Bull. Nov. Comp. Center, Comp. Science, 19 (2003), 51–59

The wall cells in the cellular automaton simulation of fluid flows*

Yu. Medvedev

In this paper, the boundary conditions of 2D and 3D Cellular Automaton models (CA models) are considered and classified. It is shown that the simulation algorithm does not change at different boundary conditions, and the computing complexity of simulation is not increased with a large number of wall cells, even when simulating a porous medium. The numerical experiments are described, which were carried out with the CA models of fluid flows in a tube and in a porous medium. The parabolic dependence of a flow speed on a distance to the wall is attained for a flow in a pipe, which coincides with analytical results.

1. Introduction

The Cellular Automaton (CA) fluid flow models (Lattice Gas Models) were designed quite recently [2]. They have been developed intensively during the last few years [4].

These models have the following advantages as compared to conventional methods.

1. *Elimination of calculation errors.* There is no round-off errors because of the equal rights of all digits of operands.
2. *Stability of calculation.*
3. *Natural parallelism.* The CA may be cut up on into number of parts to be allocated on processors of a multiprocessor system.
4. *Simplicity of boundary conditions.* The boundary conditions are represented by special boundary cells named walls and sources. This does not change the algorithm complexity.

These advantages have resulted in the growing interest in the CA simulation of porous media [1].

In this paper, the boundary conditions of 2D and 3D CA models are considered; the simulation experiments on some models are described; the boundary conditions in 2D and 3D cases are classified.

*Supported by the Russian Foundation for Basic Research under Grant 03-00-00086.

2. The main concepts of the CA fluid models

The Cellular Automaton (CA) is a set of exactly identical finite state machines (FSM) with regular local interconnections. All the FSMs work synchronously and in parallel. The FSM being included as a component in a CA is called an *elementary automaton* or a *cell*. In the CA fluid flow models, elementary volumes of the simulated flow correspond to cells of the CA. The cell coordinates coincide with those of the volume centers. The distance unit is a distance between the neighboring cells.

The elementary automaton state is determined by a set of some hypothetical *particles*, having at this time moment the cell coordinates. The particles possess the following properties:

1. The particle mass is unity.
2. Velocity vector magnitude is unity or zero.
3. The coordinates of a particle are equal to the coordinates of one of the cells. The particle is said to be in a cell if their coordinates coincide.
4. Particle velocities are directed only towards the neighboring cells (Figure 1).
5. At any moment there may not be two or more particles, having the same velocity vector.

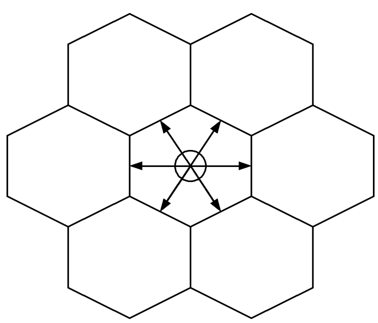
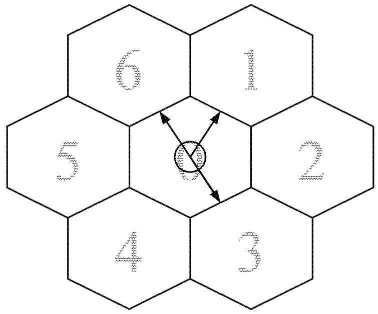


Figure 1. Directions of the velocity vector

So, a state of the cell is represented by $(n+1)$-length Boolean vector, where n is the number of neighbors. Every digit of the vector defines the presence / absence of particles with a certain velocity vector. Each digit corresponds to one neighbor-directed velocity vector and one digit – for the rest particle. An example of a cell state is shown in Figure 2. On its left, a cell with its neighbors is shown; on its right, a state Boolean vector is given. There are three particles in the cell. They have velocity vectors directed to the 1-st, the 3-d, and the 6-th neighbors. The corresponding digits of the Boolean vector are ones.

The neighbor number is a very important property of the model. It determines the elementary automaton transition table size: $s = k \times 2^{(n+1)}$, where k is the number of different transition rules in the probabilistic models; $k = 1$ for deterministic models.

There are three cell types in the CA models. They comprise *ordinary*, *wall*, and *source* cells respectively. Cells of different types have different be-



Digits						
6	5	4	3	2	1	0
1	0	0	1	0	1	0
Values						

Figure 2. Boolean vector of the cell state

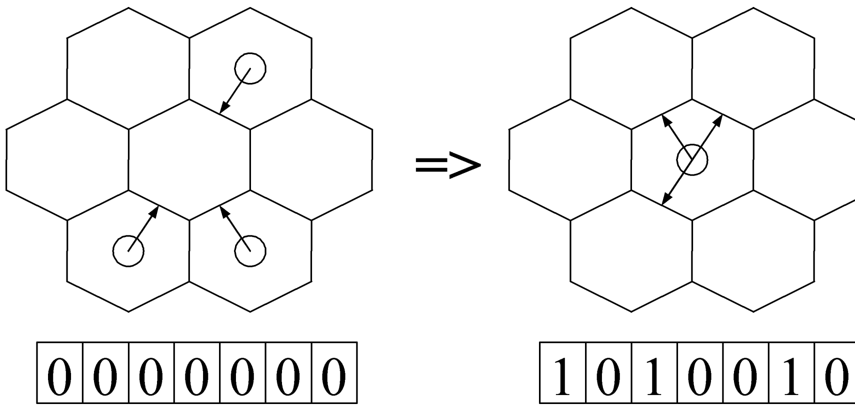


Figure 3. The propagation phase

havior, i.e., they have different transition table. The elementary automaton behavior is defined by the following rules.

1. Every time step of the CA is divided into two phases: *propagation* and *collision*.

2. At *the propagation* phase cells of all the types have the same behavior. The next automaton state at the propagation phase is a superposition of velocity vectors of its neighbors, directed to the elementary automaton (Figure 3). Note, that the automaton state affects only the next states of its neighbors, but not its own state. So, during the propagation phase each particle moves along the velocity vector to the neighboring cell. The propagation phase is deterministic even for probabilistic automata. The mass and the momentum conservation laws are satisfied at the propagation phase because the total particles number is not changed: the particles are only shifted to the neighboring cells, but they do not change their velocity vector direction.

3. At *the collision* phase, an elementary automaton next state depends only on its own state. It does not depend on the neighboring automata states. In ordinary cells, the next automaton state is equiprobably chosen

between all possible states conserving mass and momentum. In wall cells, the particles reverberate according to the different collision rules. These rules define the wall cell properties. The reverberation violates the momentum conservation. The source cells generate particles. They differ from ordinary cells in that at certain times there appear n particles. The mass conservation is violated in source cells. So, walls and sources define the automaton boundary conditions.

From the CA behavior it follows that the computational complexity depends only on the cells number but not on the their types.

The fluid flow simulation results are represented by the *averaged values* of particle velocities. These values are computed as sums of all velocity vectors in an averaging area. They coincide with the macroscopic real fluid speed values. An averaging area has an n-faced polytope shape (an n-angled polygon on a plane).

The CA models take a special place in *the porous media* simulation [5]. This is due to simplicity of the CA border conditions profile. There are solid wall cell groups in the porous media CA models. Such groups are randomly distributed over the whole CA (Figure 4). The fluid flows through the pores among these groups. Despite of that the wall cells occupy a huge part of the CA, the boundary conditions are as simple as in a model without any walls. This is because all the cells follow the same algorithm. Only collision rules are different for different cell types, but these rules are only parameters in the algorithm. The porous media simulation has the same computational complexity as non-porous media simulation, because computational complexity depends only on cells number but not on their types.

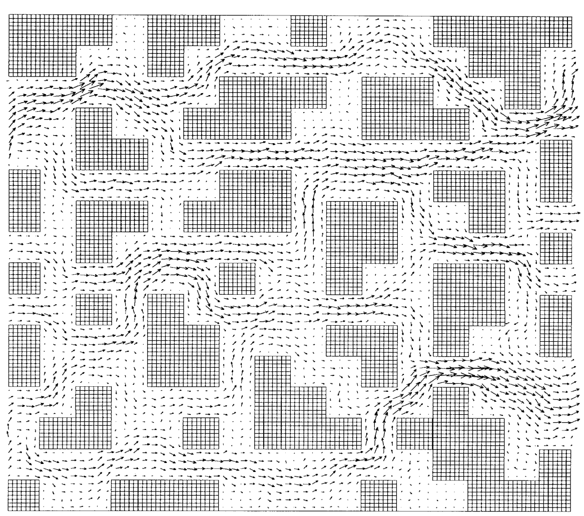


Figure 4. The speed field of the 2D flow (from [5])

3. Boundary conditions in the 2D flows

The properties of the 2D CA models, which are considered in this section, are illustrated by the well-known FHP model. The model has been called after the names of the French scientists Frish, Hasslacher, and Pomeau, who had proposed this model [2]. Every cell in the model has six neighbors.

In the model in question there are three kinds of the wall cells. They differ in the wall friction factor. Wall cells of each kind have their own collision rules. These rules are as follows:

1. Each particle velocity vector in a wall cell changes its direction to the opposite one (Figure 5). The friction factor of a wall consisting of this kind of cells, is large, i.e., the flow speed is equal to zero near the wall.
2. Each particle velocity vector changes its direction to the symmetrical one, relative to a special line. This line is perpendicular to the bisectrix between two half lines, drawn from the cell to those wall neighbors, which have an ordinary neighbor among the cell neighbors (Figure 6).

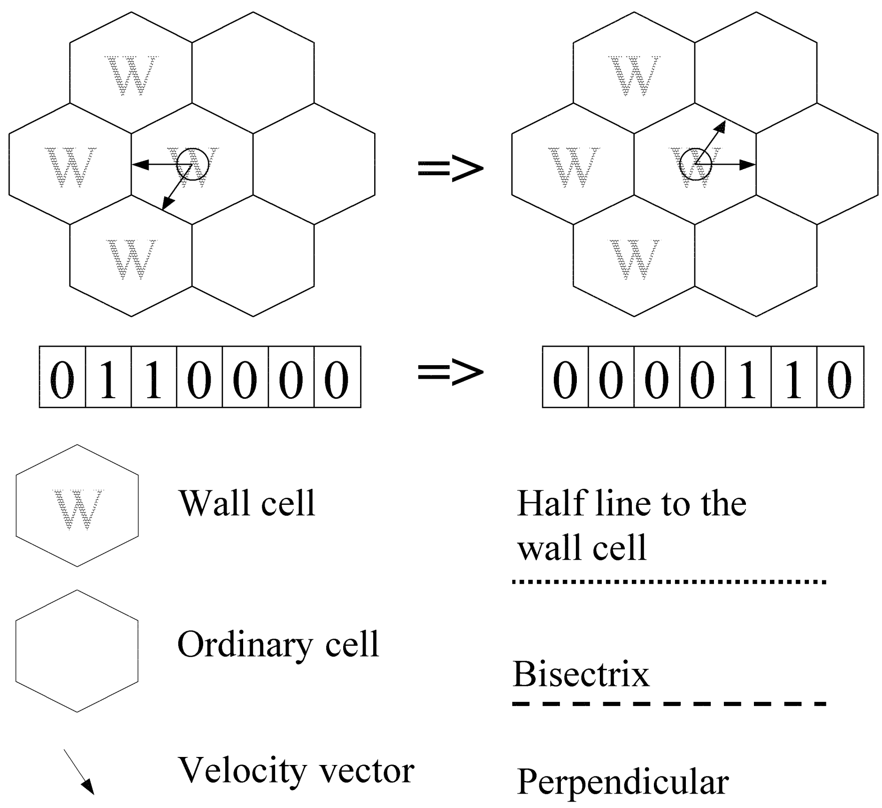


Figure 5. Reflections from the wall cell (wall with friction)

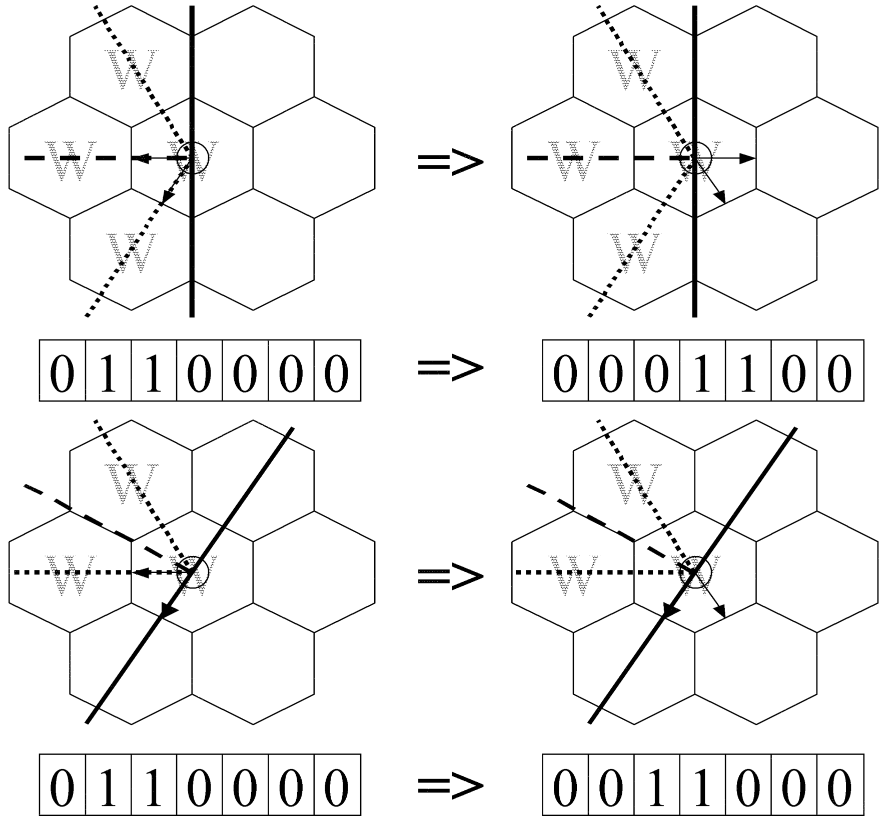


Figure 6. Reflections from the wall cell (smooth wall)

The friction factor of a wall, consisting of this kind of cells, is equal to zero because the wall reflects particles according to the optics laws.

3. Each particle velocity vector changes its direction according to the above rules 1 or rule 2 with probabilities p and $1 - p$. The friction factor of a wall, consisting of this kind of wall cells, varies between zero and its maximum value according to probability p.

Usually, one checks the conformity of a model and a real fluid flow by well-known analytical results. Such results are available for the fluid flow speed field in a pipe with a large friction of walls [1]. So, the fluid flow simulation in the 2D pipe has been done for the experimental validation of the boundary conditions algorithm in the CA model. In the experiment, two parallel lines on a plane form a 2D pipe. These lines consist of the wall cells. According to the simulation, the parabolic dependence of the flow speed on the distance to the wall has been found for the first and the second kinds of wall cells. It has been found that for the first kind of wall cells the dependence of speed values of the distance on the walls is parabolic

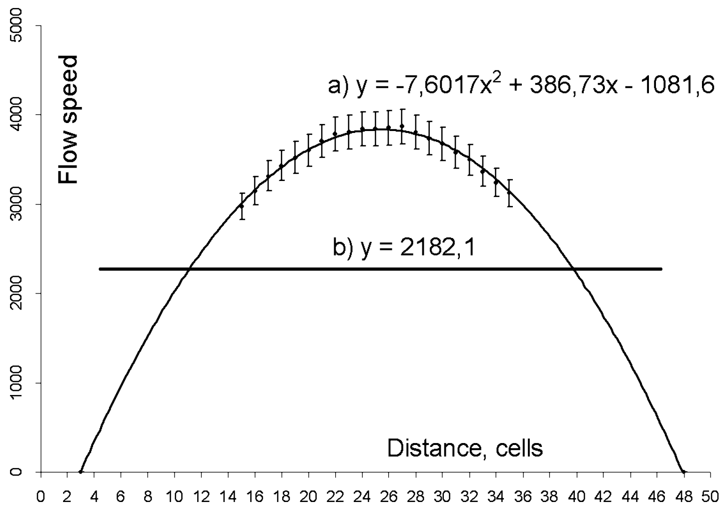


Figure 7. Dependence the flow speed from the distance to the wall

(Figure 7, curve a). This coincides with the results from [5] that the fluid flow speed in a pipe with considerable friction of the walls forms a parabola. For the second kind of wall cells the longitudinal component of the flow speed does not depend of the distance from the walls (Figure 7, curve b). For the third type of wall cells one can obtain an intermediate dependence.

In the models discussed the probability p defines the friction factor between the wall and the flow. On the boundary conditions of the first type ($p = 0$) the friction is absent. On the second type boundary conditions ($p = 1$), the friction is maximal, and the flow speed is equal to zero near the wall.

When simulating a porous 2D medium, the boundary conditions are defined for some wall cells groups (see Figure 4). The fluid is infiltrated through the medium. In Figure 4, the fluid flow speed is given for the 2D model. The experiments were carried out by Daniel H. Rothman [5]. The flow speed at a point is shown by an arrow. The length of an arrow is proportional to the fluid speed.

4. Boundary conditions in the 3D flows

In paper [3], the 3D model of a fluid flow is proposed. The cells of this model have the shape of the rhombic dodecahedrons (Figure 8). They fill in the 3D space without interspace. Each cell has 12 neighbors. Therefore, the velocity vector of a particle can be oriented in one of 12 directions.

In the 3D model, it is possible to distinguish seven kinds of walls. In each of them the collision rules are different.

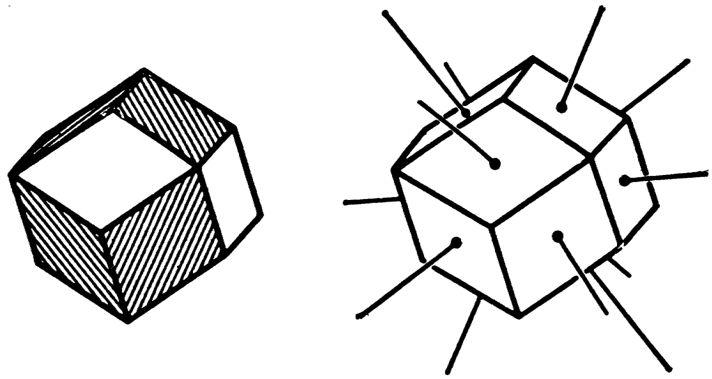


Figure 8. Rhombic dodecahedron

1. The velocity vector of any particle in a cell changes its direction to the inverse one.
2. The velocity vector of any particle in a cell changes its direction to the symmetrical one relative to the plane a) Oxy; b) Oxz; c) Oyz.
3. The velocity vector of any particle in a cell changes its direction according to rule 1 or rule 2 (a, b or c) with probabilities p and $1 - p$.

The first rule is similar to that of a 2D case. It is used in the simulation of flows with wall friction. The second rule is used only for simulation of flows with a smooth wall. In the second rule, only particular cases of walls (a, b and c), orthogonal to the Cartesian axes are considered.

5. Conclusion

In this paper, the boundary conditions of the CA models of fluid flows in 2D and 3D cases are discussed. The types of wall cells are distinguished depending on a friction factor of a fluid and a wall. It is shown that the algorithm of simulation does not change at different boundary conditions, and the computing complexity of simulation is not increased with a large number of wall cells, even when simulating a porous medium. The numerical experiments are described, which were carried out with the CA models of fluid flows in a pipe and in porous media. The parabolic dependence between the distance to wall and the flow speed is attained for a flow in a pipe, which coincides with analytical results.

The obtained results are useful for determining the transport coefficients for models under study. Such coefficients are parameters of models (the quantity of cells, probability) connected with parameters of simulated media (speed, pressure, viscosity, the Reynolds number). The results also prove the validity of the CA fluid flow models.

References

[1] Di Pietro L.B., Melayah A., Zaleski S. Modeling water infiltration in unsaturated porous media by interacting lattice gas – Cellular automata // Water Recourses Research. – Vol. 30, № 10. – P 2785–2792.

[2] Frisch U. et al. Lattice gas hydrodynamics in two and three dimensions // Complex Systems. – 1987. – Vol. 1. – P. 649–707.

[3] Medvedev Yu. Gas-lattice simulation of high viscous fluid flows // NCC Bulletin, Series Computer Science. – Novosibirsk: NCC Publisher, 2002. – Issue 17. – P. 63–73.

[4] Rothman D.H., Zaleski S. Lattice-Gas Cellular Automata: Simple Models of Complex Hydrodynamics. – Cambridge University Press, 1997.

[5] Rothman D.H. Cellular-automaton fluids: a model for flow in porous media // Geophysics. – 1988. – Vol. 53, № 4. – P. 509–518.