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Designing a collision matrix for a cellular automaton with rest particles for simulation of wave processes*

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Abstract. We consider the single-particle HPPrp Lattice Gas Cellular Automata for simulation of modeling wave processes. The HPPrp Cellular Automaton is defined on a two-dimensional square lattice. Each cell of the automaton contains particles of the two types: the moving particles and the rest particles. Inserting the rest particles leads to non-deterministic collision rules. In this paper, the design of a procedure collision matrix for a cellular automaton with rest particles for simulation wave processes is presented. The entries of the collision matrix are transition probabilities from one state to another. As the condition that ensures the existence of a wave process, the semi-detailed balance condition is used.

Introduction

The HPPrp Lattice Gas Cellular Automata are a powerful instrument for the simulation of a complex event[1–4] due to a set of the key features: absolute computational stability, simplicity of boundary conditions, locality of operational interactions, and inherent spatial parallelism.

In the HPPrp Cellular Automata (CA) [1, 2], the dynamics of an event is described by a set of hypothetical particles. They move in the lattice discrete space according to certain rules. These rules present the modeling process on a micro-level, based on the general laws of physics. In the HPPrp CA, the space is represented as a two-dimensional square lattice, whose nodes can contain a quantity of hypothetical particles. Each lattice node is assigned to a HPPrp cell. Each cell is associated with the unit vectors which connect the cell with its nearest neighbor.

The initial state of a HPPrp cell is determined by a set of some particles, locating in the cell at this time instant. There are two types of particles: the moving particles and the rest particles. The moving particles have the unit mass and the unit velocity. The rest particles have velocity equal to zero and different masses. Interactions between particles are simple. Each interaction consists of two successive steps: collision and propagation. Collision rules are chosen in such a way that mass and moment conservation laws are satisfied. All cells update their own states simultaneously and synchronously. An iterative change in the HPPrp global state (evolution of the HPPrp)

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describes the dynamics of a wave process. In published works regarding the Lattice Gas Cellular Automata, a formal procedure for designing a cellular automaton, the collision matrix with an arbitrary number of rest particles is unknown. That is why we present the procedure of this kind.

This paper is organized as follows. In Section 1, the main concepts of the HPPrp CA are given. Section 2 deals with the construction procedure of the collision matrix. In Section 3, the influence of the semi-detailed balance on wave processes is investigated.

1. The HPPrp cellular automata for simulating wave propagation. The basic definitions

Formally, the HPPrp lattice gas automaton is defined by the set $\mathcal{N} = \langle M, A, \Theta \rangle$, where M is a discrete space, A is the state alphabet, Θ is a set of transition functions.

The space M is represented as a regular two-dimensional four-neighbor Euclidean lattice $M = \{(i,j) : \ i = 0, 1, \ldots, I, \ j = 0, 1, \ldots, J\}$. For simplicity, the (i,j)-th node of the lattice is a HPPrp *cell* which is labeled by its position $\boldsymbol{r} = (i,j)$. Each cell is associated with the vectors (links) $\boldsymbol{e}_k$, $k = 1, 2, 3, 4$, which connect a cell with its nearest neighbor in one of the directions k (Figure 1).

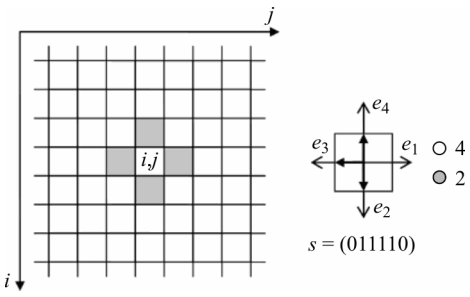

Figure 1. The HPPrp lattice and the HPPrp cell

Each cell can contain particles of two types: the moving particles and the rest particles. *Moving* particles have the unit mass and the unit velocity and moving particles are undistinguished. To each moving particle a momentum is assigned. No more than one moving particle can be found in the same cell at the same time with the same direction. This means that the moving particles locally obey the Pauli exclusion principle and are Fermi–Dirac distributed consequently. *Rest* particles have zero velocity and a different mass (2, 4, 8, ...).

The alphabet A is a set of 2^{4+b} Boolean vectors (states) $\boldsymbol{s} = (a_{4+b}, \ldots, a_4, a_3, a_2, a_1)$, $a_p \in \{0, 1\}$, where b is the number of the rest particles. The vector $\boldsymbol{s}$ contains the whole information about particles placed in a cell. The first four digit values of the vector $\boldsymbol{s}$ from the right show the presence ($a_p = 1$) or the absence ($a_p = 0$) of a moving particle in the direction to the k-th neighbor. The other digit values of the vector $\boldsymbol{s}$ show the presence ($a_p = 1$) or the absence ($a_p = 0$), $p = 5, \ldots, 4 + b$, of the mass 2^{p-4} rest particle. The total sum of particle mass in a cell is called *the model density.*

It is defined as

$$d(\boldsymbol{s}, \vec{\boldsymbol{r}}) = \sum_{i=1}^{4} a_i + \sum_{i=5}^{4+b} a_i 2^{i-4}.$$

For example, if a cell has the state $\boldsymbol{s} = (11011)$, this implies that it contains one the mass-2 rest particle and three moving particles with velocities in the directions $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ and $\boldsymbol{e}_4$, the model density of this cell being 5.

A pair $(\boldsymbol{s}, \boldsymbol{r})$, $\boldsymbol{s} \in A$, $\boldsymbol{r} \in M$, is called *a cell*. A set of cells, in which all cells have different names, forms *a cellular array* Ω. A set of the state of a cellular array at the time t is called *a global state* $\Omega(t)$ of the cellular array.

A set of transition functions $\Theta = \{\theta_s\}$ is defined by functioning rules of the HPPrp cellular automaton. The HPPrp CA operates synchronously: all the cells update their own states simultaneously at each iteration step. The iteration step consists of the two successive phases: collision and propagation. We introduce $a_p(\boldsymbol{r}, t)$ as the number of particles (which can be either 0 or 1) entering a cell with the name $\boldsymbol{r}$ at the time t with the unit velocity along the vector $\boldsymbol{e}_p$, where $p = 1, 2, 3, 4$.

At *the collision* phase, particles at each cell collide with each other in such a way that the total particle mass ($\sum_{p=1}^{4+b} a_p$) and the total momentum ($\sum_{p=1}^{4} a_p \boldsymbol{e}_p$) are conserved in each cell. At *the propagation* phase, the moving particles from each cell shift to the nearest neighbors with the unit velocity along the vectors $\boldsymbol{e}_p$. As a result, the microdynamics of the HPPrp cellular automaton is written down as

$$a_p(\boldsymbol{r} + \boldsymbol{e}_p, t+1) = a_p(\boldsymbol{r}, t) + \Lambda_p(\boldsymbol{a}(\boldsymbol{r}, t)),$$

where $\Lambda_p(\boldsymbol{a}(\boldsymbol{r}, t))$ represents the *collision operator*. The collision is carried out locally and transforms a *current* state $\boldsymbol{s} = (a_{4+b}, \ldots, a_4, a_3, a_2, a_1)$ of the cell to the *next* state $\hat{\boldsymbol{s}} = (\hat{a}_{4+b}, \ldots, \hat{a}_4, \hat{a}_3, \hat{a}_2, \hat{a}_1)$ with a certain transition probability $p_{\boldsymbol{s} \to \hat{\boldsymbol{s}}} \geq 0$. The set of transition probabilities forms *the collision matrix*.

In the HPPrp cellular automata, the collision rules are both deterministic and non-deterministic. They can be divided into three groups. (Here the empty circle stands for the absence of rest particle.)

Group 1 (head-on collision). If two particles enter a cell in one of the two opposite directions (either $(i, i+2)$ or $(i+1, i+3)$), these particles collide and change the vector direction by 90 degrees (Figure 2).

Figure 2. Head-on collision rules

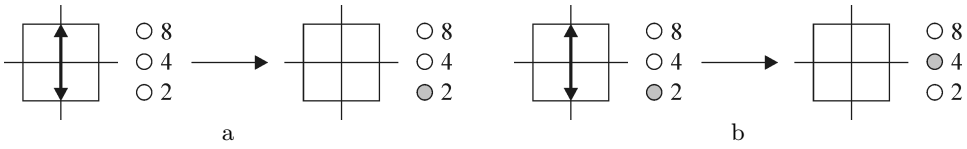

Figure 3. The rest particle creation rules

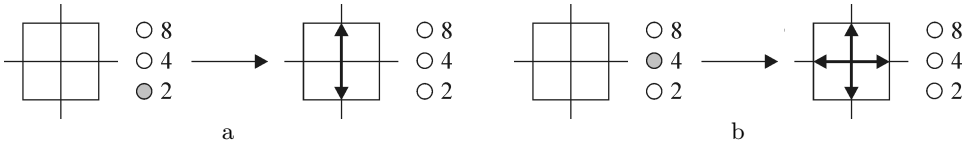

Figure 4. The rest particle annihilation rule

Group 2 (Creation of the rest particle). If two moving particles enter a cell in opposite directions and the mass-2 rest particle is absent, then moving particles will be annihilated and the mass-2 rest particle will be created. (Figure 3a). If either two moving particles enter a cell in opposite directions and the mass-2 rest particle exists (Figure 3b) or four moving particles enter a cell, then the mass-4 rest particle will be created and all particles in the current state of a cell will be annihilated.

Group 3 (rest particle annihilation). If the mass-2 rest particle exists in a cell and any of the two moving particles entering a cell in opposite directions are absent, then two moving particles will be created and the mass-2 rest particle will be annihilated (Figure 4a). If the mass-4 rest particle exists in a cell and all moving particles are absent, then four moving particles will be created, and all particles in the current state of a cell will be annihilated (Figure 4b).

As a result of the iteration step execution, the cellular automaton changes a current global state $\Omega(t)$ to a new global state $\Omega(t+1)$. An iterative change in the HPPrp global state (*evolution*) in the HPPrp CA describes the wave process dynamics.

Figure 5 shows the iteration step for one HPPrp cell with the two rest particles: the mass-2 and the mass-4. The current cell state is $\boldsymbol{s} = (010101)(\mathbf{21})$, $(\mathbf{21})$ is the decimal representation of a current cell state $\boldsymbol{s}$. The collision operator transforms this current state into one of the four states: $\hat{\boldsymbol{s}}_1 = (011010)(\mathbf{26})$, $\hat{\boldsymbol{s}}_2 = (001111)(\mathbf{15})$, $\hat{\boldsymbol{s}}_3 = (100000)(\mathbf{32})$, $\hat{\boldsymbol{s}}_4 = (011010)(\mathbf{21})$ with a certain transition probability $p_{\boldsymbol{s}\to\hat{\boldsymbol{s}}_k} \geq 0$, $k = 1, 2, 3, 4$. The transition probabilities satisfy the *normalization*

$$\forall \boldsymbol{s} \in A \quad \sum_{k=1}^{4} p_{\boldsymbol{s}\to\hat{\boldsymbol{s}}_k} = 1.$$

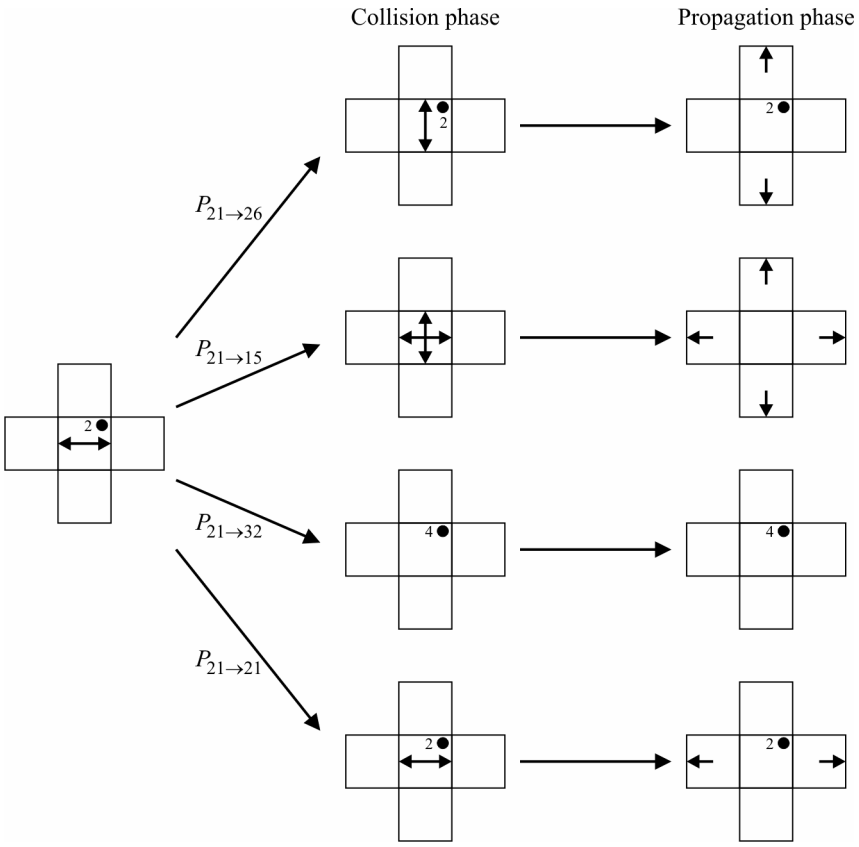

Figure 5. One iteration step for cell in the current state $\boldsymbol{s} = (010101)$

A set of states where all states have the same value for the invariant quantities for a HPPrp CA (mass and momentum) will be called *equivalence* class and denoted as Q_B, where B is a set of states for a given equivalence class. In the equivalence class for any state, which is a current state, all other states are the next states. For a given HPPrp CA, the equivalence classes are disjoint. The number of states in the class Q_B will be called the equivalence class *cardinality*.

2. The construction of the collision matrix

The collision matrix is defined as a matrix P of $2^{4+b} \times 2^{4+b}$ size, where b is the number of rest particles. A matrix entry p_{ij} is the transition probability of a cell from the current state $p_{\boldsymbol{s}}$ to the next state $p_{\hat{\boldsymbol{s}}}$. Indices i, j are the decimal representation of the current cell state $\boldsymbol{s}$ and the next cell state $\hat{\boldsymbol{s}}$. Since a set of the states for the HPPrp cells can be partitioned into mutually exclusive classes, then constructing the collision matrix can be reduced to

the construction of the collision matrix for each equivalence class. The transformed collision matrix $\boldsymbol{P}$ for the HPPrp with a mass-2 rest particle takes the following diagonal form:

$$\boldsymbol{P} = \mathrm{diag}(P_{Q_{5,10,16}}, P_{Q_{7,18}}, P_{Q_{11,17}}, P_{Q_{13,24}}, P_{Q_{14,20}}, P_{Q_{15,21,26}}).$$

Each diagonal entry in the matrix $\boldsymbol{P}$ presents a collision matrix for a given equivalence class. There are six equivalence classes — two classes of cardinality 3: $Q_{5,10,16}$ and $Q_{15,21,26}$ and four classes of cardinality 2: $Q_{7,18}$, $Q_{11,17}$, $Q_{13,24}$, and $Q_{1,18}$. For example, the collision matrix for the equivalence class $Q_{5,10,16}$ has the following form:

$$P_{Q_{5,10,16}} = \begin{pmatrix} p_{5\to5} & p_{5\to10} & p_{5\to16} \\ p_{10\to5} & p_{10\to10} & p_{10\to16} \\ p_{16\to5} & p_{16\to10} & p_{16\to16} \end{pmatrix}.$$

In such a manner, the construction of the collision matrix for the HPPrp CA is reduced to:

- derivation of equivalence classes for a given HPPrp CA and
- construction of the collision matrix for each equivalence class.

Entries of each collision matrix for a given class of equivalence satisfy:

- laws of conservation of mass and momentum,
- normalization condition $\forall \boldsymbol{s} \ \sum_{\hat{\boldsymbol{s}}} p_{\boldsymbol{s}\to\hat{\boldsymbol{s}}} = 1$, and
- semi-detailed balance propriety $\forall \hat{\boldsymbol{s}} \ \sum_{\boldsymbol{s}} p_{\boldsymbol{s}\to\hat{\boldsymbol{s}}} = 1$.

The procedure of constructing the collision matrix procedure for the equivalence class cardinality B is based on the formulation and solution to a system of 2B linear equations. Below a system of equations to the class $Q_{5,10,16}$ is shown:

$$\begin{aligned} p_{5\to5} + p_{5\to10} + p_{5\to16} &= 1, \\ p_{10\to5} + p_{10\to10} + p_{10\to16} &= 1, \\ p_{16\to5} + p_{16\to10} + p_{16\to16} &= 1, \\ p_{5\to5} + p_{10\to5} + p_{16\to5} &= 1, \\ p_{5\to10} + p_{10\to10} + p_{16\to10} &= 1, \\ p_{5\to16} + p_{10\to16} + p_{16\to16} &= 1. \end{aligned}$$

The first three equations are formed according to the normalization property. The second three equations are formed according to the semi-detailed balance. If the number of variables in a system of equations exceeds the number of equations in this system, then one has to set fixed values for probability of a transition cell from one state $p_{\boldsymbol{s}}$ to another state $p_{\hat{\boldsymbol{s}}}$. For

example, one can set a fixed value for probability of a cell remaining in the same state or a probability of a transition cell into the state when a cell contains a rest particle with a given mass. Then any method for solving a system of linear equations may be used. A simple version of the collision matrix is that with equally probable transitions:

$$P_{Q_{5,10,16}} = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}.$$

3. Investigation of the influence of the semi-detailed balance on wave processes

In the experiments carried out, the wave process propagation is presented by evolution of the HPPrp CA with the mass-2 rest particle. The cellular array size is 800×800 cells. The perturbation generation source is located at the array center and forms a sub-array of 20×300 cells size.

The initial states of the array cells (model densities) are given by particles distribution with a certain probability in each cell. Further, a cellular array for the wave process simulation will be called *a medium*. The medium model density is 3.3: four moving particles are generated in cells with probability 1, one the mass-2 rest particle is generated with probability 0.75 within one iteration. The model density of perturbation source cells are 5.5: four moving particles are generated in the cells with probability 0.7, one the mass-2 rest particle is generated with probability 0.25 within one iteration. The boundary conditions are periodical.

In order to observe the wave process in the usual representation of a physical phenomenon, the medium global states are twice averaged [3]. First, a value of particles density for each cell from a global state is averaged over a 5×5 cells square. Second, the values obtained are averaged over the array column. Further, a twice averaged global state of a medium at the t-th iteration of the cellular automaton evolution will be called *a wave profile* at the t-th iteration of the single wave propagation. The following parameters (model velocity, profile amplitude and profile median) are used for investigation of the wave processes obtained.

Figure 6 presents the profiles at different iterations of single wave propagation. The used collision matrix $\boldsymbol{P}^{(1)}$ has equal-probability blocks:

$$P^{(1)}_{Q_{5,10,16}} = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}, \quad P^{(1)}_{Q_{7,18}} = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \quad P^{(1)}_{Q_{11,17}} = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix},$$

$$P^{(1)}_{Q_{13,24}} = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \quad P^{(1)}_{Q_{14,20}} = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \quad P^{(1)}_{Q_{15,21,26}} = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}.$$

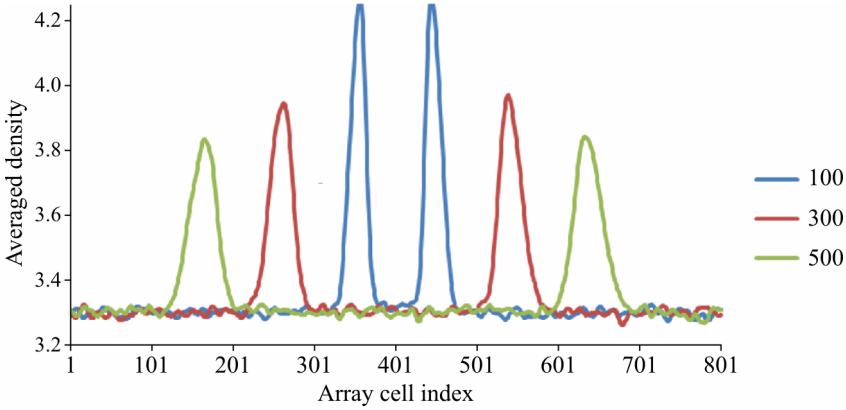

Figure 6. Wave profiles at different iterations of single wave propagation in the HPPrp medium for collision matrix $\boldsymbol{P}^{(1)}$

The simulation shows the following:

- A single wave propagates from a perturbation source with equal model velocity.
- Wave profiles vary with time: the amplitude profile is reduced, the width profile is increased, while the total mass and momentum of all the particles of the cell array are conserved.
- Wave profiles have the same parameters (amplitude and median) from a perturbation source.

Below we present the results of several computational experiments in which different collision matrices are used for modeling the wave process.

Experiment 1 (*Collision matrices obey the semi-detailed balance*). Computational experiments show that the profiles of different wave processes coincide regardless the transition probabilities values in collision matrices. Figure 7 shows the wave profiles for different iterations (200 and 500) for the two wave processes.

In the first wave processes, the collision matrix $\boldsymbol{P}^{(1)}$ was used and, in the second wave process, the matrix $\boldsymbol{P}^{(2)}$ with the following blocks was used:

$$P^{(2)}_{Q_{5,10,16}} = \begin{pmatrix} 0.1 & 0.9 & 0 \\ 0.8 & 0.1 & 0.1 \\ 0.1 & 0 & 0.9 \end{pmatrix}, \quad P^{(2)}_{Q_{7,18}} = \begin{pmatrix} 0.3 & 0.7 \\ 0.7 & 0.3 \end{pmatrix}, \quad P^{(2)}_{Q_{11,17}} = \begin{pmatrix} 0.95 & 0.05 \\ 0.05 & 0.95 \end{pmatrix},$$

$$P^{(2)}_{Q_{13,24}} = \begin{pmatrix} 0.05 & 0.95 \\ 0.95 & 0.05 \end{pmatrix}, \quad P^{(2)}_{Q_{14,20}} = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \quad P^{(2)}_{Q_{15,21,26}} = \begin{pmatrix} 0.2 & 0.8 & 0 \\ 0 & 0 & 1 \\ 0.8 & 0.2 & 0 \end{pmatrix}.$$

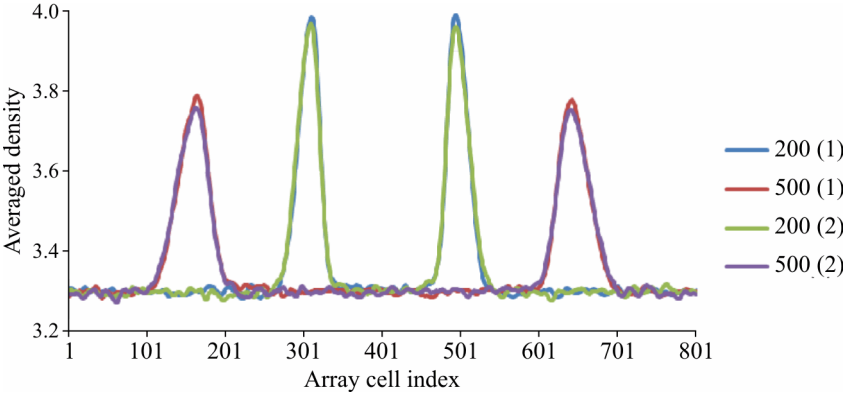

Figure 7. Wave profiles at different iterations of single wave propagation in the HPPrp medium for collision matrices $\boldsymbol{P}^{(1)}$ and $\boldsymbol{P}^{(2)}$

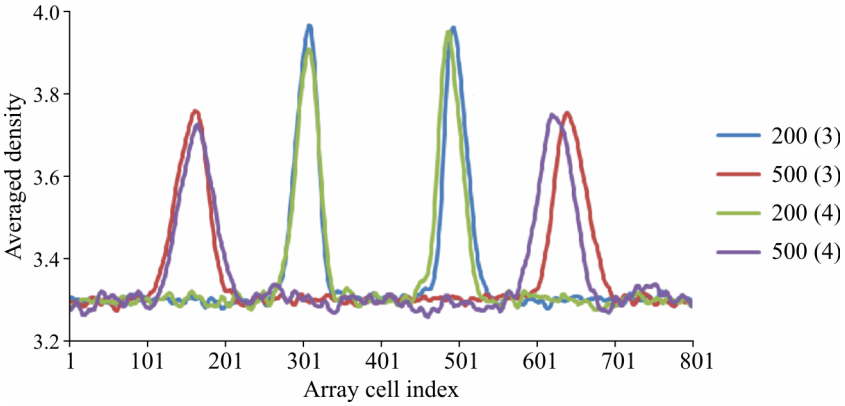

Figure 8. Wave profiles at different iterations of single wave propagation in the HPPrp medium for collision matrices $\boldsymbol{P}^{(3)}$ and $\boldsymbol{P}^{(4)}$

Experiment 2 (*Collision matrices do not obey the semi-detailed balance*). Computational experiments show that despite the fact that the used collision matrices do not obey the semi-detailed balance, the HPPrp evolution simulates a wave process. Figure 8 shows the wave profiles for different iterations (200 and 500) for the two wave processes.

The collision matrix $\boldsymbol{P}^{(3)}$ used in the first wave process differs from $\boldsymbol{P}^{(2)}$ in the blocks

$$P^{(3)}_{Q_{5,10,16}} = \begin{pmatrix} 0.1 & 0.9 & 0 \\ 0.8 & 0.2 & 0 \\ 0.8 & 0.2 & 0 \end{pmatrix}, \quad P^{(3)}_{Q_{15,21,26}} = \begin{pmatrix} 0.2 & 0.8 & 0 \\ 0 & 0 & 1 \\ 0.1 & 0.1 & 0.8 \end{pmatrix}$$

and the matrix $\boldsymbol{P}^{(4)}$ used in the second wave process differs from $\boldsymbol{P}^{(1)}$ in the blocks

$$P^{(4)}_{Q_{5,10,16}} = \begin{pmatrix} 0.7 & 0.2 & 0.1 \\ 0.2 & 0.7 & 0.1 \\ 0.5 & 0.5 & 0 \end{pmatrix}, \quad P^{(4)}_{Q_{15,21,26}} = \begin{pmatrix} 0.2 & 0.7 & 0.1 \\ 0.7 & 0.3 & 0 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$$

Moreover, the collision matrices $\boldsymbol{P}^{(4)}$ describes the particle dynamics which simulates wave processes with different velocities in the different directions from the perturbation source. The reason for this phenomenon is subject to further study.

Conclusion

In this paper, the procedure of designing the collision matrix for a cellular automaton with the rest particles for simulating wave processes is proposed. Entries in the collision matrix are transition probabilities from one state to anther. As the condition that guarantees the existence of a wave process the semi-detailed balance condition is used. The influence of the semi-detailed balance on characteristics of the wave process (velocity, amplitude and median of wave profile) is investigated. A large body of computational experiments has shown the following:

- If the semi-detailed balance condition holds in the HPPrp CA, the characteristics of the wave process coincide regardless of the transition probabilities values in the collision matrices.
- The HPPrp evolution simulates wave processes despite the fact that the semi-detailed balance condition is violated.
- In certain cases, the collision matrix simulates wave processes with different velocities in different directions from the perturbation source. The reason for this phenomenon is subject to further study.

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