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On the influence of a grid on temperature evaluation in Particle-in-Cell method*

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Abstract. A technique for evaluation of temperature in the Particle-in-Cell method is proposed. A number of computational experiments were conducted in order to reveal how a grid step affects the temperature evaluation according to the proposed technique both in 1D and 3D cases for electrostatic plasma. In order to prove the correctness of the temperature evaluation, the energy of the short-wave temperature harmonics is considered for grids with different steps. The non-physical heating is studied in the self-consistent electrical field as well as the dependence of a temperature decrease on the grid step. It is shown that the temperature values converge with a decrease of the grid step. This allows to conclude that temperature evaluated with the proposed technique is of the physical nature.

1. Introduction

In the Particle-in-Cell (PIC) method, every particle carries some attributes of a medium, such as charge, mass, impulse, kinetic energy, etc. In order to assign temperature to each particle in the same way, it is necessary to presume some form of a distribution function at a given point (for example, as is done in the SPH method [1]). On the other hand, it is possible to compute temperature with an ensemble of particles. In the latter case, it is necessary to separate temperature from non-physical effects (noises) that occur in the PIC method.

The main source of non-physical noises in PIC method is a grid used for evaluation of density, velocity, current. Because of the grid the question arises: how strongly is the computed temperature affected by the grid? How much are the temperature values alter when the number of grid nodes is changed, or when a grid step is decreased? The objective of the present work is to answer these questions in the case of electrostatic computer plasma.

In the case, when temperature in the PIC method is non-physical, it essentially depends on the number of particles in each cell, on the value of the grid step and on the stochastic drift of particles from one cell to another. Thus, if one shows that the computed temperature does not depend on the number of particles, that the dependence of temperature on the grid step is not strong, and, finally, a stochastic drift of particles does not play the major

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role, then it will be possible to say that temperature is correctly evaluated. The stochastic drift is shown by the amount of energy in the short-wave temperature harmonics.

Consequently, it is necessary to define the following:

- values of temperature with a different number of particles
- the dependence of temperature on a grid step
- the amount of energy in the short-wave temperature harmonics

The plasma electron temperature was chosen for this study, because it is mostly subject to all changes including those non-physical. The values of all the quantities are given in non-dimensional units.

2. Temperature evaluation with an ensemble of particles

Let us compute temperature, as in [2], as dispersion of the particles velocity

$$T = \left\langle \frac{m\vec{v}^2}{2} \right\rangle.$$

A difference with a physical definition is that in the PIC simulation we have model particles with a sufficiently larger size than real physical particles. So, it should be proved that the temperature evaluated with these large particles is of the physical nature.

Temperature in the simulation could be evaluated either in the whole computational domain

$$T = \frac{1}{N_P} \sum_{n=1}^{N_P} \frac{m(\vec{v}^n - \vec{v}^0)^2}{2}, \qquad \vec{v}^0 = \frac{1}{N_P} \sum_{n=1}^{N_P} \vec{v}^n,$$

or in a separate grid cell

$$T_{i,j,k} = \frac{1}{N_{i,j,k}} \sum_{n=1}^{N_{i,j,k}} \frac{m(\vec{v}^n_{i,j,k} - \vec{v}^0_{i,j,k})^2}{2}, \qquad \vec{v}^0_{i,j,k} = \frac{1}{N_{i,j,k}} \sum_{n=1}^{N_{i,j,k}} \vec{v}^n_{i,j,k},$$

here N_P is the total number of model particles, $N_{i,j,k}$ is the number of model particles in a cell with numbers i, j, k. Let $T_{i,j,k}$ stand for the grid temperature.

3. The influence of a grid step in the 1D case: experiments and estimates

3.1. The shape of temperature computed on grids with different steps. To study the influence of a grid step on the evaluation of temperature, a 1D particle ensemble was set with a Gaussian velocity distribution and the following parameters: the initial temperature $T = 1$, the number of particles $N_P = 5 \cdot 10^5$, a distance between particles $h_p = 1/N_P$. Particles were distributed along the interval with the length $L = 1$, thus the coordinate of the particle number j is $x_j = jh_p$.

This particle ensemble was applied to grids of a different size:

$$N = 2^k, \qquad k = 5, \ldots, 12.$$

It should be noted that particles did not move, and for every new grid the same particle ensemble was used.

The coordinates of the grid nodes are

$$X_i = ih, \qquad i = 1, \ldots, N-1, \qquad h = \frac{1}{N}.$$

It is easy to conclude from Figure 1 that the temperature values are in fact considerably different. One can see the temperature oscillations that occur with the frequency increase with a grid size. It is possible to propose that short-wave harmonics play a major role in the evaluation of temperature.

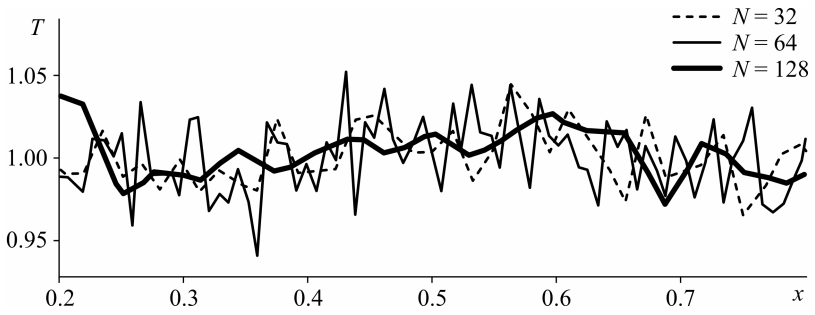

Figure 1. Grid temperature on a sequence of nested grids

3.2. The impact of the grid step on the amount of energy in the short-wave temperature harmonics. Following [3], let us define the spectral form of the grid value G_j as

$$G(k) = \Delta x \sum_{j=0}^{N-1} G_j \exp(-ikX_j), \qquad \Delta x = h, \quad X_j = jh. \tag{1}$$

Wavenumber k depends on the harmonic number n as $k = \frac{2\pi n}{L}$, where L is the size of the computational domain. Let us assume the harmonics with the number from $0.9N$ to $N-1$ as short-wave harmonics; here N is the number of grid nodes. The amount of energy in short-wave harmonics of the temperature could be derived as a ratio of the short-wave energy to the total energy of the spectrum

$$S = \sum_{n=0.9N}^{N-1} |G(n)|^2 \Big/ \sum_{n=0}^{N-1} |G(n)|^2.$$

In order to estimate the quantity S it could be proposed that all the grid values G_j are nearly equal (for the electrostatic plasma with uniform density in the self-consistent field this proposition is true). Therefore, if we consider the sum of the squares of absolute values of the harmonic amplitudes, and the number of these harmonics is equal to one tenth of the total number of harmonics, then the sum must be nearly equal to one tenth of the whole sum (that is, the sum of the squares of absolute values of all the harmonic amplitudes).

The above passage could be illustrated by the following expression. Let us first denote two average values: A_{sh} for the squares of absolute values of amplitudes of short-wave harmonics, and A_{wh} for the squares of absolute values of amplitudes of the whole spectrum:

$$A_{sh} = \frac{1}{0.1N} \sum_{n=0.9N}^{N-1} |G(n)|^2, \qquad A_{wh} = \frac{1}{N} \sum_{n=0}^{N-1} |G(n)|^2.$$

Then the quantity S, as defined above, has the following form:

$$S = \frac{0.1NA_{sh}}{NA_{wh}} = \frac{1}{10}\frac{A_{sh}}{A_{wh}}.$$

Thus we can make an estimate of the amount of energy in short-wave harmonics of the temperature, provided $A_{sh} \leq A_{wh}$

$$S \leq \frac{1}{10}.$$

The meaning of this estimate is quite clear: if in a numerical experiment the amount of energy in short-wave harmonics (the quantity S) exceeds one tenth (it means that $A_{sh} > A_{wh}$ or even $A_{sh} \gg A_{wh}$), then the course of the experiment in mainly governed by the short-wave harmonics with the wavelength near the value of grid step. It cannot be true for plasma simulated with the PIC method, because at least four grid steps must correspond the plasma Debye length. The Debye length is the minimal wavelength in

plasma. Thus if the quantity S exceeds one tenth, then the experiment has no physical sence. In the experiments that pretend to have physical sence S must be significantly lower than one tenth.

In order to define the amount of energy in short-wave harmonics an experiment was conducted. The particles with the above given initial parameters moved without any force ($\frac{\partial v}{\partial t} = 0$) within the time interval $\Delta T = 1$. Periodical boundary conditions were set for the particles.

For the grid with the number of nodes $N = 128$ timestep is $\tau = 0.01$, number of timesteps $M = 100$, for other grids

$$\tau_n = 0.01\frac{128}{2^n}, \quad M_n = 100\frac{2^n}{128}, \qquad n = 5, \ldots, 12.$$

The amount of energy in short-wave harmonics of the temperature is computed as follows:

$$S = \sum_{i=0.9N}^{N} |\hat{T(i)}|^2 \Big/ \sum_{i=0}^{N} |\hat{T(i)}|^2.$$

Figure 2 shows the quantity S versus the number of grid nodes.

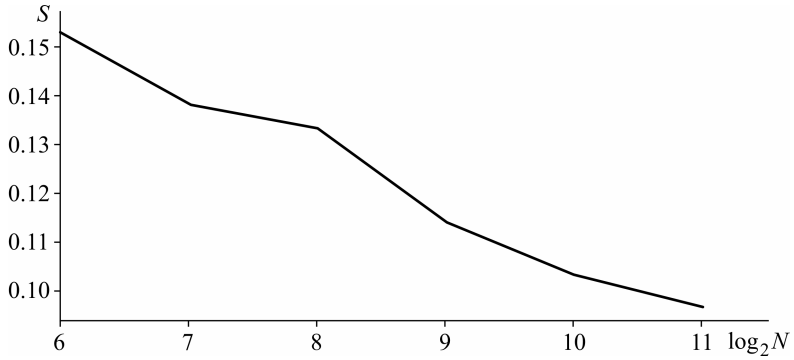

Figure 2. The amount of energy in short-wave harmonics depending on the number of grid nodes; $N = 2^n$, $n = 6, \ldots, 11$

A decrease of S with decreasing the value of a grid step (the increasing number of nodes) is confirmed by the fluctuation level estimate in a 1D case given in [3]:

$$(\rho)^2_{k,\omega} \approx \rho_0 q \Delta t \left(1 - \frac{2}{3}\sin^2\frac{k\Delta x}{2}\right),$$

here $\Delta t = \tau$, $\Delta x = h$, q is the number of the time Fourier harmonics. The time step τ in the computations was decreased together with decreasing the grid step h.

It is possible to compare the fluctuation level and the energy of the short-wave harmonics. The reason is the following: the shortest harmonics

with the corresponding lengths of h or $2h$ store the effect of smallest-scale processes. These processes either lack a correct approximation with a grid (at least four nodes at a characteristic length of the process are necessary) or the processes are non-physical at all, like a stochastic drift of model particles from one cell to another. Let us imagine a particle going exactly along the border of two cells. Just a very small deviation of the velocity and the particle will go to one cell or to another, resulting in a significant change of the corresponding density harmonic. Both cases — the absence of approximation and a stochastic drift — could be called fluctuations.

3.3. Impact of the grid step on the computer plasma heating. The objective of this computation was to study how the non-physical heating of the computer plasma depends on the value of a grid step h. For each value of h, different values were set for the time step τ, the initial temperature of the particles T_0, the total charge of positively charged particles q_0 and the number of particles N_P. All the combinations of values of these parameters were set to ensure the result depending only on h but not on a random choice of other parameters.

The computation involves no external forces, no sources of thermal energy. There are no peculiarities leading to thermalization (density shears, for example). Thus, any heating could be only non-physical [4, 5].

The following conditions were set for the experiment: the number of grid nodes 100 (the size of the domain L changes together with h, $L = 100h$), the number of particles, at least, 100 for each cell, the equal number of positively and negatively charged particles of the same mass (like the electron-hole plasma in a semiconductor or the electron-positron plasma). The electrical field is computed with the Poisson equation, solved by the sweeping method. Particles were reflected at the boundaries of the domain.

The initial parameters for particles are: the coordinate $x_j = jh_p$, here h_p changes together with h, $h_p = h\frac{N}{N_P}$ the charge $x_j = (-1)^j\frac{2q_0}{N_P}$, velocities were set according to the Maxwellian distribution with the initial temperature T_0.

Parameters of the computation h, τ, T_0, q_0, N_P were set as follows:

$$\begin{aligned} h &= \frac{0.01}{2^i}, & i &= 0, \ldots, 3, \\ T_0 &= 0.1 \times 2^j, & j &= 0, \ldots, 10, \\ \tau &= \frac{h}{2\sqrt{T_0} i_\tau}, & i_\tau &= 1, \ldots, 5, \\ q_0 &= 0.0001 \times 2^k, & k &= 0, \ldots, 8, \\ N_P &= 10^{p+4}, & p &= 0, \ldots, 2. \end{aligned}$$

Thus, 5,940 different combinations of parameters were set. Each combination could be given its number

$$J = 1485i + 135j + 27i_\tau + 3k + p,$$

corresponding to a definite combination.

In all the cases, heating is of interest. Heating here is the ratio of the temperature at the end of computation to the initial temperature. And the main objective of this study is the dependence of this ratio on the grid step h.

Let us take the grid temperature T_i at the end of computation and evaluate the two quantities:

$$R_{\min} = \frac{1}{T_0} \min_i T_i, \qquad R_{\max} = \frac{1}{T_0} \max_i T_i, \qquad i = 1, \ldots, N,$$

corresponding to a maximal and a minimal grid temperature at the end of computation.

First, let us consider a change of $R_{\min}$ and $R_{\max}$ when only h is changed (Figure 3). Each marked point in this figure is an average over 1,485 computations. It is clear that the dependence is only minor.

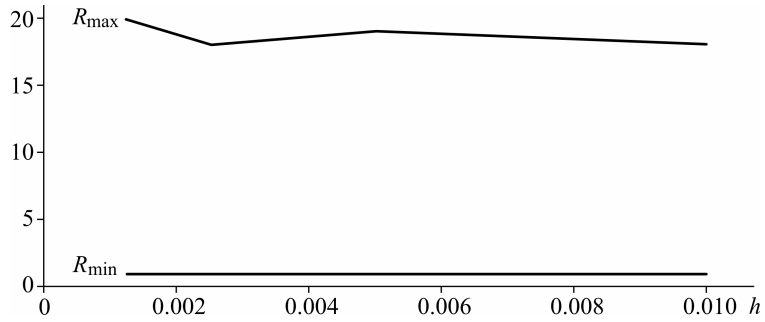

Figure 3. The ratio of a minimal and a maximal grid temperatures after the computation to the initial temperature depending on the grid step, $R_{\min}(h), R_{\max}(h)$

Furthermore, the dependence of $R_{\min}$ and $R_{\max}$ on h takes place when the number of particles is changed (Figure 4). It is clear from the figures that the heating does not dramatically depend on a grid step with any (big enough) number of particles.

It should be noted that the lack of a significant relation between the heating and a grid step is in a qualitative agreement with the results [5], in particular, with the estimate of the grid fluctuations given:

$$\frac{\langle E^2 \rangle}{nmv_{th}^2} = \frac{0.12}{\lambda_D^2 + W^2},$$

here v_{th} is a thermal velocity of the model electron, λ_D^2 is the Debye length, $W = h$. This means that the value of grid fluctuations does not depend on the number of particles at all, and if $h \ll \lambda_D$, it depends on h only slightly.

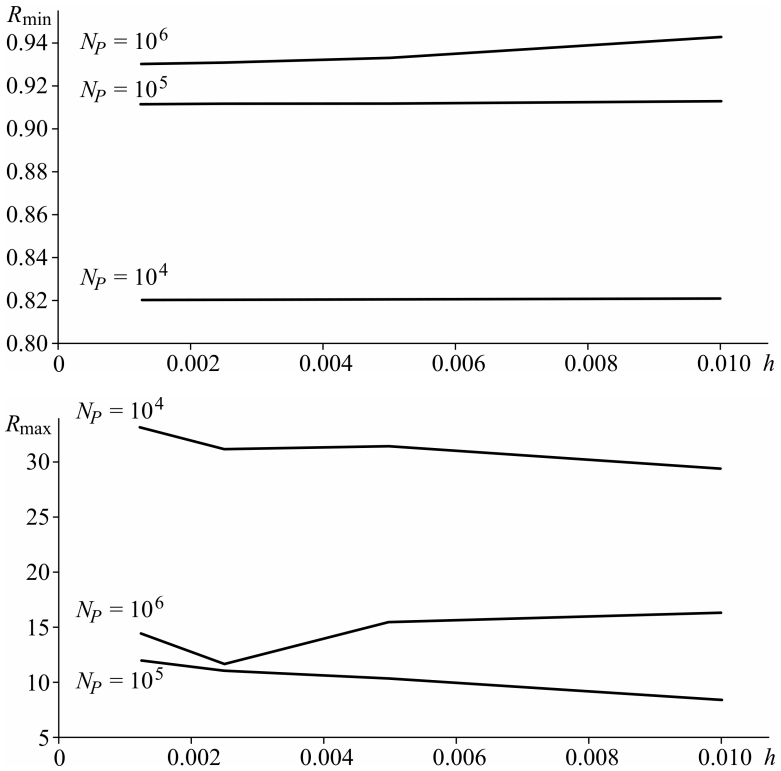

Figure 4. The ratio of minimal grid temperatures after the computation to the initial temperature depending on a grid step with a different number of particles, $R_{\min}(h, N_P)$ and $R_{\max}(h, N_P)$

4. The impact of a grid step on temperature in 3D computations

In this section, the 1D results are confirmed by the 3D electrostatic plasma simulations. The focus as well as in the 1D case is on the dependence of temperature on a grid step.

4.1. Computation parameters. The following values of parameters were chosen for the computation:

The number of grid nodes along one dimension	16
The size of a domain	3.2, 1.6, 0.8, 0.4
The number of particles in each cell	50
Ion mass (in relation to electron mass)	1
Initial temperature of electrons	0.8, 0.4, 0.2, 0.1
Density	1.0, 0.5, 0.25, 0.125

Every parameter combination could be given a number as follows:

$$J = 16i + 4j + k. \tag{2}$$

Here i, j, k define values of the domain size L, the initial electron temperature T^0 and the density of electrons n_e, respectively:

$$\begin{aligned} L &= 0.4 \cdot 2^i, & i &= 0, \ldots, 3, \\ T^0 &= 0.1 \cdot 2^j, & j &= 0, \ldots, 3, \\ n_e &= 0.125 \cdot 2^k, & k &= 0, \ldots, 3. \end{aligned}$$

Thus, 64 different combinations were set.

A grid of such a small size enables us to test the temperature evaluation technique with an ensemble of particles. Since the ion mass is equal to the electron mass, the properties of the computer plasma are far from the real plasma properties, but the energy exchange between the plasma components goes much faster. Thus it is possible to study computer plasma fluctuations in a shot period.

4.2. The impact of a grid step on the electron temperature change rate. To study the impact of a grid step on the temperature evaluation, a relative change rate for the electron temperature was computed

$$\xi = \frac{\delta T}{T_0}, \qquad \delta T = T_0 - T.$$

Here T_0 is the initial electron temperature. The initial temperature of ions is 0. A relative change is studied since the quantity T_0 computed with an ensemble of particles, slightly differs from one grid to another. The temperature in this case is evaluated in the whole computational domain.

The number of particles was constant when the number of nodes was changed. The size of a domain was also constant, thus a grid step was changed.

It is seen from Figure 5 that ξ decreases with decreasing a grid step, thus there is some relation between ξ and h. Nevertheless, this relation converges with a decrease of h, and starting with a sufficiently big number of grid nodes (64 in the case in question) this dependence comes to a steady state. The same conclusion could be made from Figure 6.

4.3. The impact of a grid step on the amount of energy in short-wave harmonics of temperature and density. The Fourier transform was conducted for both the temperature and the density of electrons. Density is considered here in order to show the temperature spectrum stability. Density affects particle velocities through the electric field, and a velocity

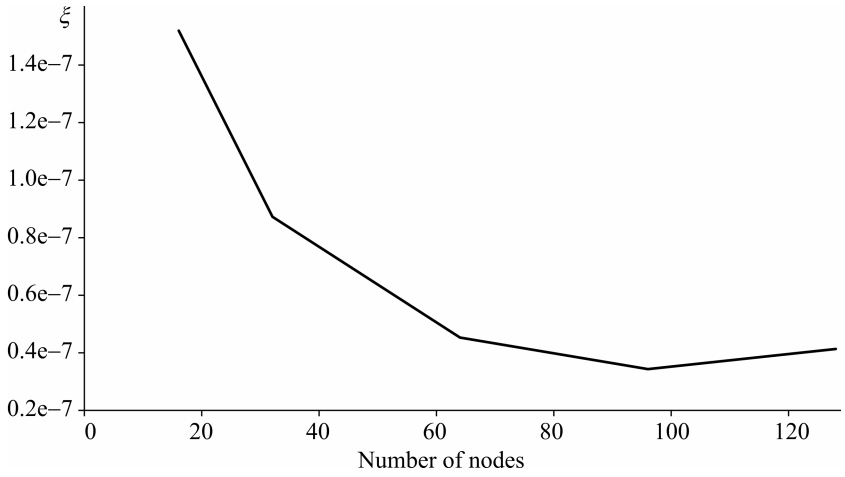

Figure 5. The temperature change rate versus a grid step, $L = 0.05$, the computation time $\delta = 0.01$

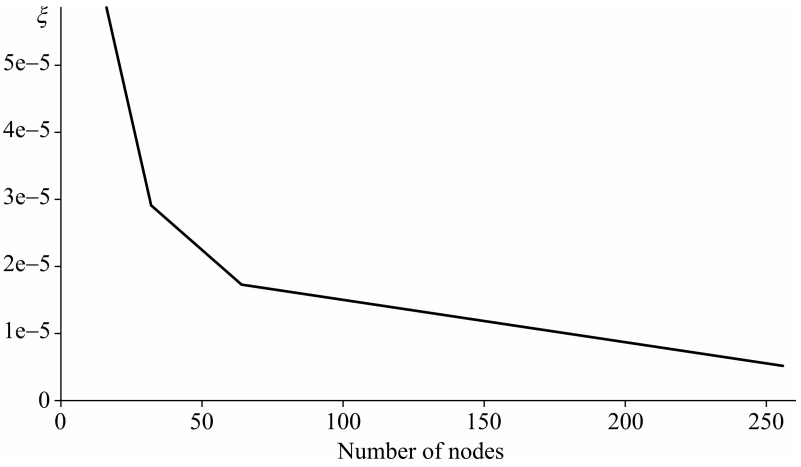

Figure 6. The temperature change rate versus a grid step, $L = 0.4$, the computation time $\delta = 0.36$

distribution defines temperature. This means that if density contains a lot of non-physical harmonics, the temperature distribution will be the same soon.

The amount of energy in the short-wave harmonics S is computed in the same way as in the 1D case. The sum should be, of course, three-dimensional and the expression for S becomes

$$S_f = \sum_{n_x=0.9n_{\max}}^{n_{\max}} \sum_{n_y=0.9n_{\max}}^{n_{\max}} \sum_{n_z=0.9n_{\max}}^{n_{\max}} f^2_{n_x,n_y,n_z} \Bigg/ \sum_{n_x=1}^{n_{\max}} \sum_{n_y=1}^{n_{\max}} \sum_{n_z=1}^{n_{\max}} f^2_{n_x,n_y,n_z}.$$

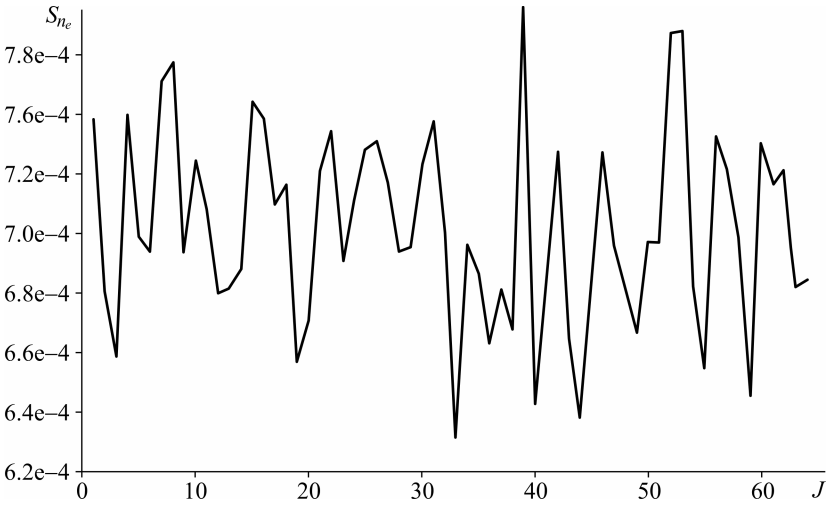

Figure 7. The amount of energy in the short-wave harmonics S_{n_e} of the electron density depending on J

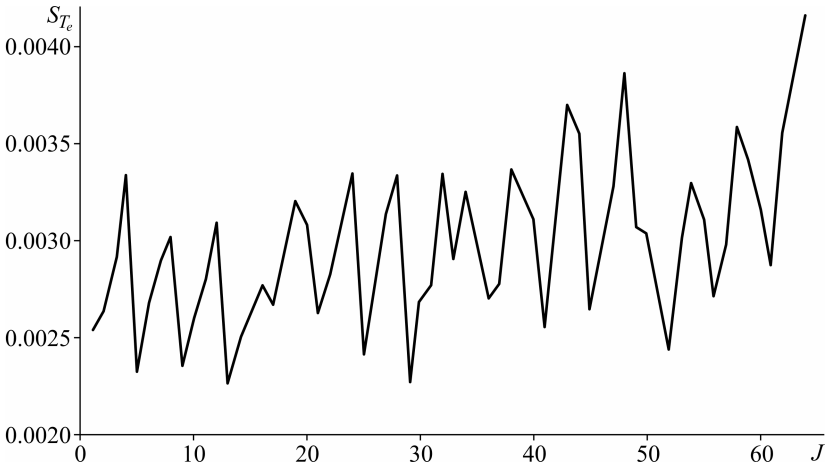

Figure 8. The amount of energy in the short-wave harmonics S_{T_e} of the electron temperature depending on J

Here N is a grid size, f is the quantity for the Fourier transform computation, either electron density n_e or electron temperature T_e.

Figures 7 and 8 show the dependence of the amount of energy in the short-wave harmonics S on the number of experiment J (2).

It is seen from Figures 7 and 8, the short-wave harmonics contain a small amount of energy in comparison to the rest of the spectrum — less than 1 % for temperature and less than 0.1 % for density.

5. Conclusion

A technique for evaluation of temperature in the Particle-in-Cell method is proposed: the temperature is computed as particle velocity dispersion and confirmed by the estimate of the non-physical (short-wave) harmonics.

For the 1D computations, it is shown that the amount of energy in short-wave harmonics decreases with a decrease of the grid step. The electron heating in the self-consistent electric field is shown to have no dependence on the grid step. Both results are in the qualitative agreement with theoretical estimates.

For the 3D computations, the relaxation of the electron and the ion temperatures was considered. The change rate for the electron temperature appeared to be converging with decreasing a grid step. Finally, it is shown that the amount of energy in the short-wave harmonics is very small in the 3D case as well.

Thus it is possible to state that the temperature computed with the proposed technique does not depend on the grid step provided a sufficiently large size of the grid and a large number of particles per cell.

References

[1] Springel V. The Cosmological Simulation Code "GADGET-2". — MNRAS, 2005.

[2] Krall N., Trivelpiece A. Principles of Plasma Physics. — McGraw-Hill, 1973.

[3] Bidsall Ch., Langdon B. Plasma Physics via Computer Simulation. — McGraw-Hill, 1985.

[4] Vshivkov V.A., Romanov D.V., Snytnikov V.N. The problem of self-heating of model plasma in Particle-in-Cell method // Vychislitel'nye Tecknologii. — 1999. — Vol. 4, No. 3. — P. 62–72 (In Russian).

[5] Hockney R.W. Measurements of collision and heating times in a two-dimensional thermal computer plasma // J. Computational Physics. — 1971. — No. 8. — P. 19–44.