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Exact charge conservation scheme for Particle-in-Cell simulation with an arbitrary form-factor

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Abstract

The new method of local electric current density assignment in the Particle-in-Cell code in Cartesian geometry is presented. The method is valid for an arbitrary quasi-particle form-factor assuming that quasi-particle trajectory over time step is a straight line. The method allows one to implement the PIC code without solving Poisson equation. The presented formula for the current density associated with the motion of a single quasi-particle is the unique linear combination of form-factor differences in consistency with the discrete continuity equation. The computation scheme is demonstrated in 2D and 3D.

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1. Introduction

It is well known that Particle-in-Cell (PIC) method for plasma simulation can be implemented without solving Poisson equation for the electric potential. Usually Poisson solver is used for a correction of the electric field. Instead of incorporating Gauss law in the form of Poisson equation one need to solve the continuity equation in finite differences.

There are several methods for satisfying the continuity equation locally, i.e. charge and current densities are associated with each quasi-particle. These methods use the special definition for the current density which is connected with the change of the charge density due to quasi-particle motion.

The most general derivation of charge conserving scheme is presented in [1] for Cartesian geometry and [2] for general curvilinear meshes in one, two and three dimensions. The authors split the quasi-particle trajectory into segments, each segment lie wholly in an appropriate cell. The current density is assigned to each segment with some fixed assignment pattern.

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In Refs. [3–5] authors present charge conserving schemes designed for simple shapes of quasi-particles, for the zero- and the first-order form-factors.

We present a new charge conserving scheme — *Density Decomposition*. The scheme is valid for an arbitrary form-factor. It is limited to Cartesian geometry. Quasi-particle trajectory over time step is assumed to be a straight line, like in a simple leap-frog scheme for quasi-particle motion equations. The scheme is formulated for quasi-particle moving less than one cell per time step. We show that under these limitations the Density Decomposition is the unique linear procedure of computation of the current density associated with the motion of a quasi-particle. The Density Decomposition scheme is the generalization of the method developed by Villasenor and Buneman [4]. Both schemes can be considered as special cases of impulse approximation scheme described by Eastwood [1].

It is known that the use of quasi-particle form-factors of the high-order reduces the numerical noise significantly. The main advantage of the Density Decomposition method is that it is suitable for high-order form-factors. The new method would be useful for overdense plasma simulation [6].

Other methods of incorporating Gauss law into Maxwell solver use trivial definition of local current density, see Refs. [7,8].

Very detailed study of PIC method can be found in [9–11].

2. Continuity equation in finite differences

Let us consider the local Maxwell solver, which is equivalent to Finite Difference Time Domain (FDTD) method [12]

$$\frac{\mathbf{E}^{n+1} - \mathbf{E}^n}{dt} = \nabla^+ \times \mathbf{B}^{n+1/2} - \mathcal{J}^{n+1/2}, \tag{1}$$

$$\frac{\mathbf{B}^{n+1/2} - \mathbf{B}^{n-1/2}}{dt} = -\nabla^- \times \mathbf{E}^n, \tag{2}$$

$$\nabla^+ \cdot \mathbf{E}^n = \rho^n, \tag{3}$$

$$\nabla^- \cdot \mathbf{B}^{n+1/2} = 0, \tag{4}$$

and the particle mover

$$\frac{\mathbf{u}_\alpha^{n+1/2} - \mathbf{u}_\alpha^{n-1/2}}{dt} = 2\pi \frac{q_\alpha}{m_\alpha} \frac{m_e}{e} \left(\mathbf{E}^n\left(\mathbf{x}_\alpha^n, t\right) + \frac{\mathbf{u}_\alpha^n}{\gamma_\alpha} \times \mathbf{B}^n\left(\mathbf{x}_\alpha^n, t\right) \right), \tag{5}$$

$$\frac{\mathbf{x}_\alpha^{n+1} - \mathbf{x}_\alpha^n}{dt} = \frac{\mathbf{u}_\alpha^{n+1/2}}{\gamma_\alpha^{n+1/2}}, \tag{6}$$

$$\gamma_\alpha = \left(1 + (\mathbf{u}_\alpha)^2\right)^{1/2}. \tag{7}$$

Eqs. (1)–(4) are discretized Maxwell equations and Eqs. (5)–(6) are the leap-frog scheme of Newton–Lorentz equations. Here we use dimensionless variables defined by transformations $t \to 2\pi\omega_0^{-1} t$, $\mathbf{x} \to \lambda_0 \mathbf{x}$, $(\mathbf{E}, \mathbf{B}) \to (m_e c\omega_0/e)(\mathbf{E}, \mathbf{B})$, where m_e, e are electron mass and charge, c is the speed of light, ω_0 and λ_0 are characteristic frequency and length (e.g., the frequency and wavelength of incident EM radiation). Index n denotes integer time step and α stands for the index of a quasi-particle; dt, dx, dy, dz are discretizations of time and space coordinates.

Different components of electromagnetic fields and charge density ρ and current density $\mathcal{J}$ are defined on different grids and at different time steps,

$$\mathbf{E}^n = \left(E^1_{i,j+1/2,k+1/2}, E^2_{i+1/2,j,k+1/2}, E^3_{i+1/2,j+1/2,k}\right)^n,$$

$$\mathbf{B}^{n+1/2} = \left(B^1_{i+1/2,j,k}, B^2_{i,j+1/2,k}, B^3_{i,j,k+1/2}\right)^{n+1/2},$$

$$\rho^n = \rho^n_{i+1/2,j+1/2,k+1/2},$$
$$\mathcal{J}^{n+1/2} = \left(\mathcal{J}^1_{i,j+1/2,k+1/2}, \mathcal{J}^2_{i+1/2,j,k+1/2}, \mathcal{J}^3_{i+1/2,j+1/2,k}\right)^{n+1/2}, \tag{8}$$

where i, j, k are integer grid indices. Discrete operators $\nabla^{\pm}$ in Eqs. (1)–(4) are vectors,

$$\nabla^+ f_{i,j,k} = \left(\frac{f_{i+1,j,k} - f_{i,j,k}}{dx}, \frac{f_{i,j+1,k} - f_{i,j,k}}{dy}, \frac{f_{i,j,k+1} - f_{i,j,k}}{dz}\right),$$
$$\nabla^- f_{i,j,k} = \left(\frac{f_{i,j,k} - f_{i-1,j,k}}{dx}, \frac{f_{i,j,k} - f_{i,j-1,k}}{dy}, \frac{f_{i,j,k} - f_{i,j,k-1}}{dz}\right). \tag{9}$$

These operators have the following properties

$$\nabla^- \cdot \nabla^- \times = \nabla^+ \cdot \nabla^+ \times = 0, \qquad \nabla^- \cdot \nabla^+ = \nabla^+ \cdot \nabla^- = \Delta, \tag{10}$$

where Δ is the discrete Poisson operator in central differences,

$$\Delta f_{i,j,k} = \frac{f_{i-1,j,k} - 2f_{i,j,k} + f_{i+1,j,k}}{dx^2} + \frac{f_{i,j-1,k} - 2f_{i,j,k} + f_{i,j+1,k}}{dy^2} + \frac{f_{i,j,k-1} - 2f_{i,j,k} + f_{i,j,k+1}}{dz^2}. \tag{11}$$

Acting on Eqs. (1) and (2) by operators $(\nabla^+ \cdot)$ and $(\nabla^- \cdot)$, respectively, we obtain

$$\frac{\rho^{n+1} - \rho^n}{dt} + \nabla^+ \cdot \mathcal{J}^{n+1/2} = 0, \tag{12}$$
$$\frac{\nabla^- \mathbf{B}^{n+1/2} - \nabla^- \mathbf{B}^{n-1/2}}{dt} = 0. \tag{13}$$

It means that if the continuity equation (12) is fulfilled then the divergence of **E** is always equal to charge density (Gauss law), and if the initial discrete divergence of **B** is zero then it remains zero forever.

Thus, to solve Maxwell equations we need Eqs. (1), (2) and (12) with initial conditions

$$\nabla^+ \cdot \mathbf{E} = \rho \quad \text{and} \quad \nabla^- \cdot \mathbf{B} = 0 \quad \text{at } t = 0. \tag{14}$$

Let us consider the continuity equation in finite differences

$$\frac{\rho^{n+1}_{i+1/2,j+1/2,k+1/2} - \rho^n_{i+1/2,j+1/2,k+1/2}}{dt} + \frac{\mathcal{J}^1_{i+1,j+1/2,k+1/2} - \mathcal{J}^1_{i,j+1/2,k+1/2}}{dx}$$
$$+ \frac{\mathcal{J}^2_{i+1/2,j+1,k+1/2} - \mathcal{J}^2_{i+1/2,j,k+1/2}}{dy} + \frac{\mathcal{J}^3_{i+1/2,j+1/2,k+1} - \mathcal{J}^3_{i+1/2,j+1/2,k}}{dz} = 0. \tag{15}$$

Further we drop indices and modificators like $\pm 1/2$. The charge density ρ is constructed from form-factors of separate quasi-particles

$$\rho_{i,j,k} = \sum_\alpha \mathsf{Q}_\alpha S_{i,j,k}(x_\alpha, y_\alpha, z_\alpha), \tag{16}$$

where Q_α is the charge and S is the form-factor (or density) of a quasi-particle,

$$S_{i,j,k}(x_\alpha, y_\alpha, z_\alpha) = S(X_i - x_\alpha, Y_j - y_\alpha, Z_k - z_\alpha), \tag{17}$$

where X_i, Y_j, Z_k denote coordinates of the grid, $(x_\alpha, y_\alpha, z_\alpha)$ is the location of the quasi-particle with the index α. Here the form-factor can be interpreted as a charge density of a single quasi-particle. The quasi-particle is considered as if it is a charged cloud. During quasi-particle motion the total charge should not change, therefore the form-factor must obey the condition

$$\sum_{i,j,k} S_{i,j,k}(x_\alpha, y_\alpha, z_\alpha) = 1, \tag{18}$$

where the sum is taken over all grid nodes.

3. Density decomposition

Due to linearity of the continuity equation (15), it is sufficient to define the current density associated with the motion of a single quasi-particle.

Let us consider a single quasi-particle with the form-factor, Eq. (17), and coordinates (x, y, z). Consider the vector W defined by equations:

$$\begin{aligned}
&\mathcal{J}^1_{i+1,j,k} - \mathcal{J}^1_{i,j,k} = -\mathsf{Q}\frac{dx}{dt}W^1_{i,j,k},\\
&\mathcal{J}^2_{i,j+1,k} - \mathcal{J}^2_{i,j,k} = -\mathsf{Q}\frac{dy}{dt}W^2_{i,j,k},\\
&\mathcal{J}^3_{i,j,k+1} - \mathcal{J}^3_{i,j,k} = -\mathsf{Q}\frac{dz}{dt}W^3_{i,j,k}.
\end{aligned} \tag{19}$$

Then according to the continuity equation we can write (dropping grid indices),

$$W^1 + W^2 + W^3 = S(x+\Delta x, y+\Delta y, z+\Delta z) - S(x, y, z). \tag{20}$$

Here $(\Delta x, \Delta y, \Delta z)$ is 3-dimensional shift of the quasi-particle due to the motion.

Shift of the quasi-particle generates eight functions

$$\begin{aligned}
&S(x, y, z),\quad S(x+\Delta x, y, z),\quad S(x, y+\Delta y, z),\quad S(x, y, z+\Delta z),\\
&S(x+\Delta x, y+\Delta y, z),\quad S(x+\Delta x, y, z+\Delta z),\quad S(x, y+\Delta y, z+\Delta z),\\
&S(x+\Delta x, y+\Delta y, z+\Delta z).
\end{aligned} \tag{21}$$

We assume that the vector W and corresponding current density linearly depend on these functions. The base for this assumption is the following. (1) We can consider the form-factor to be the charge density of the quasi-particle. If the form-factor magnitude is increasing, the current density associated with a shift of the form-factor must increase proportionally. (2) The quasi-particle trajectory over time step is treated as a straight line. We can decompose any three-dimensional shift of the form-factor $S(x, y, z)$ into three one-dimensional shifts:

$$\begin{aligned}
&S(x+\Delta x, y+\Delta y, z+\Delta z) - S(x, y, z)\\
&\quad = S(x+\Delta x, y, z) - S(x, y, z)\\
&\qquad + S(x+\Delta x, y+\Delta y, z) - S(x+\Delta x, y, z)\\
&\qquad + S(x+\Delta x, y+\Delta y, z+\Delta z) - S(x+\Delta x, y+\Delta y, z).
\end{aligned} \tag{22}$$

Current densities corresponding to one-dimensional shifts must be additive.

Let us formulate the properties of the vector W.

(1) The vector $(W^1_{i,j,k}, W^2_{i,j,k}, W^3_{i,j,k})$ is a linear combination of eight functions, Eq. (21).
(2) The sum of components of the vector W is equal to the finite difference of form-factors, Eq. (20).
(3) If one of the shifts Δx, Δy, Δz is zero, the corresponding component of W is also zero:

$$\Delta x = 0 \Rightarrow W^1 = 0,\quad \Delta y = 0 \Rightarrow W^2 = 0,\quad \Delta z = 0 \Rightarrow W^3 = 0.$$

(4) If $S(x, y, z)$ is symmetrical with respect to the permutation of (x, y), $S(x, y, z) = S(y, x, z)$, and $\Delta x = \Delta y$, then $W^1 = W^2$. The same property is assumed for symmetries with respect to permutations of pairs (x, z) and (y, z).

Lemma. *Only one linear combination of eight functions, Eq.* (21), *obeys the conditions* (1)–(4):

$$
\begin{aligned}
W^1 = {} & \tfrac{1}{3}S(x+\Delta x, y+\Delta y, z+\Delta z) - \tfrac{1}{3}S(x, y+\Delta y, z+\Delta z) \\
& + \tfrac{1}{6}S(x+\Delta x, y, z+\Delta z) - \tfrac{1}{6}S(x, y, z+\Delta z) \\
& + \tfrac{1}{6}S(x+\Delta x, y+\Delta y, z) - \tfrac{1}{6}S(x, y+\Delta y, z) \\
& + \tfrac{1}{3}S(x+\Delta x, y, z) - \tfrac{1}{3}S(x, y, z), \\
W^2 = {} & \tfrac{1}{3}S(x+\Delta x, y+\Delta y, z+\Delta z) - \tfrac{1}{3}S(x+\Delta x, y, z+\Delta z) \\
& + \tfrac{1}{6}S(x, y+\Delta y, z+\Delta z) - \tfrac{1}{6}S(x, y, z+\Delta z) \\
& + \tfrac{1}{6}S(x+\Delta x, y+\Delta y, z) - \tfrac{1}{6}S(x+\Delta x, y, z) \\
& + \tfrac{1}{3}S(x, y+\Delta y, z) - \tfrac{1}{3}S(x, y, z), \\
W^3 = {} & \tfrac{1}{3}S(x+\Delta x, y+\Delta y, z+\Delta z) - \tfrac{1}{3}S(x+\Delta x, y+\Delta y, z) \\
& + \tfrac{1}{6}S(x, y+\Delta y, z+\Delta z) - \tfrac{1}{6}S(x, y+\Delta y, z) \\
& + \tfrac{1}{6}S(x+\Delta x, y, z+\Delta z) - \tfrac{1}{6}S(x+\Delta x, y, z) \\
& + \tfrac{1}{3}S(x, y, z+\Delta z) - \tfrac{1}{3}S(x, y, z).
\end{aligned}
\tag{23}
$$

Proof. (Scenario). We can write the properties (2)–(4) in the form of linear equations with unknown coefficients of eight functions S, Eq. (21). Using Eq. (18) we can obtain additional equations for coefficients taking the sum of each linear combination of eight functions S over all grid points (i, j, k). Solving 10 linear equations for all S, we find all the coefficients. Of course, eight values, Eq. (21), are not independent. We have six independent variables $x, y, z, \Delta x, \Delta y, \Delta z$, hence in the most general case only six values S can be independent, for example, all excluding $S(x, y, z)$ and $S(x+\Delta x, y+\Delta y, z+\Delta z)$. Among possible solutions we must keep only one, which does not assume specific numerical values for excluded functions. □

The formulae (23) define the Density Decomposition. Solving Eq. (19) we obtain the current density associated with the motion of a single quasi-particle. It is important to emphasize that uniqueness claimed in the lemma depends on the quasi-particle path over time step. We assume that quasi-particle moves from (x, y, z) to $(x+\Delta x, y+\Delta y, z+\Delta z)$ along a straight line.

One can easily show that the Density Decomposition, Eq. (23), is the generalization of methods proposed in [3–5].

4. Computation scheme for the second-order polynomial form-factor

In this section we present the scheme of an implementation of the Density Decomposition for the second-order piecewise-polynomial form-factor.

Let us consider well-known one-dimensional form-factor

$$
\begin{aligned}
& S_i^{(1\mathrm{D})}(x) = \tfrac{3}{4} - (X_i - x)^2, \\
& S_{i\pm 1}^{(1\mathrm{D})}(x) = \tfrac{1}{2}\bigl(\tfrac{1}{2} \mp (X_i - x)\bigr)^2, \quad |X_i - x| < 1/2,
\end{aligned}
\tag{24}
$$

which is the second-order spline. The quasi-particle is bell-shaped. The correspondent 3-dimensional form-factor is

$$
S_{i,j,k}^{3\mathrm{D}}(x, y, z) = S_i^{1\mathrm{D}}(x) S_j^{1\mathrm{D}}(y) S_k^{1\mathrm{D}}(z). \tag{25}
$$

Now we can formulate a recipe for computing the current density based on the Density Decomposition, Eq. (23). We assume that the Finite Difference Time Domain (FDTD) technique [12] is used for computation of electromagnetic fields. In FDTD the fields and the current density are defined on different regular grids. Here we do not pretend to show the most optimal or fastest algorithm.

(1) Prepare 15-component array $\mathsf{S0}$ which contains one-dimensional form-factors corresponding to quasi-particle coordinates $(\mathsf{x0}, \mathsf{y0}, \mathsf{z0})$ with respect to the grid of the charge density ρ:

$$\begin{aligned} \mathsf{S0}(i,1) &= S_i^{(1\mathrm{D})}(\mathsf{x0}), \quad i=-2,2,\\ \mathsf{S0}(j,2) &= S_j^{(1\mathrm{D})}(\mathsf{y0}), \quad j=-2,2,\\ \mathsf{S0}(k,3) &= S_k^{(1\mathrm{D})}(\mathsf{z0}), \quad k=-2,2. \end{aligned} \tag{26}$$

The components $\mathsf{S0}(-2,m)$ and $\mathsf{S0}(2,m)$ are zero, but we need these additional components for further calculations.
The actual 3-dimensional form-factor is 27-component array

$$S^{(3\mathrm{D})}(i,j,k) = \mathsf{S0}(i,1) * \mathsf{S0}(j,2) * \mathsf{S0}(k,3). \tag{27}$$

(2) Using $\mathsf{S0}$ or precomputed $S^{(3\mathrm{D})}$, compute the force acting on the quasi-particle. Here we can use fields spatially averaged to the grid of ρ or compute additional form-factors for each grid. Advance the quasi-particle and compute new coordinates $(\mathsf{x1}, \mathsf{y1}, \mathsf{z1})$. Note here that quasi-particle shift in any direction must be smaller or equal than grid step in this direction,

$$\mathsf{x1} - \mathsf{x0} \leqslant dx, \quad \mathsf{y1} - \mathsf{y0} \leqslant dy, \quad \mathsf{z1} - \mathsf{z0} \leqslant dz. \tag{28}$$

(3) Using the new coordinates compute a new array $\mathsf{S1}$ containing new one-dimensional form-factors:

$$\begin{aligned} \mathsf{S1}(i,1) &= S_i^{(1\mathrm{D})}(\mathsf{x1}), \quad i=-2,2,\\ \mathsf{S1}(j,2) &= S_j^{(1\mathrm{D})}(\mathsf{y1}), \quad j=-2,2,\\ \mathsf{S1}(k,3) &= S_k^{(1\mathrm{D})}(\mathsf{z1}), \quad k=-2,2. \end{aligned} \tag{29}$$

Components $\mathsf{S1}(-2,m)$ and $\mathsf{S1}(2,m)$ are not zero in general, because of quasi-particle motion. If conditions Eq. (28) are satisfied, the array $\mathsf{S1}(i,m)$ does not have non-zero components out of $i=-2,2$.

(4) Compute auxiliary array of differences of new and old form-factors:

$$\begin{aligned} \mathsf{DS}(i,1) &= \mathsf{S1}(i,1) - \mathsf{S0}(i,1), \quad i=-2,2,\\ \mathsf{DS}(j,2) &= \mathsf{S1}(j,2) - \mathsf{S0}(j,2), \quad j=-2,2,\\ \mathsf{DS}(k,3) &= \mathsf{S1}(k,3) - \mathsf{S0}(k,3), \quad k=-2,2. \end{aligned} \tag{30}$$

It is possible to use $\mathsf{S1}$ for storage of differences DS.

(5) Compute 125*3-component array containing density decomposition $\mathsf{W}(i,j,k,m)$, in accordance with Eq. (23). We need so many components because we have the current density with components defined on different regular grids (in FDTD technique).

$$\begin{aligned} \mathsf{W}(i,j,k,1) = {} & \mathsf{DS}(i,1) * \big(\mathsf{S0}(j,2) * \mathsf{S0}(k,3) + \tfrac{1}{2} * \mathsf{DS}(j,2) * \mathsf{S0}(k,3)\\ & + \tfrac{1}{2} * \mathsf{S0}(j,2) * \mathsf{DS}(k,3) + \tfrac{1}{3} * \mathsf{DS}(j,2) * \mathsf{DS}(k,3)\big),\\ \mathsf{W}(i,j,k,2) = {} & \mathsf{DS}(j,2) * \big(\mathsf{S0}(i,1) * \mathsf{S0}(k,3) + \tfrac{1}{2} * \mathsf{DS}(i,1) * \mathsf{S0}(k,3)\\ & + \tfrac{1}{2} * \mathsf{S0}(i,1) * \mathsf{DS}(k,3) + \tfrac{1}{3} * \mathsf{DS}(i,1) * \mathsf{DS}(k,3)\big),\\ \mathsf{W}(i,j,k,3) = {} & \mathsf{DS}(k,3) * \big(\mathsf{S0}(i,1) * \mathsf{S0}(j,2) + \tfrac{1}{2} * \mathsf{DS}(i,1) * \mathsf{S0}(j,2)\\ & + \tfrac{1}{2} * \mathsf{S0}(i,1) * \mathsf{DS}(j,2) + \tfrac{1}{3} * \mathsf{DS}(i,1) * \mathsf{DS}(j,2)\big). \end{aligned} \tag{31}$$

Of course, this computation is easy to optimize. In fact, only 48*3 components are necessary.

(6) Compute three components of the current density $\mathcal{J}^1, \mathcal{J}^2, \mathcal{J}^3$ associated with the motion of the quasi-particle, using Eq. (19) and boundary condition (there is no current in nodes far from the quasi-particle location),

$$\begin{aligned}
\mathcal{J}^1_{i+1,j,k} - \mathcal{J}^1_{i,j,k} &= -\mathsf{Q}\frac{dx}{dt}\mathsf{W}(i,j,k,1),\\
\mathcal{J}^2_{i,j+1,k} - \mathcal{J}^2_{i,j,k} &= -\mathsf{Q}\frac{dy}{dt}\mathsf{W}(i,j,k,2),\\
\mathcal{J}^3_{i,j,k+1} - \mathcal{J}^3_{i,j,k} &= -\mathsf{Q}\frac{dz}{dt}\mathsf{W}(i,j,k,3),
\end{aligned} \tag{32}$$

where Q is the charge of the quasi-particle.

(7) Add computed contribution from the single quasi-particle to the total array of the current density.

As this algorithm uses only simple polynomes, its accuracy is equivalent to the accuracy of the last digit of numerical representation (e.g., 10^{-7} in single precision Fortran real*4 data or 10^{-14} in double precision Fortran real*8 data).

The computation scheme described in this section can be generalized to an arbitrary form-factor which is the product of one-dimensional form-factors Eq. (25).

5. Reduction to two dimensions

Suppose we have the two-dimensional problem, when all the variables depend on (x, y) only. In this case the Density Decomposition equation (23) provides only two first components of the current density. How to construct the third one, in consistency with the rest?

The simplest idea is to derive the third component from three-dimensional case assuming the homogeneity of all dependent variables on z. One can easily show that if the electric current density $\mathcal{J}$ is homogeneous along z at each time step and the electromagnetic fields **E**, **B** and the charge density ρ are initially homogeneous along z then the electromagnetic fields and the charge density remain homogeneous along z in time. This is valid for both continuous Maxwell equations and finite differences scheme of FDTD method. Therefore, to make 3D problem essentially two-dimensional it is sufficient to construct the current density homogeneous along z.

Consider a form-factor $S_{i,j,k}(x, y, z)$ which occupies $2N+1$ cells along z-axis. Suppose that this form-factor is sufficiently smooth and in the limit $N \to \infty$ tends to some function $\overline{S}_{i,j}(x, y)$. For all N we assume that the total sum of $S_{i,j,k}(x, y, z)$ over the grid indices k does not depend on z:

$$\sum_{k=-N}^{N} S_{i,j,k}(x, y, z) = S^N_{i,j}(x, y) > 0. \tag{33}$$

Eq. (33) is the version of Eq. (18). Here we assume that the grid node nearest to the centre of the quasi-particle is the zeroth. Of course, this sum must tend to the infinity in the limit $N \to \infty$, to allow the existence of positive quantity

$$\overline{S}_{i,j}(x, y) = \lim_{N\to\infty} \frac{S^N_{i,j}(x, y)}{2N+1}. \tag{34}$$

Here $S^N_{i,j}(x, y)/(2N+1)$ plays the role of the density of the charged “fibre” with length $2N+1$.

Suppose that the quasi-particle have moved from (x, y, z) to $(x+\Delta x, y+\Delta y, z+\Delta z)$ during dt. We assume that $\Delta x < dx$, $\Delta y < dy$, $\Delta z < dz$. The corresponding contribution to the z-component of the current density is given by Eqs. (19), (23):

$$\begin{aligned}\mathcal{J}^3_{i,j,k+1}-\mathcal{J}^3_{i,j,k} &= -\mathsf{Q}\frac{dz}{dt}\big\{\tfrac{1}{3}S(x+\Delta x,y+\Delta y,z+\Delta z)-\tfrac{1}{3}S(x+\Delta x,y+\Delta y,z)\\&\quad+\tfrac{1}{6}S(x,y+\Delta y,z+\Delta z)-\tfrac{1}{6}S(x,y+\Delta y,z)\\&\quad+\tfrac{1}{6}S(x+\Delta x,y,z+\Delta z)-\tfrac{1}{6}S(x+\Delta x,y,z)\\&\quad+\tfrac{1}{3}S(x,y,z+\Delta z)-\tfrac{1}{3}S(x,y,z)\big\}.\end{aligned}\tag{35}$$

Note that the expression in the curly braces have the form $F(z+\Delta z)-F(z)$, where

$$\begin{aligned}F(z) &= \tfrac{1}{3}S(x+\Delta x,y+\Delta y,z)+\tfrac{1}{6}S(x,y+\Delta y,z)\\&\quad+\tfrac{1}{6}S(x+\Delta x,y,z)+\tfrac{1}{3}S(x,y,z).\end{aligned}$$

Let us compute the current density at $k=0$:

$$\begin{aligned}\mathcal{J}^3_{i,j,0} &= \mathcal{J}^3_{i,j,0}-\mathcal{J}^3_{i,j,-1}+\mathcal{J}^3_{i,j,-1}-\mathcal{J}^3_{i,j,-2}+\cdots\\&= \sum_{k=-N}^{-1}\big(\mathcal{J}^3_{i,j,k+1}-\mathcal{J}^3_{i,j,k}\big)\\&= -\mathsf{Q}\frac{dz}{dt}\sum_{k=-N}^{-1}\big(F(z+\Delta z)-F(z)\big)\\&\approx \mathsf{Q}\frac{1}{dt}\int_{-\infty}^{0}\big(F(z+\Delta z)-F(z)\big)\,dz\\&\approx \mathsf{Q}\frac{1}{dt}F(0)\Delta z=\mathsf{Q}V_zF(0).\end{aligned}\tag{36}$$

Here we replace the sum by an approximate integral, the change in the sign is due to Eq. (17). The ratio $\Delta z/dt=V_z$ is the z-component of the quasi-particle velocity. Finally, in the limit $N\to\infty$ we obtain

$$\begin{aligned}\mathcal{J}^1_{i+1,j,0}-\mathcal{J}^1_{i,j,0} &= -\mathsf{Q}\frac{dx}{dt}\big\{\tfrac{1}{2}\overline{S}(x+\Delta x,y+\Delta y)-\tfrac{1}{2}\overline{S}(x,y+\Delta y)\\&\quad+\tfrac{1}{2}\overline{S}(x+\Delta x,y)-\tfrac{1}{2}\overline{S}(x,y)\big\},\\ \mathcal{J}^2_{i,j+1,0}-\mathcal{J}^2_{i,j,0} &= -\mathsf{Q}\frac{dy}{dt}\big\{\tfrac{1}{2}\overline{S}(x+\Delta x,y+\Delta y)-\tfrac{1}{2}\overline{S}(x+\Delta x,y)\\&\quad+\tfrac{1}{2}\overline{S}(x,y+\Delta y)-\tfrac{1}{2}\overline{S}(x,y)\big\},\\ \mathcal{J}^3_{i,j,0} &= \mathsf{Q}V_z\big\{\tfrac{1}{3}\overline{S}(x+\Delta x,y+\Delta y)+\tfrac{1}{6}\overline{S}(x,y+\Delta y)\\&\quad+\tfrac{1}{6}\overline{S}(x+\Delta x,y)+\tfrac{1}{3}\overline{S}(x,y)\big\}.\end{aligned}\tag{37}$$

These formulae define the Density Decomposition for two-dimensional problem.

In the case of the algorithm described in the previous section we must change formulae of items (5) and (6) in the following way:

$$\begin{aligned}\mathsf{W}(i,j,1) &= \mathsf{DS}(i,1)*\big(\mathsf{S0}(j,2)+\tfrac{1}{2}*\mathsf{DS}(j,2)\big),\\ \mathsf{W}(i,j,2) &= \mathsf{DS}(j,2)*\big(\mathsf{S0}(i,1)+\tfrac{1}{2}*\mathsf{DS}(i,1)\big),\\ \mathsf{W}(i,j,3) &= \mathsf{S0}(i,1)*\mathsf{S0}(j,2)+\tfrac{1}{2}*\mathsf{DS}(i,1)*\mathsf{S0}(j,2)\\&\quad+\tfrac{1}{2}*\mathsf{S0}(i,1)*\mathsf{DS}(j,2)+\tfrac{1}{3}*\mathsf{DS}(i,1)*\mathsf{DS}(j,2).\end{aligned}\tag{38}$$

$$
\begin{aligned}
&\mathcal{J}^1_{i+1,j} - \mathcal{J}^1_{i,j} = -\mathsf{Q}\frac{dx}{dt}\mathsf{W}(i,j,1),\\
&\mathcal{J}^2_{i,j+1} - \mathcal{J}^2_{i,j} = -\mathsf{Q}\frac{dy}{dt}\mathsf{W}(i,j,2),\\
&\mathcal{J}^3_{i,j} = \mathsf{Q}\mathsf{V}_\mathsf{z}\mathsf{W}(i,j,3),
\end{aligned}
\tag{39}
$$

where V_z is the third component of the quasi-particle velocity. These formulae are similar to that of 3D-case, Eqs. (31)–(32).

6. Conclusion

In this paper we develop the Density Decomposition, a new charge conserving scheme for Particle-in-Cell code in Cartesian geometry. This scheme allows one to implement the PIC code without solving Poisson equation. The described current density assignment is the unique linear procedure in consistency with the continuity equation, assuming that quasi-particle trajectory over time step is a straight line.

The new method is valid for an arbitrary form-factor of quasi-particles. The method can be used to reduce the numerical noise, when applied to high-order form-factors.

One can see that this method is not restricted by special Maxwell solver, but is based on discretized continuity equation in Cartesian geometry.

We do not discuss how to treat boundary conditions in this paper. It is easy to implement described scheme in the simplest case of periodic boundary condition.

The Density Decomposition was implemented by the author in three-dimensional and two-dimensional PIC codes. It was used for the simulation of collisionless plasma in intense electromagnetic field, [13–17].

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