

Development and analysis of computational algorithm of the Maxwell's equations in flat domains

M A Boronina¹ and V A Vshivkov^{2,3}

¹ Institute of Computational Mathematics and Mathematical Geophysics SB RAS, Novosibirsk, Russia

² Novosibirsk State University, Novosibirsk, Russia

³ Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia

E-mail: boronina@ssd.sccc.ru

Abstract. We present a new scheme for the Maxwell's equations computations in three-dimensional domains, where size in one direction is much smaller than the other sizes. The scheme is based on the Langdon-Lasinski scheme, which is standard for numerical experiments in plasma physics. Our study is devoted to analysis of correct wave propagation due to the effects of using a finite-difference approximation. To show the main dependencies we present numerical results in one-dimensional case. The results demonstrate, that the new scheme maintains the wave amplitude, the propagation speed and allows using of bigger time step in comparison with the Langdon-Lasinski scheme.

1. Introduction

The scheme of A. Langdon and B. Lasinski [1] is widely used in numerical experiments in plasma physics. The advantages of the scheme are the second order of accuracy in space and time and simplicity of its realization. However, the stability condition defines the maximal ratio of the time step to the spatial step. In cases of flat domains (where one domain size is much smaller than the other sizes), the time step depends on the minimal spatial step and leads to a bigger number of the time steps with the spatial grid refinement. The computations with the unnecessary small time step become longer and ineffective. For example, in problem of ultrarelativistic beam dynamics in supercolliders, the ratio of the beam sizes may achieve 1 : 200 : 60000 [2] and the domain sizes depend on the beam sizes. A three-dimensional parallel algorithm with mixed decomposition and load-balancing makes it possible to perform numerical experiments with the beam sizes ratio 1 : 50 : 500 [3].

A new scheme for the Maxwell's equations is presented. The scheme is based on the Langdon-Lasinski scheme. The weakened stability condition allows using the bigger time steps and decreasing of the computation time. The new scheme must be validated in terms of correct wave propagation: the numerical errors may change the solution significantly, in the same time it is impossible to distinguish the numerical errors from the physical effects [4]. The scheme effects for the simplest solutions must be studied to predict the scheme influence in real numerical experiments.

The implicit scheme was analyzed and compared with the Langdon-Lasinski scheme. It was shown that the new scheme maintains the wave amplitude, the propagation speed and allows



using the bigger time step in comparison with the Langdon-Lasinski scheme. The implicit scheme may be applied in a variety of problems with the Maxwell's equations solutions in flat domains.

2. The scheme development and analysis

Let one consider the Maxwell's equations in dimensionless units:

$$\begin{aligned} \text{rot} \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \text{rot} \vec{B} &= \frac{\partial \vec{E}}{\partial t} + \vec{j} \\ \text{div} \vec{E} &= \rho \\ \text{div} \vec{B} &= 0 \end{aligned}$$

The Langdon-Lasinski scheme uses grids, which are shifted in half-step in time and space:

$$\frac{H^{m+1/2} - H^{m-1/2}}{\tau} = -\text{rot}_h E^m \quad (1)$$

$$\frac{E^{m+1} - E^m}{\tau} = j^{m+1/2} + \text{rot}_h H^{m+1/2}, \quad (2)$$

where

$$\begin{aligned} \text{rot}_h H &= \begin{vmatrix} \frac{Hz_{i,k,l-1/2} - Hz_{i,k-1,l-1/2}}{h_y} - \frac{Hy_{i,k-1/2,l} - Hy_{i,k-1/2,l-1}}{h_z} \\ \frac{Hx_{i-1/2,k,l} - Hx_{i-1/2,k,l-1}}{h_z} - \frac{Hz_{i,k,l-1/2} - Hz_{i-1,k,l-1/2}}{h_x} \\ \frac{Hy_{i,k-1/2,l} - Hy_{i-1,k-1/2,l}}{h_x} - \frac{Hx_{i-1/2,k,l} - Hx_{i-1/2,k-1,l}}{h_y} \end{vmatrix}, \\ \text{rot}_h E &= \begin{vmatrix} \frac{Ez_{i-1/2,k+1/2,l} - Ez_{i-1/2,k-1/2,l}}{h_y} - \frac{Ey_{i-1/2,k,l+1/2} - Ey_{i-1/2,k,l-1/2}}{h_z} \\ \frac{Ex_{i,k-1/2,l+1/2} - Ex_{i,k-1/2,l-1/2}}{h_z} - \frac{Ez_{i+1/2,k-1/2,l} - Ez_{i-1/2,k-1/2,l}}{h_x} \\ \frac{Ey_{i+1/2,k,l-1/2} - Ey_{i-1/2,k,l-1/2}}{h_x} - \frac{Ex_{i,k+1/2,l-1/2} - Ex_{i,k-1/2,l-1/2}}{h_y} \end{vmatrix}. \end{aligned}$$

The scheme may be reduced to the following:

$$\frac{y_i^{m+1} - 2y_i^m + y_i^{m-1}}{\tau^2} = \frac{y_{i+1}^m - 2y_i^m + y_{i-1}^m}{h^2}, \quad (3)$$

where y is any of the electric or magnetic field components.

The stability condition for scheme (1-2) $\tau/h \leq 1$ provides the amplitude conservation.

Let one consider scheme [5], which is implicit in the direction of the smallest domain size:

$$\frac{y_i^{m+1} - 2y_i^m + y_i^{m-1}}{\tau^2} = \delta \Delta_{xx} y_i^{m+1} + (1 - 2\delta) \Delta_{xx} y_i^m + \delta \Delta_{xx} y_i^{m-1} \quad (4)$$

where

$$\Delta_{xx} y_i^m = \frac{y_{i+1}^m - 2y_i^m + y_{i-1}^m}{h^2},$$

and $0 \leq \delta \leq 1/2$. For $\delta = 0$ the original Langdon-Lasinski scheme is obtained. For $\delta \geq 1/4$, the scheme is absolutely stable and maintains the wave amplitude.

Considering the solution as $y_l^m = A \exp(-i(\omega t m - k l h))$, one obtains the dispersion relations for the Langdon-Lasinski scheme:

$$\sin^2 \frac{\omega \tau}{2} = \frac{\tau^2}{h^2} \sin^2 \frac{kh}{2},$$

and for the second scheme:

$$\sin^2 \frac{\omega \tau}{2} = \frac{\tau^2}{h^2} \frac{\sin^2 \frac{kh}{2}}{1 + 4\delta \frac{\tau^2}{h^2} \sin^2 \frac{kh}{2}}.$$

Having expressed ω through k and having used Taylor series for τ and h we obtain the relations for the wave speed respectively:

$$u_1 = \frac{\omega}{k} = 1 + k^2 \left(\frac{\tau^2 - h^2}{24} \right) + O(h^3, \tau^3, h\tau^2, h^2\tau) \quad (5)$$

$$u_2 = \frac{\omega}{k} = 1 + k^2 \left(\frac{\tau^2 - h^2}{24} + \frac{\delta \tau^2}{2} \right) + O(h^3, \tau^3, h\tau^2, h^2\tau) \quad (6)$$

The formula (5) for the Langdon-Lasinski scheme demonstrates the fact, that the numerical wave speed is always smaller than 1 in dimensionless units (which corresponds to the light speed in dimensional units), because $\tau/h \leq 1$. The opposite conclusion is held for the second scheme (6) when $\tau > h/\sqrt{1 + 12\delta} \geq h/2$ the wave has the speed bigger then 1, which is not a physical effect. For both schemes the error arises with increasing of the wavenumber k . Thus, the high-frequency modes of numerical solutions must be described with a proper spatial grid. However, the difference between the two scheme errors is not big, and the new scheme is very promising.

The same idea can be used to obtain the corresponding schemes in a three-dimensional case. Let x be the direction of the smallest domain size. Then the Langdon-Lasinski scheme turns into

$$\frac{y^{m+1} - 2y^m + y^{m-1}}{\tau^2} = \Delta_{xx}y^m + \delta\Delta_{xx}y^{m-1} + \Delta_{yy}y^m + \Delta_{zz}y^m \quad (7)$$

and the second scheme turns into the following:

$$\frac{y^{m+1} - 2y^m + y^{m-1}}{\tau^2} = \delta\Delta_{xx}y^{m+1} + (1 - 2\delta)\Delta_{xx}y^m + \delta\Delta_{xx}y^{m-1} + \Delta_{yy}y^m + \Delta_{zz}y^m \quad (8)$$

The stability condition of the explicit scheme (7) is $\tau^2/h_x^2 + \tau^2/h_y^2 + \tau^2/h_z^2 \leq 1$, while the stability condition of the second scheme (8), which contains the implicitness, does not depend on h_x for $\delta \geq 1/4$: $\tau^2/h_y^2 + \tau^2/h_z^2 \leq 1$. The symmetrical scheme ($\delta = 1/4$) provides the second order of accuracy in time, and both schemes (7,8) have the second order of approximation in space and time.

To create a new scheme for the Maxwell's equations, one applies the changes of the magnetic field in the original scheme (1,2) using $\delta = 1/4$ [6]:

$$\begin{aligned}
 \frac{Hx^{m+1/2} - Hx^{m-1/2}}{\tau} &= \Delta_z Ey^m - \Delta_y Ez^m \\
 \frac{Hy^{m+1/2} - 2Hy^{m-1/2} + Hy^{m-3/2}}{\tau^2} &= \Delta_{yy} Hy^{m-1/2} + \Delta_{zz} Hy^{m-1/2} + \\
 &+ \frac{1}{4} \Delta_{xx} Hy^{m+1/2} + \frac{1}{2} \Delta_{xx} Hy^{m-1/2} + \frac{1}{4} \Delta_{xx} Hy^{m-3/2} \\
 \frac{Hz^{m+1/2} - 2Hz^{m-1/2} + Hz^{m-3/2}}{\tau^2} &= \Delta_{yy} Hz^{m-1/2} + \Delta_{zz} Hz^{m-1/2} + \\
 &+ \frac{1}{4} \Delta_{xx} Hz^{m+1/2} + \frac{1}{2} \Delta_{xx} Hz^{m-1/2} + \frac{1}{4} \Delta_{xx} Hz^{m-3/2} \\
 \frac{Ex^{m+1} - Ex^m}{\tau} &= \Delta_y Hz^{m+1/2} - \Delta_z Hy^{m+1/2} - jx^{m+1/2} \\
 \frac{Ey^{m+1} - Ey^m}{\tau} &= \Delta_z Hx^{m+1/2} - \Delta_x Hz^{m+1/2} - jy^{m+1/2} \\
 \frac{Ez^{m+1} - Ez^m}{\tau} &= \Delta_x Hy^{m+1/2} - \Delta_y Hx^{m+1/2} - jz^{m+1/2}
 \end{aligned} \tag{9}$$

The Gauss laws in this case for the dimensionless units are following:

$$\frac{1}{4} \Delta_x Hx^{m+1/2} + \frac{1}{2} Hx^{m-1/2} + \frac{1}{4} Hx^{m-3/2} + \Delta_y Hy^{m-1/2} + \Delta_z Hz^{m-1/2} = 0$$

for $\text{div} H = 0$ and

$$\Delta_x Ex^m + \Delta_y Ey^m + \Delta_z Ez^m = \rho^m$$

for $\text{div} E = \rho$.

Another scheme, based on the changes of electric the field computation

$$\begin{aligned}
 \frac{Hx^{m+1/2} - Hx^{m-1/2}}{\tau} &= \Delta_z Ey^m - \Delta_y Ez^m \\
 \frac{Hy^{m+1/2} - Hy^{m-1/2}}{\tau} &= \Delta_x Ez^m - \Delta_z Ex^m \\
 \frac{Hz^{m+1/2} - Hz^{m-1/2}}{\tau} &= \Delta_y Ex^m - \Delta_x Ey^m \\
 \frac{Ex^{m+1} - Ex^m}{\tau} &= \Delta_y Hz^{m+1/2} - \Delta_z Hy^{m+1/2} - jx^{m+1/2} \\
 \frac{Ey^{m+1} - 2Ey^m + Ey^{m-1}}{\tau^2} &= \frac{1}{4} \Delta_{xx} Ey^{m+1} + \frac{1}{2} \Delta_{xx} Ey^m + \frac{1}{4} \Delta_{xx} Ey^{m-1} + \\
 &+ \Delta_{yy} Ey^m + \Delta_{zz} Ey^m - \Delta_y \rho^m - \frac{jy^{m+1/2} - jy^{m-1/2}}{\tau} \\
 \frac{Ez^{m+1} - 2Ez^m + Ez^{m-1}}{\tau^2} &= \frac{1}{4} \Delta_{xx} Ez^{m+1} + \frac{1}{2} \Delta_{xx} Ez^m + \frac{1}{4} \Delta_{xx} Ez^{m-1} + \\
 &+ \Delta_{yy} Ez^m + \Delta_{zz} Ez^m - \Delta_z \rho^m - \frac{jz^{m+1/2} - jz^{m-1/2}}{\tau}
 \end{aligned} \tag{10}$$

with corresponding Gauss laws

$$\Delta_x H x^{m+1/2} + \Delta_y H y^{m+1/2} + \Delta_z H z^{m+1/2} = 0$$

for $\text{div} H = 0$ and

$$\frac{1}{4} \Delta_x E x^{m+1} + \frac{1}{2} E x^m + \frac{1}{4} E x^{m-1} + \Delta_y E y^m + \Delta_z E z^m = \rho^m$$

for $\text{div} E = \rho$ is advantageous for the cases with boundary conditions for electric field. For example, cycle of the original beam dynamics algorithm [7] consists of the following computational steps:

1. Magnetic field for time moment m : $\frac{H^m - H^{m-1/2}}{\tau/2} = -\text{rot}_h E^m$.
2. Particle motion.
3. Magnetic field for time moment $m + 1/2$: $\frac{H^{m+1/2} - H^{m-1/2}}{\tau} = -\text{rot}_h E^m$.
4. Boundary conditions for the electric field.
5. The electric field in the whole domain.

The two new equations in finite differences on the step 5 may be sold with tridiagonal matrix algorithm. This method requires $O(n)$ times more operations in comparison with the Langdon-Lasinski scheme. Besides, the three-dimensional array of the currents $j^{m-1/2}$ on the previous times step must be stored. The Langdon-Lasinski doesn't require the density computation, but the array is needed to calculate the boundary conditions for the electric field [8]. In the case of ultrarelativistic beam dynamics code, the main group processors compute the density arrays and send the corresponding contributions into the electric field. The interprocessor communications increase significantly the total computation time. It is effective the electric field grid to have 2 additional nodes more in each direction, then the magnetic field can be computed as the electric field derivative, and there is no need to set the boundary conditions for the magnetic field. The new scheme will allow performing the numerical experiments with bigger time step and thus with more seldom computations of the boundary conditions in comparison with the original scheme. The application of the implicit scheme makes possible significant decreasing of the calculation time, especially in cases of computationally difficult time steps.

3. Numerical results

The basic study requires the consideration of the one-dimensional case. The solution of flat wave $E_z(x, t) = \sin(kx - \omega t)$ in domain $[0 : L], L = 0.01$ without charges was studied. The boundary conditions are considered as periodic ones. The cyclic tridiagonal matrix algorithm was used to apply the implicit scheme. The solution in finite differences was taken as $E z_i^m = \sin\left(\frac{2\pi}{L}(k(i - 1.5)h - \omega m\tau)\right)$. In the dimensionless units $c = 1$. The numerical wave speed was calculated with second order of accuracy as the speed of the solution root point. One considers the error $\epsilon_{num} = \omega/k - 1$ for the numerical solution, $\epsilon_{theor_1} = k^2(h^2 - \tau^2)/24$ for the original Langdon-Lasinski scheme (1-2,5) and $\epsilon_{theor_2} = k^2(h^2 + 2\tau^2)/24$ (10,6) for the new scheme with $\delta = 1/4$.

Figure 1 demonstrates the errors ϵ_{num_1} with color lines and ϵ_{th_1} with thin horizontal lines for $k=10$ and different steps with $\tau/h = 0.4$. The red line corresponds to $h = 2 \cdot 10^{-4}$, the blue line to $h = 10^{-4}$, the black line to $h = 5 \cdot 10^{-5}$. The same notations are used for figure 2, where the errors ϵ_{num_2} and ϵ_{th_2} are presented. For $k = 1$ with the same steps the errors of both schemes do not exceed 0.001, for $k = 10$ and $\tau/h = 0.4$ the errors are higher. The numerical and theoretical errors are in good coincidence and decrease with the step decreasing. The differences between the two schemes are low.

When $k = 100$, the errors for both schemes become extremely high. The minimal spatial resolution for description of the wave is 400 nodes (that is $h = 2.5 \cdot 10^{-5}$). Figure 3 and figure

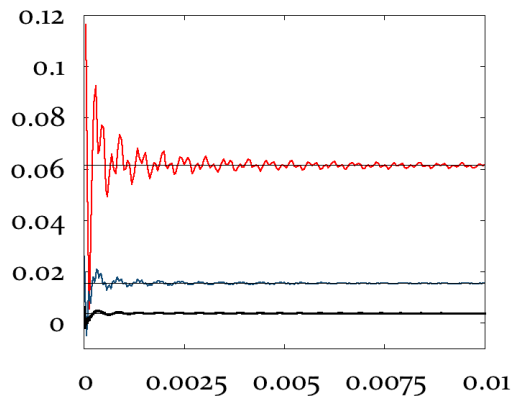


Figure 1. The errors ϵ_{num_1} and ϵ_{theor_1} for different step values, $k=10$.

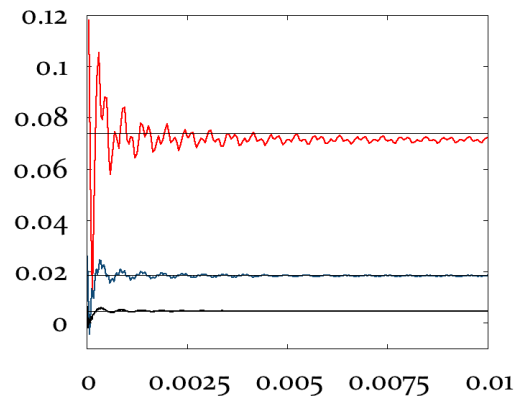


Figure 2. The errors ϵ_{num_2} and ϵ_{theor_2} for different step values, $k=10$.

4 demonstrate the numerical and theoretical error behaviour for $k = 100$ and $\tau/h = 0.4$ for the explicit and implicit schemes correspondingly. The red lines denote $h = 5 \cdot 10^{-5}$, the blue lines denote $h = 1.25 \cdot 10^{-5}$, the black lines denote $h = 6.25 \cdot 10^{-6}$. The second order of accuracy leads to the error decrease with the spatial step refinement. The differences between the two schemes are also low.

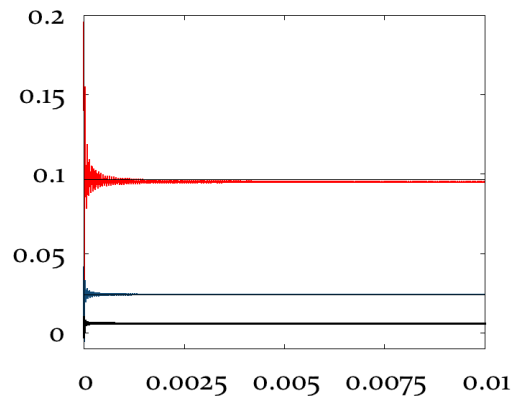


Figure 3. The errors ϵ_{num_1} and ϵ_{theor_1} for different step values, $k=100$.

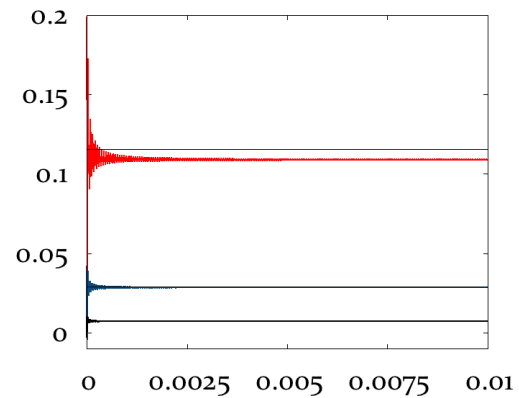


Figure 4. The errors ϵ_{num_2} and ϵ_{theor_2} for different step values, $k=100$.

Figure 5 demonstrates the analytical solution (black line), the numerical solution with the original scheme (blue line), and the solution with the new scheme (red line) after 6400 time steps with $k = 100, h = 6.25 \cdot 10^{-6}, \tau/h = 0.4$. One can see that the numerical solution accumulates the errors, and although the amplitude is precise enough, the numerical results are far away from the analytical solution. However, the numerical solutions obtained with the two schemes coincide the better, the smaller is the spatial step.

The advantage of the implicit scheme is a possibility to perform calculations with $\tau/h > 1$. This fact is demonstrated on figure 6, where the ϵ_{num_2} with $k = 10$ for $h = 2.5 \cdot 10^{-5}, \tau/h = 2$ (red line) $\tau/h = 4$ (black line) are shown.

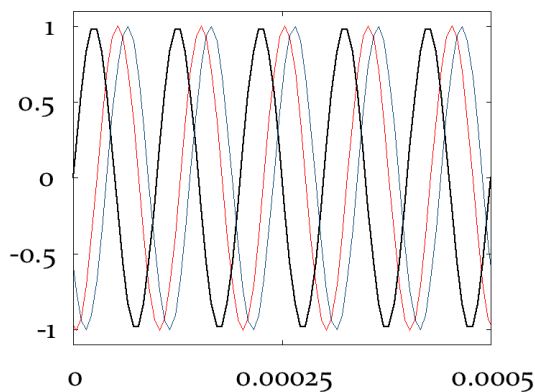


Figure 5. The numerical solutions with considered schemes and the analytical solution, $k=100$.

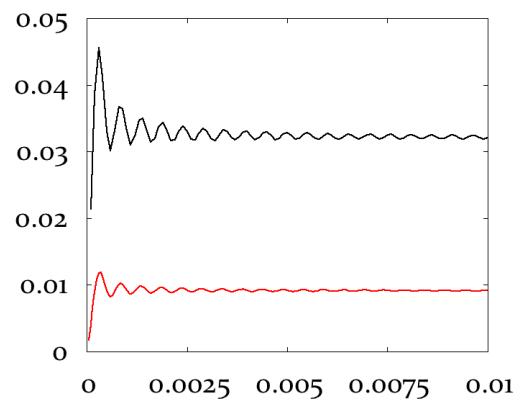


Figure 6. The errors ϵ_{num2} for different Courant numbers, $k=10$.

4. Conclusion

The new scheme for the Maxwell's equations computations in three-dimensional flat domains is presented. The scheme is based on the Langdon-Lasinski scheme. The theoretical and numerical analyses of the new scheme demonstrate the maintenance of the wave amplitude and the propagation speed with the second order of accuracy. The error increases with the increase of the wave number for both schemes, and the spatial step in numerical experiments must be taken appropriately small to describe correctly the high-frequency modes. The difference between the numerical errors of the two schemes is low, but the main advantage of the new scheme is a possibility to use a bigger time step in comparison with the Langdon-Lasinski scheme, which is standard for numerical experiments in plasma physics.

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