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Threshold functions for inserting or deleting particles in the PIC method with adaptive mass*

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1. Introduction

The Particle-in-Cell methods (PIC) [1–4] are widely used in the numerical simulation. The media under study in these methods are represented with a sufficiently large number of model particles with definite characteristics such as mass, charge, velocity. The evolution of a system of particles at each time step is evaluated in two steps. First, the Euler step computes the impact of particles on a medium with fixed particles in grid values. Second, the Lagrange step computes the positions and velocities of particles from the equation of motion with the right-hand side computed at the Euler stage.

Since it is possible to trace trajectories of model particles, the PIC method allows studying the evolution of a medium. But it is necessary to keep in mind that model particles do not exactly correspond the real prototypes. Thus, it would be a mistake to directly compare them. The number of e model and the real particles significantly differ.

The PIC method has a relatively low precision due to several sources of errors. One of them is the interpolation of forces from the Euler grid nodes into the position of particles as well as approximation of grid functions. Another source of an error is the so-called self-force. It is the impact of the particle field on the particle itself through a spatial grid. To decrease errors of the above two given sorts, various particle form-factors are used [1,3,5,6].

One more source of errors is statistical fluctuations and noise that arise due to a difference of model particles and real particles. It was proved [4] that the precision of computation depends not only on the time and the spatial steps but, also, on the number of model particles. Thus, the only universal way to reduce the noise is to increase the number of particles. But it is not always possible, especially for the 2D and the 3D computations. Moreover, this greatly increases computer costs.

Nevertheless, the PIC method is capable of simulating many physical effects that are unreachable for other computational schemes.

Due to this reason, new methods are being developed that enable us to control the number of particles in a cell [7,8,10] to add new particles if their number is lower than some definite number, or to remove particles if their

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number is too high. The main characteristics such as density, momentum, the center of mass and energy in a cell, must not be changed in the course of adding or removing model particles. At this point, model particles start having different masses. This may improve the precision of computation when the process involves masses or numbers of atoms less than the size of one model particle. This situation may take place in the following problems: gas dynamics at the boundary with vacuum, chemical processes with a low concentration of reagents, multistream flows.

There was found that not only the method of inserting or deleting particles has a meaning, but also the choice of particle number limits (the threshold functions). Three types of threshold functions are given and compared: constant functions, spatial averaged functions and local averaged functions.

In Section 2, the PIC method with an adaptive mass is presented. In Section 3, threshold functions for inserting and deleting particles in a cell are described. In Section 4, the model problem statement and methods of its solution are described. In Section 5, computing experiments for the PIC method with adaptive mass with different threshold functions and an adaptive mass are given and their results are compared with results of the PIC method with a constant mass.

2. Definition of the PIC method with adaptive mass

It is known [4] that the precision of calculation for the PIC method depends on the number of model particles in a cell. Therefore, when solving equations, it is necessary to know the number k of cells, in which the number of particles N_k is reduced below the threshold. In this case, it is necessary to add particles to a cell for reaching the given level N^*. In addition, one should decide how mass, velocity and position of new particles are determined. The conservation laws and velocity distribution should be satisfied. The latter condition is necessary for a multi-stream velocity distribution to be undestroyed.

For satisfying the above conditions, we place an auxiliary 2D grid by space and velocity into a cell, in which the number of particles should be changed. Experiments show that 5×5 grid is sufficient in this case.

The following characters are computed in each subcell:

- the total mass of particles

$$M_i = \sum_{j \in N_i} m_j; \tag{1}$$

- the total energy

$$Q_i = \sum_{j \in N_i} \frac{m_j v_j^2}{2}; \tag{2}$$

- The weighed average velocity

$$V_i = \sum_{j \in N_i} \frac{m_j v_j}{M_i}; \tag{3}$$

- The center of mass

$$X_i = \sum_{j \in N_i} \frac{m_j x_j}{M_i}. \tag{4}$$

Now, the procedure of adding or deleting a particle is split to the following steps for every subcell:

1. Calculating the number of particles k_i;
2. Calculating the mass m'_j so that $M'_i = M_i$;
3. Calculating the velocity v'_j so that $V'_i = V_i$ and $Q'_i = Q_i$;
4. Calculating the position x'_j so that $X'_i = X_i$.

We use the weight averaged method for calculation the number of particles:

$$k_i = \begin{cases} \left\lfloor \dfrac{N^* M_i}{\sum M_i} + 0.5 \right\rfloor, & \dfrac{N^* M_i}{\sum M_i} \geq 1, \\ 1, & 0 < \dfrac{N^* M_i}{\sum M_i} < 1, \\ 2, & \dfrac{N^* M_i}{\sum M_i} < 2, \ \dfrac{M_i V_i^2}{2} < Q_i, \\ 0, & M_i = 0. \end{cases}$$

The first condition provides a greater number of particles in subcells, where the total mass is greater. The second condition prevents the loss of particles in a subcell when the total mass is less than the mass of one particle. The third condition prevents the loss of energy in the case when several particles are united into one. If energy is badly conserved, then the number of particles must be at least 2. This provides the choice between 2 and $\left\lfloor \frac{N^* M_i}{\sum M_i} + 0.5 \right\rfloor$.

The mass is calculated in the following way:

$$m'_j = \frac{M_i}{k_i}. \tag{5}$$

On the one hand, this distribution is natural, and on the other hand it enables making even the mass of particles in a cell.

The velocities are specified as follows: $v'_j = V_i + \nu_j$, where ν_j satisfies the condition $\sum \nu_j = 0$, and $\sum \nu^2 = 2k_i Q_i / M_i - V_i^2$.

The new positions are calculated as $x'_j = X_i + \delta_j$, where δ_j satisfies the following conditions: $h(l-1) < X_i + \delta \leq hl$ and $\sum \delta_j = 0$, here l is the cell number. The first condition provides the presence of particles in the lth cell. The second condition provides conservation the position of the mass center. This means that the density in grid nodes does not change.

3. Threshold functions for changing the number of particles

Since the PIC method is sensitive to the number of particles in a cell, the following questions arise: when it is reasonable to change the number of particles, and how much the number of particles should be changed?

The constant threshold functions. Particles are inserted when their number has lowered below N_{low}, and particles are deleted when their number has enlarged above N_{high}.

These are the simplest threshold functions, which do not need an expanded calculation. The number of particles in a cell is strictly restricted. On the one hand, this prevents an essential increase of the total number of particles, but on the other hand, this can add noise to the density calculation because of a difference in mass values.

Note that the initial distribution should satisfy the threshold values.

The spatially averaged functions. The recommended number of particles is the value of the following function of density

$$N(\rho) = \frac{\rho}{\rho^*} n^*.$$

Here $\rho = \max(\rho_{i-1}, \rho_i)$ is a maximum density of nodes of the ith cell, ρ^* is the averaged density of computational domain, and n^* is the averaged number of particles.

The threshold functions are $N_{\text{low}}(\rho) = \frac{2}{3}N(\rho)$ and $N_{\text{high}}(\rho) = 2N(\rho)$ in this case.

The recommended number of particles depends on the density ρ, and n^*/ρ^* is a normalization factor. In this case, particles are inserted because of the density drop, but not only because of a small number of particles. Also, a condition of the initial distribution is simplified.

However, averaging by the hole area can loose local features of the solution.

The locally averaged functions. The number of particles is chosen under assumption of averaged values in the nearest cells. In experiments with the constant and the spatially averaged threshold functions, some conditions were found, namely:

- locality: values of the nearest cells (the nearest nodes) are considered;
- the direct relation of the particle mass and density: the higher density, the greater mass of particles in a cell; the lower density, the lesser mass of particles in a cell;
- when adding particles, the averaged mass in a cell should be less than 0.9 averaged mass by the localization area;
- when deleting particles, noise in the nodes of a cell should not grow. Otherwise, the averaged mass should be not more than a minimum of the averaged mass of the adjacent cells.

Noise is considered as a maximum of particles contribution to the value of density:

$$Sh_i = {\rho_i}^{-1} \max_{|x_j - x_i| \le h} \frac{m_j}{h} \left(1 - \frac{|x_j - x_i|}{h}\right),$$

where j is the number of particles, and i is number of the node in the cell. As the value of real media is too small, the value of model media is excited by a large size of model particles.

To satisfy the above conditions, the use of the averaged mass of particles $\overline{m}_i$, but not the number of particles in the cell, is convenient.

The localization is performed by 5 cells and 4 nodes. Below, the whole indices are node indices and half-indices are cell indices. The recommended averaged mass $\overline{m}'_i$ is calculated with the following formula:

$$\overline{m}'_{i-1/2} = \frac{\rho_{i-1} + \rho_i}{2} \frac{0.2 \sum\limits_{k=-2}^{2} \overline{m}_{i+k-1/2}}{0.25 \sum\limits_{k=-2}^{1} \rho_{i+k}}.$$

The number of particles could change if $\overline{m}_{i-1/2} > 1.1\overline{m}'_{i-1/2}$ or $\overline{m}_{i-1/2} < 0.9\overline{m}'_{i-1/2}$. In this case, the new number of particles is calculated as

$$n'_{i-1/2} = n_{i-1/2} \frac{\min(\overline{m}'_{i-1/2}, \overline{m}_{i-3/2}, \overline{m}_{i+1/2})}{\overline{m}_{i-1/2}}.$$

The use of the locally averaged threshold functions needs an additional memory and calculations, but this enables one to essentially reduce the density noise.

4. Problem statement

Let us consider an example of a model 1D Riemann problem for the ion density in a dispersive medium [9]. The medium is a non-isothermal rarified plasma with the Boltzmann electron distribution.

The problem has one dimension along the spatial coordinate x. The following system of equations is the basis:

$$\begin{aligned} &\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \frac{e}{m_i}\frac{\partial \phi}{\partial x}\frac{\partial f}{\partial u} = 0, \\ &\frac{\partial^2 \phi}{\partial x^2} = 4\pi e\left[n_0 \exp(\frac{e\phi}{T_e}) - \int_{-\infty}^{\infty} f\,\partial u\right], \\ &E(x) = -\frac{\partial \phi}{\partial x}. \end{aligned} \tag{6}$$

Here f is an ion distribution function, u is the ion velocity, e is the electron charge, m_i is the ion mass, ϕ is the potential, n_0 is a non-perturbed plasma density (plasma is assumed to be quasi-neutral), T_e is the electron temperature, $E(x)$ is an electric field.

After transition to non-dimensional variables and to a finite computational domain, the system of equations has the form [4]:

$$\frac{\partial x_j}{\partial t} = u_j, \quad \frac{\partial u}{\partial t} = E(x_j), \quad \beta\frac{\partial^2 \phi}{\partial x^2} = \exp(\phi) - \rho. \tag{7}$$

Here j is the index of a particle, the potential is measured in the units of T_e/e, the velocity u is measured in the units of the ion sound $c_s = T_e/m_i$, $\beta = (D/L)^2$, $D = (4\pi n_0 e^2/T_e)^{-1/2}$ is the Debye length, $\rho = \int_0^L f\,\partial u$ is the density, L is the size of the computational domain.

Let us set the following boundary and initial conditions:

$$u(x,0) = 0, \qquad \rho(x,0) = \begin{cases} C, 0 \le x \le x_0, \\ 1, x_0 < x \le L, \end{cases} \tag{8}$$

$$u(0,t) = u(L,t) = 0, \qquad \phi(0,t) = \ln C, \qquad \phi(L,t) = 0, \tag{9}$$

where C is a shear of the ion density, x_0 is the position of the shear. The boundary conditions are set under assumption that the wave does not reach the domain boundaries, thus the velocity and the potential at the boundaries do not change.

The system of equations (7) with initial and boundary conditions (8), (9) satisfy the conservation laws for mass, impulse and energy [4]:

$$\begin{aligned} \int_0^L \rho\,dx &= \text{const}, \\ P = \int_0^L \rho u\,dx &= (e^{\phi_0} - 1)t, \\ W = \int_0^L \Big[\frac{1}{2}\rho u^2 + \frac{1}{2}\beta\phi_x^2 + e^{\phi_0}(\phi - 1)\Big]\,dx &= \text{const}\,. \end{aligned} \tag{10}$$

The computational domain is split to N_c equal cells by the nodes with the coordinates $x_k = kh$ $(k = 0, 1, \ldots, N_c)$; $h = L/N_c$ is a splitting step. At the initial moment of time, N_k immobile particles are placed in each cell $[x_{k-1}, x_k]$ ($N_p = \sum_{k=1}^{N_c} N_k$ is the total number of particles). The potential ϕ_k and the density ρ_k are computed in the grid nodes, and the electric field $E_{k-1/2}$ is computed in the centers of cells $[x_{k-1}, x_k]$.

The density ρ_k is computed in the grid nodes with the PIC form-factor

$$\bar{R}(x, x') = h^{-1} \max(0, 1 - |x - x'|/h)$$

by the formula

$$\rho_k = \sum_j m_j \bar{R}(x_k, x_j).$$

The electric field is interpolated into the position x_j, where a particle is placed, by the formula

$$E(x_j) = \frac{(x_{k+1/2} - x_j)E_{k-1/2} + (x_j - x_{k-1/2})E_{k+1/2}}{h}$$

if $x_j \in [x_{k-1/2}, x_{k+1/2}]$.

A computational loop at each time step τ is implemented in the following way.

Lagrange stage. For each particle with index j, the position x_j^{n+1} and the velocity u_j^{n+1} for the time $t = (n+1)\tau$ are computed from the values at the previous moment of time $t = n\tau$ as follows:

$$\frac{u_j^{n+1} - u_j^n}{\tau} = E(x_j^n), \qquad \frac{x_j^{n+1} - x_j^n}{\tau} = u_j^{n+1},$$

Euler stage. Values of the potential in the grid nodes ϕ_k are computed as limit of the sequence ϕ^s of solutions to the linear equation

$$\beta \frac{\phi_{k-1}^{s+1} - 2\phi_k^{s+1} + \phi_{k+1}^{s+1}}{h^2} = \exp(\phi_k^s)(1 + \phi_k^{s+1} - \phi_k^s) - \rho_k;$$
$$\phi_0^{s+1} = \ln C, \qquad \phi_{N_c}^{s+1} = 0.$$

This equation is solved by the sweep method. The value of the potential obtained at the previous time step is set as an initial approximation. The interactional process goes until the condition $\|\phi^{s+1} - \phi^s\| < \epsilon = 10^{-8}$ is satisfied.

Then the electric field is computed by the formula

$$E_{k-1/2} = \frac{\phi_{k-1} - \phi_k}{h}.$$

The problem is of interest because the particles motion essentially differs due to a different shear of the density:

- when $C < 5$, the laminar percussion moves to the right and the vacuum wave — to the left;
- when $5 \leq C \leq 13$, the percussion is frustrated with the formation of the precursor and pulsar particle reflection;
- when $13 < C \leq 225$, the percussion with a sharp front between the main wave and the precursor is formed, at the same time, the front persistently reflects particles;
- when $C > 225$, the initial shear is persistently blurred without percussion formation partial reflection.

5. Numerical experiments

To solve this problem, the following modifications of the PIC method are used:

- PIC-1 with a constant mass;
- PIC-2a with an adaptive mass and the constant threshold functions;
- PIC-2b with an adaptive mass and the spatially averaged threshold functions; and
- PIC-2c with an adaptive mass and the locally averaged threshold functions.

For all modifications, the computations were carried out on the grid with 10001 nodes ($N_c = 10^5$ cells) and $N_p = 10^7$ particles.

The laminar percussion. The computations were conducted with $C = 2$. In this case, blurring a shear step forms the laminar percussion moving to the right and the vacuum wave — to the left. The positions of some model particles are shown in Figure 1a. The result of the PIC-2c method is shown in Figure 1b. For all modifications, potential values agree with five digits.

Table 1 shows the mean noise, the maximum noise, and an error of executing the energy conservation law. When the PIC-2c method is used, application of the locally averaged functions allows one to reduce maximum noise by 12 %, whereas using the constant threshold function increases a maximum noise by 5 %.

The pulsar particle reflection. When the initial density shear $C = 5$, the motion character is changed (Figure 2). The pulsar particle reflection occurs by using all the modifications.

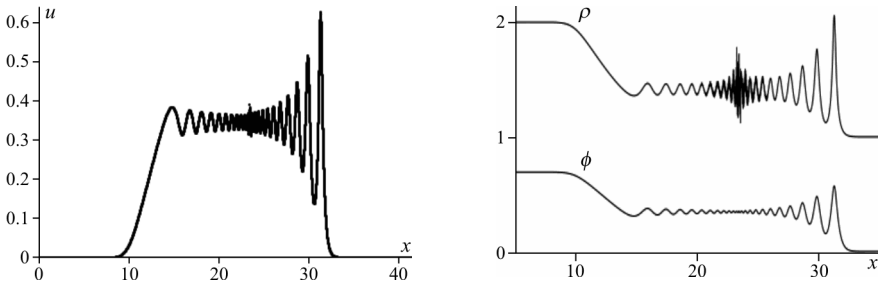


Figure 1. The laminar percussion for $C = 2$: the particle distribution (left) and the density and the potential (right)

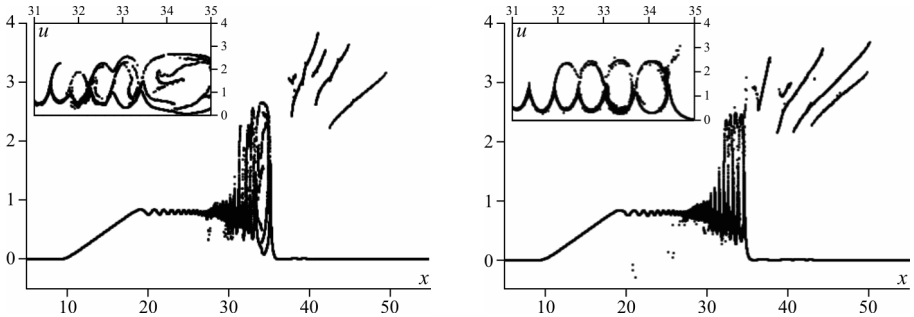
Table 1. The noise and the error of the energy conservation law (%) for different variant of PIC method for $C = 2$

Method	Mean noise	Maximum noise	Error
PIC-1	$6.0 \cdot 10^{-3}$	$1.47 \cdot 10^{-2}$	$1.044 \cdot 10^{-6}$
PIC-2a	$6.0 \cdot 10^{-3}$	$1.54 \cdot 10^{-2}$	$1.043 \cdot 10^{-6}$
PIC-2b	$6.9 \cdot 10^{-3}$	$1.33 \cdot 10^{-2}$	$1.043 \cdot 10^{-6}$
PIC-2c	$6.0 \cdot 10^{-3}$	$1.29 \cdot 10^{-2}$	$1.043 \cdot 10^{-6}$

Apparently, in Table 2, the PIC method with an adaptive mass allows one to essentially reduce the maximum noise in this case. The ratio error of the energy conservation law is reduced, too. Using the local averaged functions gives a better result than that with the use of the constant or the spatial averaged functions.

In Figure 2, the distributions of particles velocities derived by PIC-1 and PIC-2c methods are shown. The area $31 \leq x \leq 35$ is shown in the top left corner for both calculations.

Note that the motion of particles is more regular in the second case (Figure 3). This is conditioned by a sufficient quantity of smaller model



PIC-1 PIC-2c

Figure 2. The distribution of particles velocities for $C = 5$

Table 2. The noise and the error of the energy conservation law (%) for different variant of PIC method for $C = 5$

Method	Mean noise	Maximum noise	Error
PIC-1	$1.56 \cdot 10^{-2}$	$14.78 \cdot 10^{-2}$	$1.20 \cdot 10^{-4}$
PIC-2a	$1.50 \cdot 10^{-2}$	$3.40 \cdot 10^{-2}$	$0.73 \cdot 10^{-4}$
PIC-2b	$1.33 \cdot 10^{-2}$	$2.89 \cdot 10^{-2}$	$0.86 \cdot 10^{-4}$
PIC-2c	$1.41 \cdot 10^{-2}$	$2.09 \cdot 10^{-2}$	$0.44 \cdot 10^{-4}$

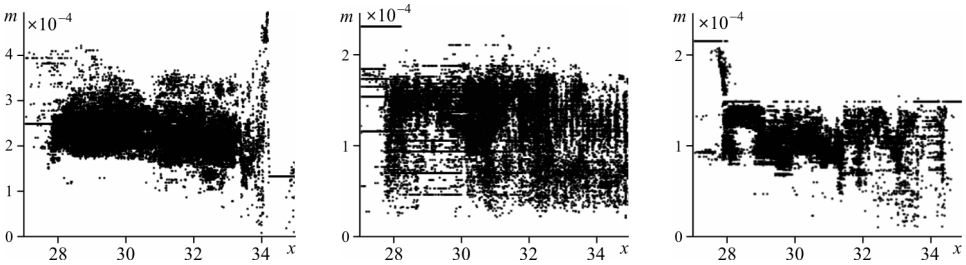


Figure 3. The distribution of particles mass for PIC-2 methods and $C = 5$

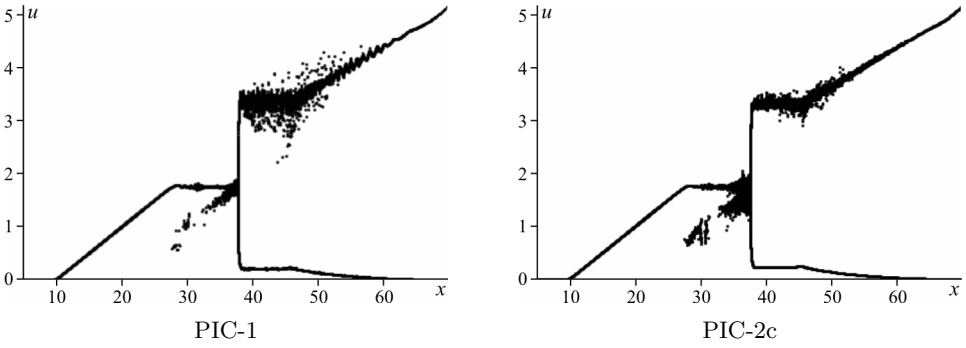


Figure 4. The distribution of particles velocities $C = 40$

Table 3. The noise and the error of the energy conservation law (%) for different variant of PIC method for $C = 40$

Method	Mean noise	Maximum noise	Error
PIC-1	$7.03 \cdot 10^{-2}$	$8.81 \cdot 10^{-2}$	$5.40 \cdot 10^{-6}$
PIC-2a	$1.76 \cdot 10^{-2}$	$5.76 \cdot 10^{-2}$	$3.04 \cdot 10^{-6}$
PIC-2b	$3.78 \cdot 10^{-2}$	$7.12 \cdot 10^{-2}$	$4.40 \cdot 10^{-6}$
PIC-2c	$2.68 \cdot 10^{-2}$	$5.51 \cdot 10^{-2}$	$3.26 \cdot 10^{-6}$

particles (from $7 \cdot 10^{-6}$ to $2.16 \cdot 10^{-4}$) as compared to model particles in PIC-1 method ($1.8 \cdot 10^{-4}$) in the area. When the constant threshold functions are used (PIC-2a), the majority of particles is bigger: the mass of particles varies from 10^{-6} to $5.96 \cdot 10^{-4}$. When the spatially averaged functions are used (PIC-2b), the mass of particles varies from $2.1 \cdot 10^{-5}$ to $2.3 \cdot 10^{-4}$.

Note, for obtaining such regular motions by the PIC method with a constant mass, the number of particles should be 10 times greater. However, this greatly increases computer costs.

The persistent reflection of particles. When $C = 40$, the particles are persistently reflected from the front, and the main wave is broken (Figure 4). In this case, the PIC method with an adaptive mass gives a gain as compared to the PIC method with a constant mass, and using the local averaged threshold functions is preferred to using the constant or the spatial averaged functions.

As in the above case, the bigger mass of particles in the PIC method with a constant mass brings about distortions. This is observed as greater dispersion and oscillatory changes of velocities of particles, which form the top stream.

6. Conclusion

In this paper, different threshold functions are presented. The constant threshold functions are simpler and more popular, but sometimes they can increase noise in the density calculation, because of an increase in the particle mass. The spatial averaged functions cannot increase noise because of the normalization factor. But they cannot detect a peculiarity of solution because of averaging over the whole area. The best results are obtained when the local averaged functions are used.

That is why for controlling the number of particles in the PIC method, one should pay attention both to using a method of inserting and deleting particles and the threshold functions.

References

[1] Hockney R.W., Eastwood J.W. Computer Simulation Using Particles. — MacGraw-Hill International Com., 1981.

[2] Birdsall C.K., Langdon A.B. Plasma Physics in Computer Simulation. — Adam-Hilger, 1991.

[3] Berezin Yu.A., Vshivkov V.A. Particle Method in Rarefied Plasma Dynamic. — Novosibirsk: Nauka, 1980.

[4] Grigoryev Yu.N., Vshivkov V.A., Fedoruk M.P. Numerical Particle-in-Cell Methods. Theory and Applications. — VSP, 2002.

[5] Vshivkov V.A., Romanov D.V., Snytnikov V.N. The problem of spontaneous heating of model plasma in the method of particles // Computational Technologies. — 1999. — Vol. 4, No. 3. — P. 62–72.

[6] Vshivkov V.A., Terekhov A.V. On the self-force in the particle-in-cell method // Numerical Methods and Programming. — 2008. — Vol. 9. — P. 48–57.

[7] Lapenta G., Brackbill J.U. Dynamic and selective control of the number of particles in kinetic plasma simulations // J. Computational Physics. — 1994. — Vol. 115. — P. 213–217.

[8] Welch D.R., Genoni T.C., Clark R.E., Rose D.V. Adaptive particle management in a particle-in-cell code // J. Computational Physics. — 2007. — Vol. 227. — P. 143–155.

[9] Sagdeev R.Z. Collective processes and shock wares in a rarefied plasma // Voprosy Teorii Plazmy. — Moscow: Atomizdat, 1964. — Vol. 4. — P. 20–80.

[10] Snytnikova T.V. Particle-in-cell method with adaptive mass // Bull. Novosibirsk Comp. Center. Ser. Numerical Analysis. — Novosibirsk, 2009. — Iss. 14. — P. 81–93.