

# CELLULAR AUTOMATON SIMULATING THE MOTION OF THE CHARGED PARTICLES BEAM

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## Abstract

In this research we formulate and formalize the rules for the cellular automaton that emulates the motion of the charged particles beam under the effect of Coulomb force for one-, two- and three-dimensional cases. In this research we also describe the main principles of the realization of this approach in a paralleled cluster environment.

## INTRODUCTION

At the present moment cellular automata are widely used as a simulating environment for complicated dynamic systems in various fields of science.

The environment that represents as a cellular automaton has a lot of opportunities for simulating the interactions of the manifold of connected homogeneous objects. We can refer to the sphere of application of cellular automata: simulating of interacting cellular systems in biology and medicine, simulating of physical processes in particle physics and nuclear physics, simulating of hydrodynamic and gasdynamic fluctuations etc. [1, 2]. To some detail about cellular automata conceptions you can go to [3].

Computer simulation tasks of the evolution of a moving beam of charged particles in accelerating installations demand advanced compute resources. For a computation constriction such models as PIC (Particle-In-Cell) [4, 5, 6], Large-particle method [7], PCM (Particle Core Models) [8, 9] etc. are used. These models assume solving of differential equations systems for the whole quasi-particle ensemble. This involves a lot of computations that demand parallelizing. The models based on cellular automata can be successfully realized in parallel computing systems owing to homogeneous discrete structure of a model. Due to this fact the idea of using cellular automata for this class of tasks of simulating appears to be challenging.

The aim of this research is to formalize the rules of cellular automaton for simulating the motion of a charged particles beam under its own Coulomb forces and develop the conception of the parallel realization of this approach.

This formalization of a cellular automaton is based on the idea of the Particle-In-Cell method [4].

## FORMAL CHARACTERIZATION OF A CELLULAR AUTOMATON FOR ONE-DIMENSIONAL CASE

Elementary charged particle  $p_n$  possesses the following characteristics:  $x$  — grid coordinate,  $m$  — particle mass,  $q$  — particle charge,  $\vec{v}$  — particle velocity.

Particle beam consists of  $N$  identical particles and has a length  $L$  in a moment of time  $t_0$  and average velocity  $\vec{v}_{avg}$ . For example we place the particles along  $Ox$  axis proportional and at random. We set the initial particle velocity as  $\vec{v}$ .

Let's choose  $\Delta t$  a step (in time) of the cellular automaton and define its working time in the interval  $[t_0, T]$ , where  $T$  is the maximal possible value  $t$  for this automaton.

Let's divide coordinate axis  $Ox$  into the similar intervals (we talk about a cell in a cellular automata theory)  $K_i = [x_i, x_{i+1})$ , where  $x_i = i\Delta x$  and  $i \in \mathbb{Z}$ . The size of a cell is chosen as  $\Delta x = \vec{v}_{avg}\Delta t$  or in any other way.

Let's formalize the rules of the automaton as an algorithm:

1. Packing a particle as a quasi-particle.

Cell  $K_i = \{p_n | x_n \in [i\Delta x, (i+1)\Delta x)\}$ . We suppose that each cell  $K_i$  is a quasi-particle that

$$x_{K_i} = i\Delta x + \frac{\Delta x}{2}, \quad q_{K_i} = \sum_{p_n \in K_i} q_{p_n},$$

$$m_{K_i} = \sum_{p_n \in K_i} m_{p_n}, \quad \vec{v}_{K_i} = \frac{\sum_{p_n \in K_i} \vec{v}_{p_n}}{n_i},$$

where  $n_i$  is the number of particles in  $K_i$  cell.

2. Reckoning of the force acting on a quasi-particle. Let us assume that  $\vec{R}_{K_i}$  is a final force that acts on  $K_i$  cell.

- (a) Neighboring cells influence. One "neighbor" from the left and one from the right.

$$\vec{R}_{K_i} = \vec{F}_{K_{i+1}} + \vec{F}_{K_{i-1}},$$

where  $\vec{F}$  is Coulomb forces acting on a cell. In projection on  $Ox$  axis we have

$$R_{K_i} = k \frac{q_{K_i} q_{K_{i-1}}}{\Delta x^2} - k \frac{q_{K_i} q_{K_{i+1}}}{\Delta x^2} =$$

$$= k \frac{q_{K_i}}{\Delta x^2} (q_{K_{i-1}} - q_{K_{i+1}}),$$

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where  $k$  is a constant of proportionality in Coulomb law.

- (b) The influence of two neighbors from the right and from the left.

$$R_{K_i} = \vec{F}_{K_{i+1}} + \vec{F}_{K_{i-1}} + \vec{F}_{K_{i+2}} + \vec{F}_{K_{i-2}}.$$

$$\begin{aligned} R_{K_i} &= k \frac{q_{K_i} q_{K_{i-1}}}{\Delta x^2} - k \frac{q_{K_i} q_{K_{i+1}}}{\Delta x^2} + \\ &+ k \frac{q_{K_i} q_{K_{i-2}}}{2\Delta x^2} - k \frac{q_{K_i} q_{K_{i+2}}}{2\Delta x^2} = \\ &= k \frac{q_{K_i}}{\Delta x^2} (q_{K_{i-1}} - q_{K_{i+1}}) + \\ &+ k \frac{q_{K_i}}{2\Delta x^2} (q_{K_{i-2}} - q_{K_{i+2}}). \end{aligned}$$

Coulomb forces are far-ranging but the influence of  $M$  remoter neighbors can be rested on.

- (c) The influence of  $M$  neighbors from the right and from the left.

$$\begin{aligned} R_{K_i} &= k \frac{q_{K_i}}{\Delta x^2} \left( \sum_{l=1}^M \frac{1}{l^2} q_{K_{i-l}} - \sum_{l=1}^M \frac{1}{l^2} q_{K_{i+l}} \right) = \\ &= k \frac{q_{K_i}}{\Delta x^2} \sum_{l=1}^M \frac{q_{K_{i-l}} - q_{K_{i+l}}}{l^2}. \end{aligned}$$

3. Acceleration that  $K_i$  cell (quasi-particle) will get is

$$a_{K_i} = \frac{R_{K_i}}{m_{K_i}},$$

and the delta of velocity

$$\Delta v_{K_i} = a_{K_i} \Delta t.$$

4. Reckoning of coordinates and velocities of  $K_i$  cell (quasi-particle) at the moment of time  $t = t + \Delta t$

$$x_{K_i} = x_{K_i} + v_{K_i} \Delta t + \frac{a_{K_i} \Delta t^2}{2},$$

$$v_{K_i} = v_{K_i} + \Delta v_{K_i}.$$

5. Unpacking of a quasi-particle into a set of particles.

- (a) Unpacking of the particle coordinate in accordance with the previous coordinates

$$x_{p_{K_i}} = x_{p_{K_i}} + (x_{K_i}^{old} - x_{K_i}^{new}).$$

- (b) Unpacking of the particle velocities with regard for the proportional change in quasi-particle velocity.

$$v_{p_{K_i}} = v_{p_{K_i}} \frac{v_{K_i}^{old}}{v_{K_i}^{new}}.$$

6. The shift of the automaton step with respect to time  $t = t + \Delta t$ . If automaton does not come out to the given interval  $t \leq T$ , let's move to the entry 1.

## FORMAL CHARACTERIZATION OF A CELLULAR AUTOMATON FOR TWO-DIMENSIONAL CASE

Let's break up  $Oxy$  subspace into square cells  $K_{i,j}$  in size  $\Delta x \times \Delta y$ , where  $\Delta x = \Delta y$ , and set the particles by analogy with one-dimensional case.

The algorithm is identical to one-dimensional case. The difference is in its dimensionality. The peculiarity of the algorithm is the reckoning of Coulomb forces for two-dimensional case. We have all of the same stages fulfilled by analogy with one-dimensional case.

We reckon Coulomb forces as follows. If the element interacting with  $K_{i,j}$  stays in place  $(i - m, j - n)$  then squared distance between them can be stated as

$$r^2 = (m^2 + n^2) \Delta x^2.$$

Coulomb force projection on  $Ox$  and  $Oy$  axes can be stated as

$$F_x^1 = k \frac{q_{K_{i,j}}}{\Delta x^2} \frac{q_{K_{i-m,j-n}}}{(m^2 + n^2)^{3/2}} m,$$

$$F_y^1 = k \frac{q_{K_{i,j}}}{\Delta x^2} \frac{q_{K_{i-m,j-n}}}{(m^2 + n^2)^{3/2}} n.$$

Taking the account of the aggregate effect of Coulomb forces of the neighboring cells on quasi-particle  $K_{i,j}$  in square  $(2M \times 2M)$  can be described with the following formula

$$R_{K_{i,j}}^x = -k \frac{q_{K_{i,j}}}{\Delta x^2} \sum_{m=-M}^M \sum_{n=-M}^M \frac{q_{K_{i+m,j+n}}}{(m^2 + n^2)^{3/2}} m,$$

$$R_{K_{i,j}}^y = -k \frac{q_{K_{i,j}}}{\Delta x^2} \sum_{m=-M}^M \sum_{n=-M}^M \frac{q_{K_{i+m,j+n}}}{(m^2 + n^2)^{3/2}} n,$$

where  $m^2 + n^2 \neq 0$ .

Acceleration, new velocities and coordinates for each quasi-particle  $K_{i,j}$  are got from the formulae of one-dimensional case for each of  $x$  and  $y$  coordinates.

## FORMAL CHARACTERIZATION OF A CELLULAR AUTOMATON FOR THREE-DIMENSIONAL CASE

Let's break up the volume  $Oxyz$  into cells  $K_{i,j,k}$  in size  $\Delta x \times \Delta y \times \Delta z$ , where  $\Delta x = \Delta y = \Delta z$  and set the particles by analogy with the previous cases. The algorithm is identical to the previous cases. The difference is in its dimensionality.

Taking the account of the aggregate effect of Coulomb forces of the neighboring cells on quasi-particle  $K_{i,j,k}$  in cube in  $(2M \times 2M \times 2M)$  can be described with formulae

$$R_{K_{i,j,k}}^x = -k \frac{q_{K_{i,j,k}}}{\Delta x^2} \sum_{m=-M}^M \sum_{n=-M}^M \sum_{l=-M}^M \frac{q_{K_{i+m,j+n,k+l}}}{(m^2 + n^2 + l^2)^{3/2}} m,$$

$$R_{K_{i,j,k}}^y = -k \frac{q_{K_{i,j,k}}}{\Delta x^2} \sum_{m=-M}^M \sum_{n=-M}^M \sum_{l=-M}^M \frac{q_{K_{i+m,j+n,k+l}}}{(m^2 + n^2 + l^2)^{3/2}} n,$$

$$R_{K_{i,j,k}}^z = -k \frac{q_{K_{i,j,k}}}{\Delta x^2} \sum_{m=-M}^M \sum_{n=-M}^M \sum_{l=-M}^M \frac{q_{K_{i+m,j+n,k+l}}}{(m^2 + n^2 + l^2)^{3/2}} l,$$

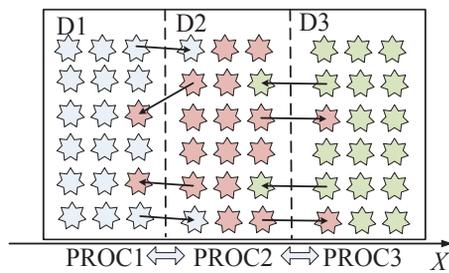


Figure 1: The distribution of quasi-particles along processors

where  $m^2 + n^2 + l^2 \neq 0$ .

Acceleration, new velocities and coordinates for each quasi-particle  $K_{i,j,k}$  are got from the formulae of one-dimensional case for each of  $x$ ,  $y$  and  $z$  coordinates.

## PARALLEL REALIZATION

Let's state the algorithm for the cases mentioned above.

1. Let's proportionally distribute the particles along processors  $PROC_n$  depending on their location. Then we break up the coordinate domain of particles into subdomains  $D_n$  along one of the dimensions, for example on  $Ox$  (see fig. 1), so that borders  $BORD_D$  of subdomains  $D$  would go through one of the points  $x \in (\Delta x \cdot \mathbb{Z})$ , and every subdomain would contain approximately equal amount of particles, i.e. to the processor  $PROC_n \in D_n$ .
2. Let's "pack" the particles into the multitude of cells  $\{K\}$ .
3. Let's redistribute the cells  $K$  containing the particles  $p \in K$  along the processors depending on their location by moving the borders  $BORD_D$  of subdomains  $D$  so that each subdomain  $D$  would contain approximately equal amount of cells  $K$  (redistribution is performed dynamically on every iteration of the algorithm).
4. For the charge reckoning  $R_D$  of the cells that are situated closer to the borders  $BORD_D$  we need the value of each cell  $K_{D-1}$  and  $K_{D+1}$  of the neighboring subdomains  $D-1$  and  $D+1$ . Due to this fact each processor  $PROC_D$  interchanges the necessary cell values  $K$  between the neighboring processors  $PROC_{D-1}$  and  $PROC_{D+1}$ .
5. For each cell  $K$  charge reckoning is performed along with the reckoning of accelerations, new velocities and coordinates.
6. After the recomputation of coordinates several cells can move into the neighboring subdomains. Due to this fact each processor  $PROC_D$  performs the interchange of such cells into the neighboring processors  $PROC_{D-1}$  and  $PROC_{D+1}$ .

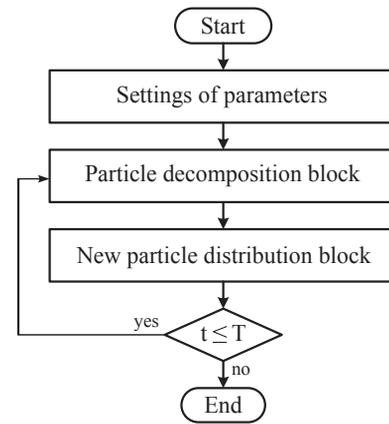


Figure 2: Control flow diagram of the automaton

7. Let's "unpack" the cells using the evaluations we made.
8. If the conditions of the secession from the algorithm are not observed then let's start a new iteration, move to enter 2.

## CONCLUSION

In this research we state and formalize the rules of a cellular automaton that simulates the motion of elementary charged particles under their own Coulomb forces for one-, two- and three-dimensional cases. We also represent the main principles of realization of this approach in a concurrent clustered environment.

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