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Numerical experiments for solving Maxwell's equations in thin domains with a new implicit scheme*

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Abstract. Conditional stability of explicit schemes in finite differences complicates the choice of a time step. The increase in the number of the grid nodes for more precise computations and the corresponding space step decrease leads to the increase in computer costs due to the decreasing of the time step. We present a new implicit scheme for computing Maxwell's equations in three-dimensional domains, where the smallest size is one tenth or less than any other size. The main advantage of the new scheme is possibility of performing the computations with bigger time steps, the disadvantage is a possible high level of errors for short-wave solutions. The first numerical results of the scheme behavior are presented.

1. Introduction

One of the widespread schemes in plasma physics for the computation of Maxwell's equations is the scheme by A. Langdon and B. Lasinsky [1]. With a supplement of the Boris scheme it represents a standard efficient method for the non-stationary plasma modeling with the particle-in-cell method. The schemes use staggered grids and provide second order of accuracy with respect to space and time, based only on the first derivatives. The algorithms allowed performing the numerical modeling for many problems, for example, those associated with electrons in nuclear fusion, wake-field acceleration by proton (electron) bunch driven plasma, self-modulation of ultra-relativistic lepton bunches in high density plasmas, generation of powerful bursts of high-energy radiation (X-ray — microwave range), relativistic bunches in pulsar magnetosphere, protoplanetary disk dynamics, beam dynamics in colliders [2–5].

However, the Langdon–Lasinsky scheme becomes inapplicable for the modeling of the thin electron/positron ultrarelativistic beams in modern colliders due to the conditional scheme stability. The beam sizes ratio in the transversal direction can reach the value of 100, and problems of the time step size arise from the minimum spatial step size. The increase in

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the number of the grid nodes for more precise computations results in the increase of computer costs due to the decreasing of the time step. For the three dimensional case, there is a basic need in developing new algorithms and in the extension of the already existing algorithms to supercomputers, with allowance of the specifics features of the beams [6].

We present a new scheme, based on the Langdon–Lasinsky scheme, which is implicit in the direction of the smallest beam size and thus allows performing computations with a bigger time step. The results of the scheme analysis and the numerical experiments are demonstrated.

2. Schemes

The Langdon–Lasinski scheme for Maxwell's equations

$$\operatorname{rot}\vec{E} = -\frac{1}{c}\frac{\partial \vec{H}}{\partial t}, \quad \operatorname{div}\vec{E} = 4\pi\rho,$$
$$\operatorname{rot}\vec{H} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c}\vec{j}, \quad \operatorname{div}\vec{H} = 0$$

has the following form:

$$\frac{H^{m+1/2} - H^{m-1/2}}{\tau} = -c\operatorname{rot}_h E^m, \tag{1}$$
$$\frac{E^{m+1} - E^m}{\tau} = c\operatorname{rot}_h H^{m+1/2} - 4\pi j^{m+1/2}, \tag{2}$$

where

$$\operatorname{rot}_h H = \begin{pmatrix} \dfrac{Hz_{i,k,l-1/2} - Hz_{i,k-1,l-1/2}}{h_y} - \dfrac{Hy_{i,k-1/2,l} - Hy_{i,k-1/2,l-1}}{h_z} \\ \dfrac{Hx_{i-1/2,k,l} - Hx_{i-1/2,k,l-1}}{h_z} - \dfrac{Hz_{i,k,l-1/2} - Hz_{i-1,k,l-1/2}}{h_x} \\ \dfrac{Hy_{i,k-1/2,l} - Hy_{i-1,k-1/2,l}}{h_x} - \dfrac{Hx_{i-1/2,k,l} - Hx_{i-1/2,k-1,l}}{h_y} \end{pmatrix},$$

$$\operatorname{rot}_h E = \begin{pmatrix} \dfrac{Ez_{i-1/2,k+1/2,l} - Ez_{i-1/2,k-1/2,l}}{h_y} - \dfrac{Ey_{i-1/2,k,l+1/2} - Ey_{i-1/2,k,l-1/2}}{h_z} \\ \dfrac{Ex_{i,k-1/2,l+1/2} - Ex_{i,k-1/2,l-1/2}}{h_z} - \dfrac{Ez_{i+1/2,k-1/2,l} - Ez_{i-1/2,k-1/2,l}}{h_x} \\ \dfrac{Ey_{i+1/2,k,l-1/2} - Ey_{i-1/2,k,l-1/2}}{h_x} - \dfrac{Ex_{i,k+1/2,l-1/2} - Ex_{i,k-1/2,l-1/2}}{h_y} \end{pmatrix}.$$

The scheme for any field component of the system without charges may be reduced to the following scheme for the wave equation:

$$\frac{y_i^{m+1} - 2y_i^m + y_i^{m-1}}{c^2\tau^2} = \Delta_{xx} y_i^m + \Delta_{yy} y^m + \Delta_{zz} y^m. \tag{3}$$

Assuming the direction of the smallest beam size as x, we are trying to use the properties of implicit schemes. On the basis of the scheme the weighted scheme may be written [7]:

$$\frac{y_i^{m+1} - 2y_i^m + y_i^{m-1}}{c^2\tau^2} = \frac{1}{4}\Delta_{xx} y_i^{m+1} + \frac{1}{2}\Delta_{xx} y_i^m + \frac{1}{4}\Delta_{xx} y_i^{m-1} + \Delta_{yy} y^m + \Delta_{zz} y^m. \tag{4}$$

This scheme has also the second order of accuracy. However, the stability condition does not depend on x direction, and allows using a bigger time step. The important question is: how correct is the description of the wave propagation? The analysis of both schemes has shown that both schemes describe the wave velocity with second order of accuracy [8]:

$$u = \frac{\omega}{k} = 1 - k^2\left(\frac{h_x^2 \cos^4\alpha + h_y^2 \cos^4\beta + h_z^2 \cos^4\gamma - \tau^2}{24}\right) + O((h+\tau)^3) \tag{5}$$

for the initial scheme and

$$u = \frac{\omega}{k} = 1 + k^2\left(\frac{h_x^2 \cos^4\alpha + h_y^2 \cos^4\beta + h_z^2 \cos^4\gamma - \tau^2 + 3\tau^2\cos^2\alpha}{24}\right) + O((h+\tau)^3) \tag{6}$$

for the new scheme, where α, β, γ are the angles between the propagation vector and the corresponding axis. We may observe the difference in the factor for k^2, and it depends on the time step and may give much bigger errors when k is high. The errors in the wave propagation velocity depend on the wave vector for both schemes, thus the short-wave solutions must be described with a correspondingly small space and time steps.

The scheme for Maxwell's equations based on the Langdon–Lasinsky scheme has the following form:

$$\begin{aligned}
\frac{Hx^{m+1/2} - Hx^{m-1/2}}{\tau} &= c\Delta_z Ey^m - c\Delta_y Ez^m,\\
\frac{Hy^{m+1/2} - Hy^{m-1/2}}{\tau} &= c\Delta_x Ez^m - c\Delta_z Ex^m,\\
\frac{Hz^{m+1/2} - Hz^{m-1/2}}{\tau} &= c\Delta_y Ex^m - c\Delta_x Ey^m,\\
\frac{Ex^{m+1} - Ex^m}{\tau} &= c\Delta_y Hz^{m+1/2} - c\Delta_z Hy^{m+1/2} - 4\pi jx^{m+1/2}, \qquad (7)\\
\frac{Ey^{m+1} - 2Ey^m + Ey^{m-1}}{\tau^2} &= c^2\Delta_{xx} Ey^m + c^2\Delta_{yy} Ey^m + c^2\Delta_{zz} Ey^m -\\
&\quad 4\pi c^2 \Delta_y \rho^m - 4\pi\frac{jy^{m+1/2} - jy^{m-1/2}}{\tau},
\end{aligned}$$

$$\frac{Ez^{m+1} - 2Ez^m + Ez^{m-1}}{\tau^2} = c^2\Delta_{xx}Ez^m + c^2\Delta_{yy}Ez^m + c^2\Delta_{zz}Ez^m - 4\pi c^2\Delta_z\rho^m - 4\pi\frac{jz^{m+1/2} - jz^{m-1/2}}{\tau}.$$

According to the scheme presented we may write down the final new scheme for Maxwell's equations:

$$\begin{aligned}
\frac{Hx^{m+1/2} - Hx^{m-1/2}}{\tau} &= c\Delta_z Ey^m - c\Delta_y Ez^m,\\
\frac{Hy^{m+1/2} - Hy^{m-1/2}}{\tau} &= c\Delta_x Ez^m - c\Delta_z Ex^m,\\
\frac{Hz^{m+1/2} - Hz^{m-1/2}}{\tau} &= c\Delta_y Ex^m - c\Delta_x Ey^m,\\
\frac{Ex^{m+1} - Ex^m}{\tau} &= c\Delta_y Hz^{m+1/2} - c\Delta_z Hy^{m+1/2} - 4\pi jx^{m+1/2},\\
\frac{Ey^{m+1} - 2Ey^m + Ey^{m-1}}{\tau^2} &= \frac{c^2}{4}\Delta_{xx}Ey^{m+1} + \frac{c^2}{2}\Delta_{xx}Ey^m + \frac{c^2}{4}\Delta_{xx}Ey^{m-1} + c^2\Delta_{yy}Ey^m + c^2\Delta_{zz}Ey^m - 4\pi c^2\Delta_y\rho^m - 4\pi\frac{jy^{m+1/2} - jy^{m-1/2}}{\tau},\\
\frac{Ez^{m+1} - 2Ez^m + Ez^{m-1}}{\tau^2} &= \frac{c^2}{4}\Delta_{xx}Ez^{m+1} + \frac{c^2}{2}\Delta_{xx}Ez^m + \frac{c^2}{4}\Delta_{xx}Ez^{m-1} + c^2\Delta_{yy}Ez^m + c^2\Delta_{zz}Ez^m - 4\pi c^2\Delta_z\rho^m - 4\pi\frac{jz^{m+1/2} - jz^{m-1/2}}{\tau}.
\end{aligned} \tag{8}$$

As is seen, the computation of the magnetic field and the field along the direction x of the minimum domain size repeats the one of the Langdon–Lasinsky scheme. The changes are made in two components of electric fields which are orthogonal to the axis x. The implicitness of the scheme allows using high values of the time step, which are impossible to be used in the Langdon–Lasinsky scheme. The "payment" for this advantage is a higher level of errors for short-wave solutions.

3. Numerical results

The code for schemes (3), (4) and (7), (8) was developed, and numerical experiments were performed for the case of the absence of particles. The boundary conditions were set to be periodic. For the second scheme the cyclic tridiagonal matrix algorithm was applied. The wave velocity was computed using the ordinary least squares method. The characteristic velocity is the light speed, thus in dimensionless units there is no c in Maxwell's equations.

For the one-dimensional case, the solution $E_z = \sin(kx - \omega t)$ was used in the domain $[0, L]$, $L = 0.01$ cm,

$$E^m_{z,i} = \sin\Big(\frac{2\pi}{L}k(i - 1.5)h - \omega m\tau\Big) \tag{7}$$

due to the shifted grids. The numerical experiments have proved that the errors decrease with decreasing the spatial and time steps, and the square-law convergence is held. The biggest errors are observed at the beginning of the process, and then the level of the errors corresponds to the analytical expressions (5), (6). The increase in the wave number k leads to the square-law increase of errors, and the error level does not correspond to expressions (5), (6). The differences between two schemes (7), (8) are insignificant. The conclusions are demonstrated in Figure 1 with the errors of the wave velocity for 50, 100, 200, 400, 800 nodes in each direction, and $\tau/h = 0.4$, $k = 10$.

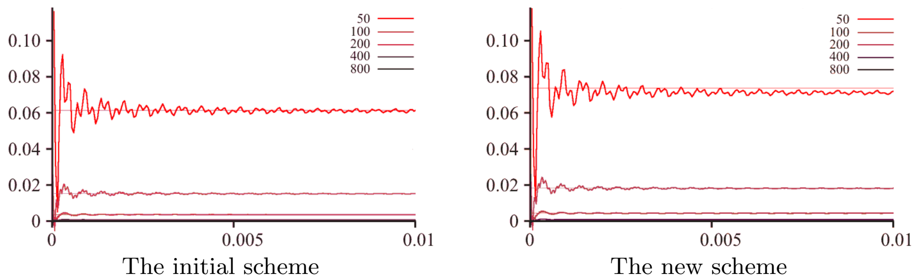
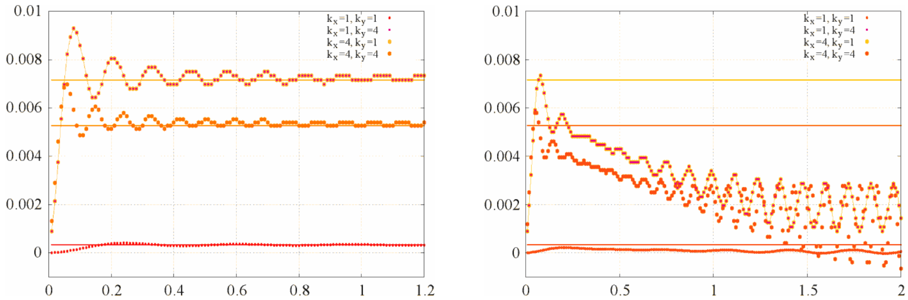


Figure 1. Errors in the wave velocity computation for $k = 10$

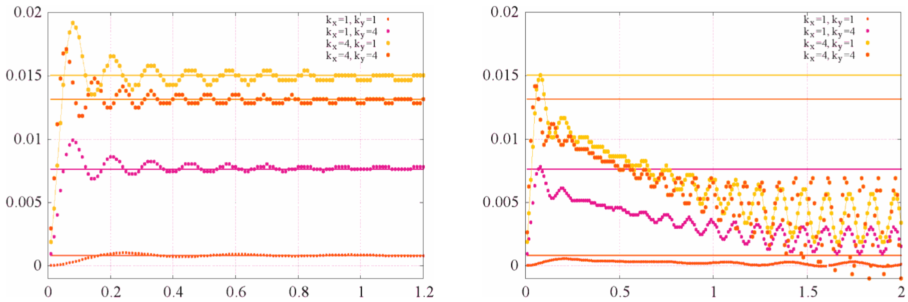
The numerical experiments for the two-dimensional case of the field $E_z = \sin(k_x x + k_y y - \omega t)$, $|k| = 1$, in the domain $[0, L] \times [0, L]$, where $L = 1$ cm, with 50 nodes in each direction, have shown similar results (Figures 2, 3). Two cases were considered: in the first one the boundary conditions were set as periodic, in the second — with explicit expression (9) (and a usual tridiagonal matrix algorithm was applied). When the boundary conditions are periodic, the errors oscillate near the analytic values (5), (6), the explicit boundary contagion brings about lower errors, thus correcting the solution phase and its speed. The initial scheme (7) does not bring any difference into the directions x and y, the new scheme (8) leading to a higher level of errors for the component k_x of the wave number k.

Figure 4 demonstrates the results of wave velocity errors for the new scheme in the domain with $L_x = 0.25$, $L_y = 1$ for $k_x = 1$, $k_y = 1$ and $k_x = 1$, $k_y = 4$. In this case, $\tau/h_x = 2$, $\tau/h_y = 0.5$, and the initial scheme (7) does not allow carrying out the computations with these parameters.



Periodic boundary conditions Explicit boundary conditions

Figure 2. Errors in the wave velocity computation for different k_x, k_y with the initial scheme



Periodic boundary conditions Explicit boundary conditions

Figure 3. Errors in the wave velocity computation for different k_x, k_y with the new scheme

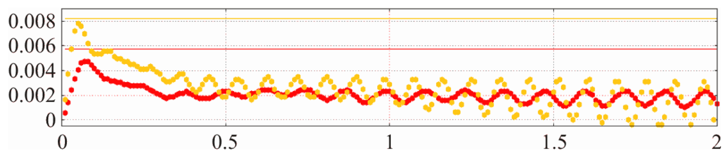
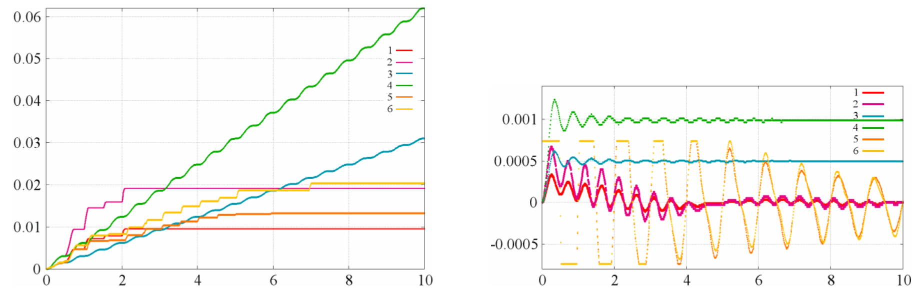


Figure 4. Errors in the wave velocity computation for $L_x = 0.25$, $L_y = 1$

In the 3D case the errors $\epsilon_1 = h_x^2 \cos^4 \alpha + h_y^2 \cos^4 \beta + h_z^2 \cos^4 \gamma - \tau^2$ for the initial scheme and $\epsilon_1 = h_x^2 \cos^4 \alpha + h_y^2 \cos^4 \beta + h_z^2 \cos^4 \gamma - \tau^2(1 - 3\cos^2 \alpha)$ for the new scheme (8) in the thin domain were considered. The selected domain sizes $L_x = 10^{-4}$ cm, $L_y = 10^{-2}$ cm, $L_z = 1$ cm are close to the parameters of the computational domain for the numerical modeling of thin ultrarelativistic beams in supercolliders. The analysis is an extension of one- and two-dimensional cases: the biggest spatial step h_z leads to the biggest errors, the errors are higher for smaller values of k_x/k and k_y/k, the time step does not significantly affect in comparison with the spacial step h_z.



a) Δy errors　　b) Velocity propagation errors

Figure 5. Errors for different schemes

The flat wave solutions $\vec{E} = \vec{E}_0 \sin(\vec{k}\vec{r} - \omega t)$, $\vec{H} = \vec{H}_0 \sin(\vec{k}\vec{r} - \omega t)$, $\vec{k}\vec{E}_0 = 0$, $\vec{k}\vec{H}_0 = 0$, $\vec{E}_0\vec{H}_0 = 0$ were considered to test the description of each field components and the propagation velocity with both schemes. In Figure 5, a) the results for $\Delta y = \max(E_y^{\mathrm{num}} - E_y^{\mathrm{an}})$ for $k = (1, 0, 0)$, $E_0 = (0, 1, 0)$, $H_0 = (0, 0, 1)$ are presented. Graph 1 corresponds to the initial scheme (7) with explicit boundary conditions, graph 2 — to the new scheme (8) with explicit boundary conditions, graph 3 — to the initial scheme (7) with periodic boundary conditions, graph 4 — to the new scheme (8) with periodic boundary conditions, 5 — to the Langdon–Lasinsky scheme (1), (2) with explicit boundary conditions on four sides of the domain (the other two can be taken from shifted grid nodes using the scheme), graph 6 — to the Langdon–Lasinsky scheme (1), (2) with explicit boundary conditions in the whole domain. From the graphs we can observe that the difference between numerical and analytic solutions for both schemes with periodic boundary conditions increases with time. This difference is the result of accumulation of constant errors in the wave velocity calculation. The lowest level of errors is provided by schemes (7), (8) with explicit boundary conditions. The error of the Langdon–Lasinsky schemes (1), (2) are low only in the beginning, but schemes (7), (8) provide better results for longer times. The same results can be observed in Figure 5, b) for the wave velocity errors.

Conclusion

The new scheme for Maxwell's equations in thin three-dimensional domains has been numerically analyzed. The second order of accuracy in space and time, the square-law dependence of the errors on the wave vector were corroborated. The dependence of the wave vector value plays a significant role for short-wave solutions and, respectively, small steps must be taken to describe the solutions correctly. The periodic boundary conditions lead to oscillations in the propagation velocity around the analytically calculated values, the explicitly set boundary conditions decrease the errors, and the errors are smaller than errors of the Langdon–Lasinsky scheme. The main advantage of the new scheme is the possibility of performing the computations with bigger time steps, the disadvantage is a possible high level of errors for short-wave solutions. The first numerical results have demonstrated the prospects of the new scheme.

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