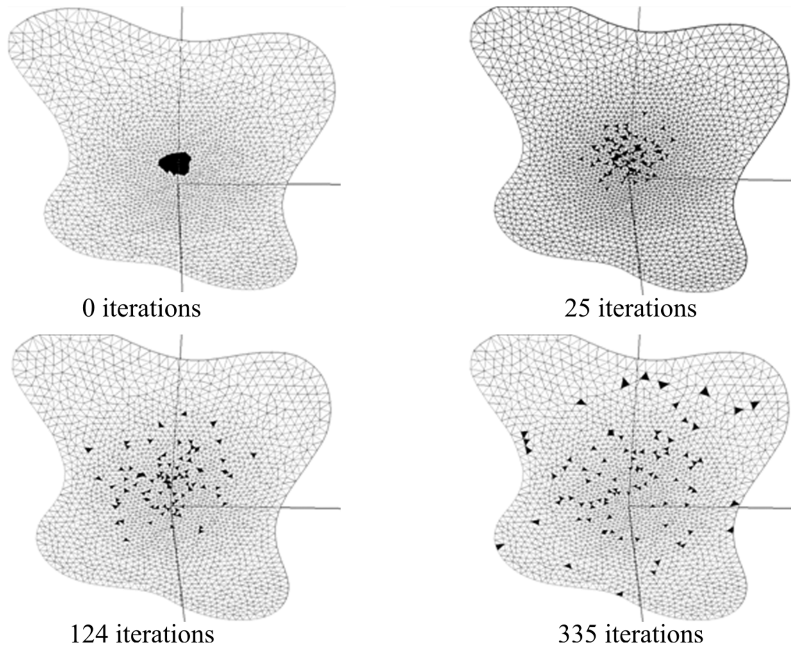

Figure 3. The diffusion process on adaptive mesh

4.2. Averaging in CA-diffusion on triangulation on the plane. Let us describe the algorithm of *averaging by circle* for cellular automaton on triangulation. We consider the center of each triangle of triangulation and draw a circle with a certain radius from this center. Let n be the total number of cells caught in this circle and n_1 be the number of cells in state 1. Thus, the concentration value will be determined by the formula:

$$u = \frac{n_1}{n}, \tag{4}$$

where $n \neq 0$ regardless of the radius, because the considered triangle is known to lie in this circle.

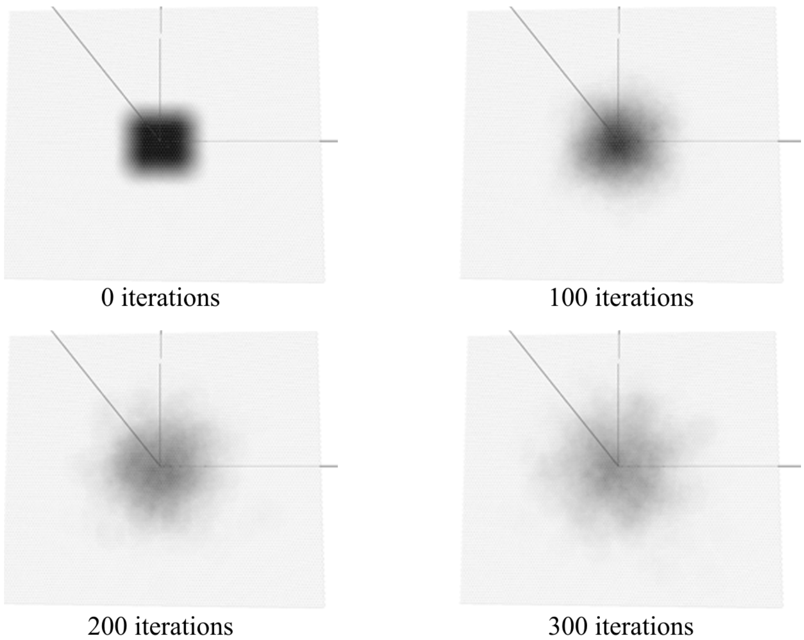

Figure 4. Diffusion process with averaging by circle

If we appropriately select a radius of the circle for averaging, we will obtain an obvious picture (Figure 4). A disadvantage of this algorithm is its computational complexity, forming $O(N^2)$, where N is the number of triangles in triangulation. In this regard, we will consider another algorithm for averaging with much less computational complexity — *averaging by the nearest neighbors*. The essence of this algorithm is to consider only the neighboring cells and computing ν_1 — the number of cells in state 1 among them. Thus,

$$u = \frac{\nu_1}{\nu + 1}, \tag{5}$$

where ν is the number of neighbors, $\nu \in \{0, 1, 2, 3\}$.

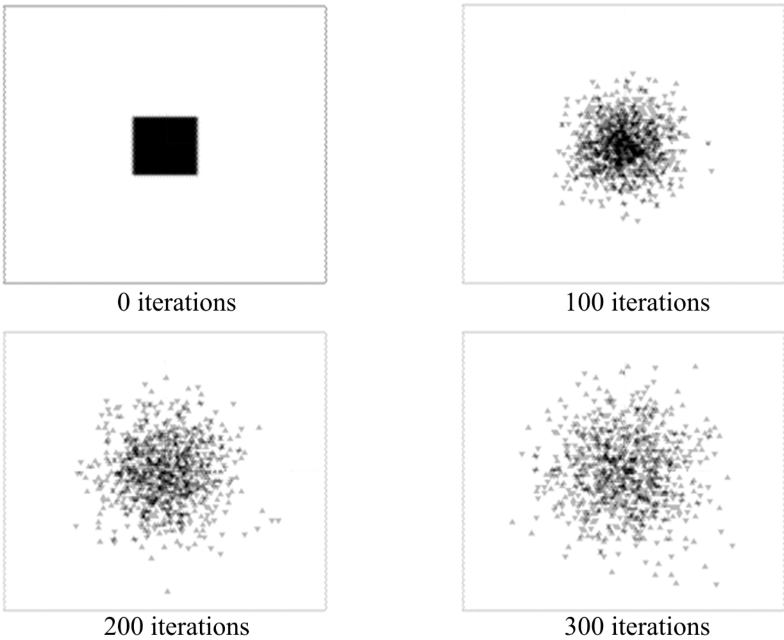

Figure 5. Diffusion process with averaging by the nearest neighbors

In the approach in question, the number of possible concentration values is only seven: 0, 1/4, 1/3, 1/2, 2/3, 3/4, 1. However, the computational complexity of this algorithm is $O(N)$, where N is the number of triangles in triangulation. This gain was achieved by introducing a naming function, which returns three neighbors by the triangle.

Despite of the small number of possible concentration values, the picture still turns to be obvious. In the center of the initial state accumulation of concentration keeps higher values for a long time, but eventually reaches its uniform distribution throughout the area (Figure 5).

This algorithm can be extended to the neighborhood of order 2, that is, to include into consideration neighbors of the second level. The picture will be more obvious. Similarly, the algorithm can be extended to the neighborhood of order n.

4.3. Comparison of CA-diffusion on triangulation with CA-diffusion on rectangular meshes. Let us introduce a criterion of correspondence of the constructed CA with cellular automata on rectangular meshes. Because of the existence of CA-diffusion model only for the planar case, the comparison is possible only in this case. We will consider a square area specified by equilateral triangles. Because the diffusion is the process of random walk of particles, comparison on Boolean alphabets is not interesting. Let us consider automata with averaging by circle.

Figure 6 illustrates the comparison of real values of concentration

$$u = \frac{u_1 + u_2}{2} \quad \longleftrightarrow \quad u_0, \qquad (6)$$

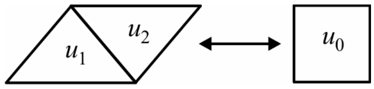

Figure 6

where u_0, u_1, u_2 are concentration values corresponding to cells.

Thus, one value of concentration in a square mesh is associated with arithmetic average of concentrations of two neighboring cells in the triangulation. In this approach, the number of cells in the cellular array on triangulation is twice as large as that in the rectangular. So, the randomly chosen cell is often empty, which subsequently, with high probability, also swaps with an empty cell. This leads to the fact that non-empty cells are rarely selected, therefore, the diffusion process is slower and the concentration of substances is high.

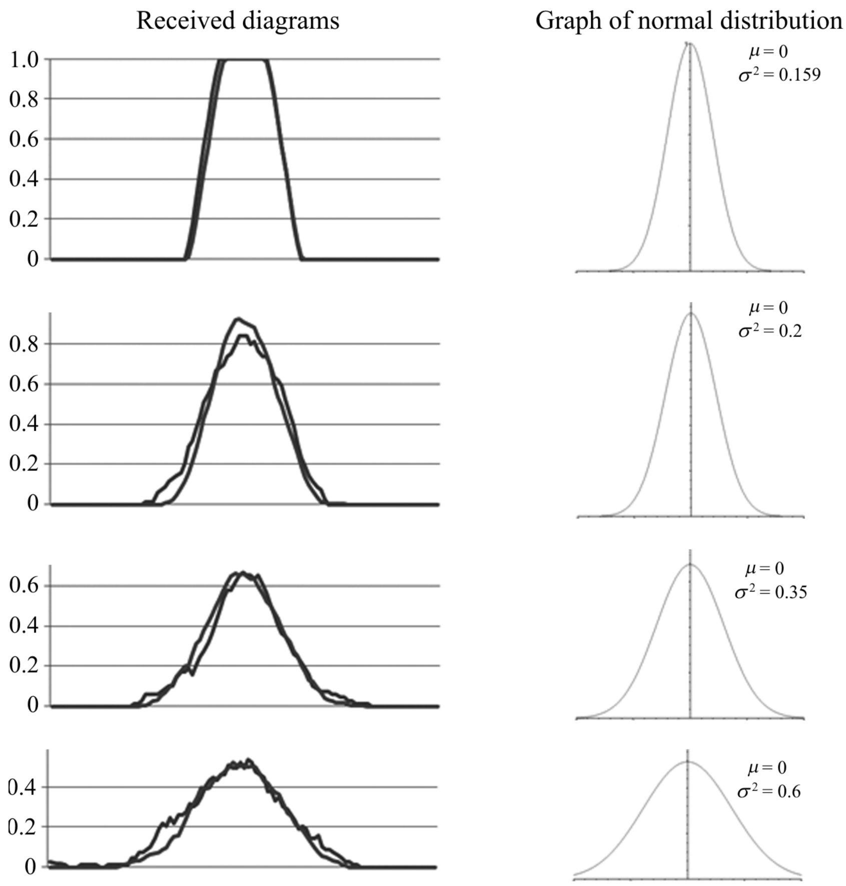

Figure 7. Comparison of CA-diffusion on triangulation (the number of iterations is doubled) with CA on a rectangular mesh and graph of normal distribution

To attain the correspondence with values of concentrations, we will twice conduct more iterations on the triangulation mesh. The comparison is made on the cells located on the horizontal midline of the cell arrays. For clearness, Figure 7 also contains a graph of the normal distribution, reflecting an analytical solution of the Laplace equation.

The criteria of compliance for CA on triangulation and on a rectangular mesh is assumed to be the analogy of the diagrams on the horizontal midline.

5. CA-diffusion on triangulation (curved surface)

5.1. The basic algorithm. With a full toolkit for further research, we will consider the behavior of CA on curved surfaces in a 3D space. The only difficulty in this case is averaging by a circle. If we form the sphere from the center of a triangle, the match is not achieved: cells located on the opposite side of the mesh can get into the scope, which is unacceptable. For obtaining real values of the substance concentration, we will use averaging by nearest neighbors. The considered mesh is the bone surface, specified by triangulation [7]. At the initial state the concentration is included into a small area of the bone (Figure 8).

As seen from the figure, the particles spread evenly over the entire surface of the bone after some time. And in the CA simulation, particles propagate in all directions homogeneously. The constructed automaton reflects the physical process on a complex surface.

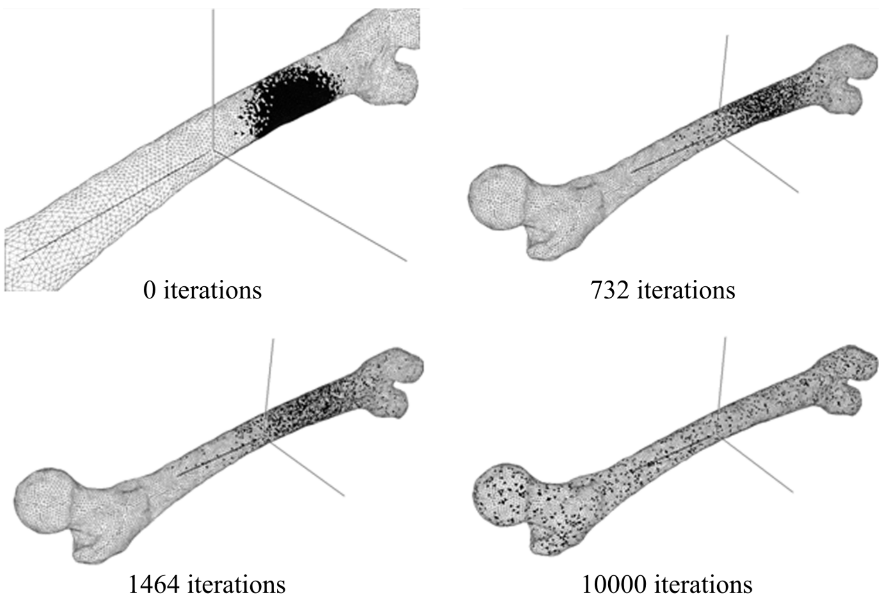

Figure 8. Diffusion process on the bone

5.2. Diffusion front propagation on curved surface. Let us consider CA of front propagation on triangulation. The considered mesh is again the bone surface with the initial state, as in Section 4.1. The process of diffusion front propagation on such a mesh can be interpreted as spread of some inflammation from the local area to the entire surface of the bone.

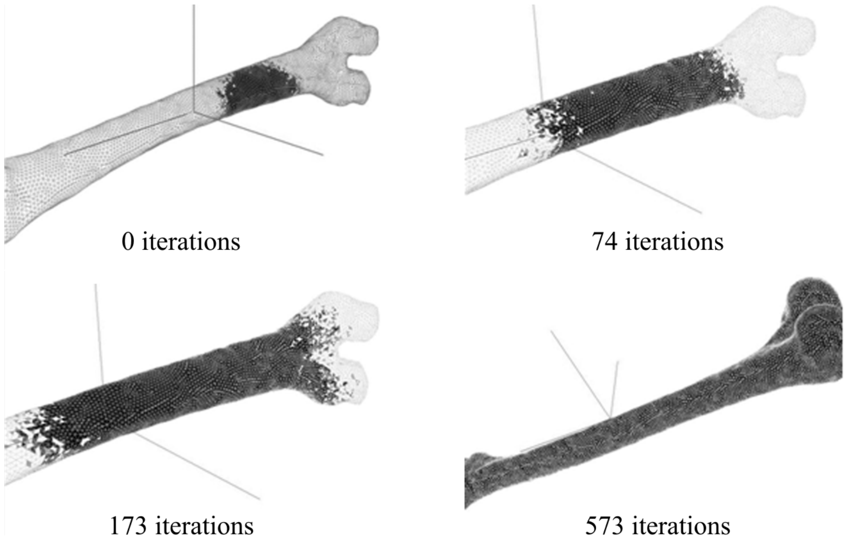

Figure 9. The front propagation process on the bone

A front propagates uniformly in all the directions and eventually covers the entire surface of the bone, which corresponds to definition of the process.

5.3. Diffusion-limited aggregation on triangulation for curved surface. The latter (above-considered) CA is a diffusion-limited aggregation cellular automaton.

At the initial state, 10 % of particles are randomly scattered throughout the mesh. One cell is the "source", it has another color and does not move. Other particles move in random directions but in contact with the "source" stop moving and change their color. The result of CA is shown in Figure 10.

5.4. Field of application. As noted above, the application area is not limited for modeling of only physical processes. The CA-diffusion can be used in many areas, up to computer games and image processing. The difference may be only in interpretation of this process in the case of its application. In models of propagation of any liquids or gases, one of components of the process is diffusion. Thus, the results of this paper can be used to construct more complex composite CA, in which one of the rules of operation will be diffusion.

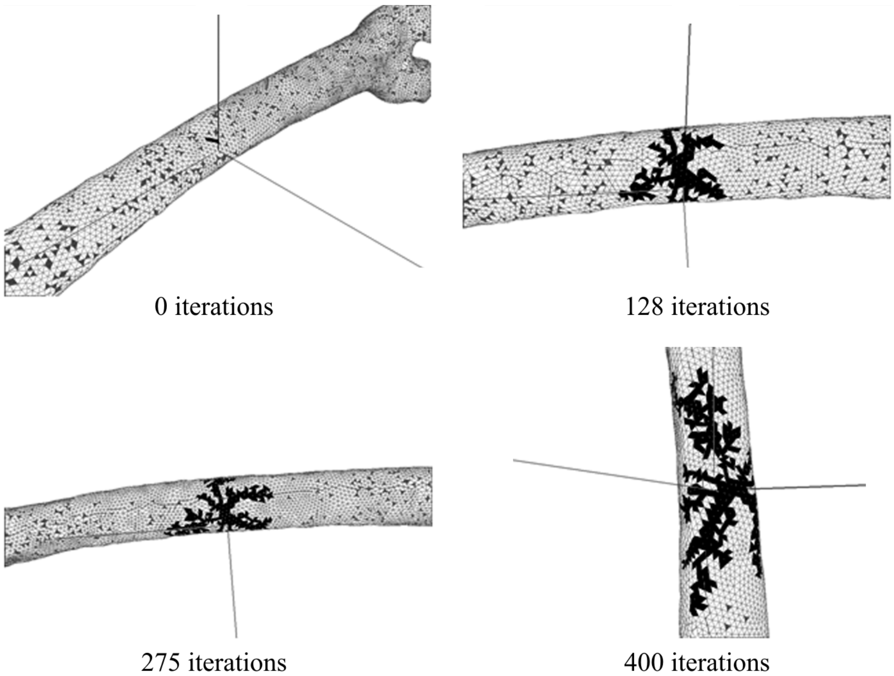

Figure 10. Diffusion-limited aggregation on the bone

6. Conclusion

We have obtained CA models of diffusion, diffusion-limited aggregation and the diffusion front propagation for any curved surface in a 3D space, specified by triangulation. The results are qualitatively similar to CA on rectangular meshes and can serve as a good basis for modeling various processes. From the above-mentioned arguments, we can conclude that the use of CA-diffusion is not limited by physical processes, and can be interpreted differently depending on a concrete problem. An example with the propagation of inflammation on the bone can be used in medicine. Note the importance of composition of cellular automata: most models of spatial dynamics have a diffusion component (for example, the considered process of diffusion front propagation). These algorithms can be applied to other cellular automaton models.

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