

# Implicit scheme for Maxwell equations solution in case of flat 3D domains

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**Abstract.** We present a new finite-difference scheme for Maxwell's equations solution for three-dimensional domains with different scales in different directions. The stability condition of the standard leap-frog scheme requires decreasing of the time-step with decreasing of the minimal spatial step, which depends on the minimal domain size. We overcome the conditional stability by modifying the standard scheme adding implicitness in the direction of the smallest size. The new scheme satisfies the Gauss law for the electric and magnetic fields in the final-differences. The approximation order, the maintenance of the wave amplitude and propagation speed, the invariance of the wave propagation on angle with the coordinate axes are analyzed.

## 1. Introduction

A standard scheme for Maxwell equation solution in plasma physics is the leap-frog scheme. The advantages of the scheme are second order of accuracy, time reversibility, simplicity, however the stability condition is  $c\tau/h < 1$ , where  $h = \min\{hx; hy; hz\}$ ,  $c$  the light speed. In case of flat ultrarelativistic beams in supercolliders the beam sizes ratio  $\sigma_x : \sigma_y : \sigma_z$  may be  $1 : 200 : 60000$ . The high ratio of vertical beam sizes provides higher luminosity, and the purpose of the experiments is to increase the maximum available luminosity. The high relativistic factor requires the domain boundaries to be close to the beam. The three-dimensional problem of ultrarelativistic beam dynamics in supercolliders is complicated [1], and the present effective parallel load-balanced algorithms based on the leap-frog scheme limit the beam sizes ratio to  $\sim 1 : 50 : 500$ . However, the stability condition in case of such flat domains (but not the accuracy condition) requires decreasing of the time-step with decreasing of the minimal spatial step, and decreasing of the number of times-steps in order to achieve a specified time moment [2].

We suggest the new scheme to be implicit in the direction of the smallest beam size and the domain. We present the study of the scheme approximation, convergence, behaviour of the wave amplitude and propagation speed in the calculations using the scheme.

## 2. The scheme study

The leap-frog scheme for Maxwell's equations is defined on the grids, which are shifted by half steps in time and space:

$$\frac{H^{m+1/2} - H^{m-1/2}}{\tau} = -rot_h E^m,$$



$$\frac{E^{m+1} - E^m}{\tau} = j^{m+1/2} + rot_h H^{m+1/2},$$

where

$$rot_h H = \begin{pmatrix} \frac{Hz_{i,k,l-1/2} - Hz_{i,k-1,l-1/2}}{h_y} - \frac{Hy_{i,k-1/2,l} - Hy_{i,k-1/2,l-1}}{h_z} \\ \frac{Hx_{i-1/2,k,l} - Hx_{i-1/2,k,l-1}}{h_z} - \frac{Hz_{i,k,l-1/2} - Hz_{i-1,k,l-1/2}}{h_x} \\ \frac{Hy_{i,k-1/2,l} - Hy_{i-1,k-1/2,l}}{h_x} - \frac{Hx_{i-1/2,k,l} - Hx_{i-1/2,k-1,l}}{h_y} \end{pmatrix},$$

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

The scheme provides the second order of accuracy in space and time because of the “central” differences. Let us consider a component of an electric field in a system without currents:

$$\frac{Ex_{i,l-1/2,k-1/2}^{m+1} - Ex_{i,l-1/2,k-1/2}^m}{\tau} = \frac{Hz_{i,l,k-1/2}^{m+1/2} - Hz_{i,l-1,k-1/2}^{m+1/2}}{h_y} - \frac{Hy_{i,l-1/2,k}^{m+1/2} - Hy_{i,l-1/2,k-1}^{m+1/2}}{h_z}$$

The magnetic field components we can exclude subtracting the values on the previous time step:

$$\frac{Ex_{i,l-1/2,k-1/2}^{m+1} - 2Ex_{i,l-1/2,k-1/2}^m + Ex_{i,l-1/2,k-1/2}^{m-1}}{\tau^2} =$$

$$\frac{Ex_{i+1,l-1/2,k-1/2}^m - 2Ex_{i,l-1/2,k-1/2}^m + Ex_{i-1,l-1/2,k-1/2}^m}{h_x^2} +$$

$$\frac{Ex_{i,l+1/2,k-1/2}^m - 2Ex_{i,l-1/2,k-1/2}^m + Ex_{i,l-3/2,k-1/2}^m}{h_y^2} +$$

$$\frac{Ex_{i,l-1/2,k+1/2}^m - 2Ex_{i,l-1/2,k-1/2}^m + Ex_{i,l-1/2,k-3/2}^m}{h_z^2}$$

The equation is hyperbolic, and looks similar for any other component of the electric and magnetic fields. The scheme for the one-dimensional case is following:

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

Let us analyze it. The solution  $y_i^m = \lambda^m e^{i\alpha l}$  provides the following relation:

$$\lambda - 2 - \frac{1}{\lambda} = \frac{\tau^2}{h^2} (e^{i\alpha} - 2 + e^{-i\alpha})$$

and the roots:

$$\lambda = 1 - 2\frac{\tau^2}{h^2} \sin^2 \frac{\alpha}{2} \pm 2\frac{\tau}{h} \sin \frac{\alpha}{2} \sqrt{\frac{\tau^2}{h^2} \sin^2 \frac{\alpha}{2} - 1}$$

The production of the roots is 1, and if the roots are real and different, then the absolute value of one root is greater than 1, and the scheme is unstable. If the roots are complex, then the absolute values of the both roots are equal to 1, what means the maintenance of the wave amplitude and the stability of the scheme. Hence, the stability condition is following:

$$\frac{\tau^2}{h^2} \sin^2 \frac{\alpha}{2} \leq \frac{\tau^2}{h^2} \leq 1 \quad (1)$$

Considering the solution as  $y_i^m = A \exp(-i(\omega t m - k l h))$  we obtain the dispersion relation:

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

and, using the Taylor series for  $\tau$  and  $h$  for

$$\omega = \frac{2}{\tau} \arcsin \left( \frac{\tau}{h} \sin \frac{k h}{2} \right),$$

we obtain the relation for the speed of the wave propagation:

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

This implies, that if the stability criterion (1) is satisfied, the speed of the wave propagation is smaller than the speed of the light. The speed decreases with the increasing of the wavenumber  $k$ . The maximum value of the wavenumber for the domain length  $L$  depends on the number of the grid nodes  $n$  for the wave description, thus  $k_{max} = 2\pi n/L = 2\pi/h$ , and the speed of the wave propagation can be negative when  $1 + 4\pi^2(\tau^2 - h^2)/24h^2 < 0$ , that is when  $\tau^2/h^2 < 1 - 6/\pi^2 \sim 0.4$ . So the leap-frog scheme has the restrictions for the steps usage for the short-wave modes.

We add the values from  $m + 1$  time step to the right hand side in order to increase the scheme stability. Having a need to keep the symmetry of the scheme in time we suggest the following scheme:

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

where

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

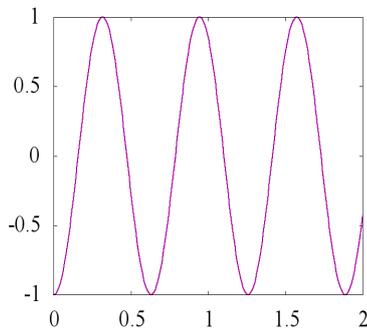
and  $0 \leq \delta \leq 1/2$ . For  $\delta = 0$  we obtain the original leap-frog scheme. Making similar deductions we analyze the scheme. The corresponding equation for the roots is following:

$$(1 + 4\delta A)\lambda^2 - 2(1 - 2(1 - 2\delta)A)\lambda + 1 + 4\delta A = 0,$$

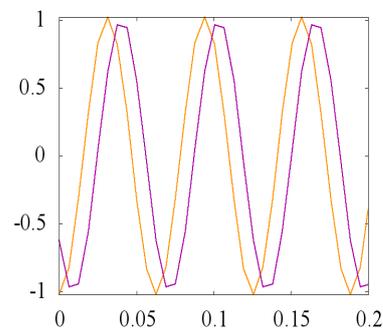
where  $A = \frac{\tau^2}{h^2} \sin^2 \frac{\alpha}{2}$ . The stability condition turns to the condition of the negativity of the discriminant  $(1 - 2(1 - 2\delta)A)^2 - (1 + 4\delta A)$ , that is  $\delta \geq 1/4$ . Hence, for  $\delta = 1/4$  the scheme is absolutely stable [3] and maintains the wave amplitude. Similarly to the previous case, the dispersion relation provides the results for the propagation speed:

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

and the speed of the wave propagation depends on the wavenumber  $k$ , the oscillations with a high wavenumber may have negative propagation speed for a certain ratio of the spatial and the time steps. For example, for  $\delta = 1/4$   $k = k_{max}$  with  $\tau^2/h^2 < (\pi^2 - 6)/4\pi^2 \sim 0.09$  the waves travel in the opposite direction. Note, that the optimal step ration for the scheme is  $\tau/h = 1$ , for the implicit scheme the optimal ratio is  $\tau/h = 0.5$ , in this case the approximation order arises. The fig. 1 demonstrates the solution for  $k = 10$ . The graphs for both schemes coincide, as the wavenumber is not high. The fig. 2 demonstrates the solutions for  $k = 100$ , the difference in the wave speeds is the result of the difference  $k^2\tau^2/8$  between the two schemes.



**Figure 1.** Figure caption for first of two sided figures.



**Figure 2.** Figure caption for second of two sided figures.

So, both schemes change the propagation speed in cases of high wavenumbers. But the implicit scheme allows using a big time step in the calculations.

Let us use the following scheme for the three-dimensional case:

$$\frac{Ex_{i,l,k}^{m+1} - 2Ex_{i,l,k}^m + Ex_{i,l,k}^{m-1}}{\tau^2} = \delta\Delta_{xx}Ex_{i,l,k}^{m+1} + (1 - 2\delta)\Delta_{xx}Ex_{i,l,k}^m + \delta\Delta_{xx}Ex_{i,l,k}^{m-1} + \delta\Delta_{yy}Ex_{i,l,k}^m + \delta\Delta_{zz}Ex_{i,l,k}^m.$$

Taking the solution as  $Ex_{j,l,k}^m = \lambda^m \exp(i(\alpha j + \beta l + \gamma k))$ , we obtain, that contrary to the stability condition of the explicit scheme  $\tau^2/h_x^2 + \tau^2/h_y^2 + \tau^2/h_z^2 \leq 1$  the stability condition of the scheme with implicitness does not depend on  $h_x$ :  $\tau^2/h_y^2 + \tau^2/h_z^2 \leq 1$ .

The analysis above was made only for one component of the electric field. However, the similar results can be obtains for any other components.

So, the final three-dimensional scheme is following:

$$\frac{Hx^{m+1/2} - Hx^{m-1/2}}{\tau} = \Delta_z Ey^m - \Delta_y Ez^m$$

$$\frac{Hy^{m+1/2} - 2Hy^{m-1/2} + Hy^{m-3/2}}{\tau^2} = \Delta_{yy} Hy^{m-1/2} + \Delta_{zz} Hy^{m-1/2} + \frac{1}{4}\Delta_{xx} Hy^{m+1/2} + \frac{1}{2}\Delta_{xx} Hy^{m-1/2} + \frac{1}{4}\Delta_{xx} Hy^{m-3/2}$$

$$\frac{Hz^{m+1/2} - 2Hz^{m-1/2} + Hz^{m-3/2}}{\tau^2} = \Delta_{yy} Hz^{m-1/2} + \Delta_{zz} Hz^{m-1/2} + \frac{1}{4}\Delta_{xx} Hz^{m+1/2} + \frac{1}{2}\Delta_{xx} Hz^{m-1/2} + \frac{1}{4}\Delta_{xx} Hz^{m-3/2}$$

$$\frac{Ex^{m+1} - Ex^m}{\tau} = \Delta_y Hz^{m+1/2} - \Delta_z Hy^{m+1/2}$$

$$\frac{Ey^{m+1} - Ey^m}{\tau} = \Delta_z Hx^{m+1/2} - \Delta_x Hz^{m+1/2}$$

$$\frac{Ez^{m+1} - Ez^m}{\tau} = \Delta_x Hy^{m+1/2} - \Delta_y Hx^{m+1/2}$$

The Gauss laws in finite differences are following:

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

for  $divH = 0$  and

$$\Delta_x Ex^m + \Delta_y Ey^m + \Delta_z Ez^m = 4\pi\rho^m$$

for  $divE = 4\pi\rho$ .

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### 3. Conclusion

A new scheme for solution of Maxwell equations in flat 3D domains is presented. The scheme is based on the standard leap-frog scheme and is implicit in the direction of the smallest domain size. The approximation order and the stability of the scheme in one-dimensional and three-dimensional cases are analyzed. The study of the wave propagation in different directions demonstrated that the both schemes are non-invariant on the angle with the coordinate axes. It is shown, that the scheme maintains the amplitude of the wave and maintains the wave propagation speed with the second order in space and time. The difference between the two schemes results are insignificant, however the new scheme allows using bigger time step in order to decrease of the calculations time.

## References

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