Fourth-order Jameson–Schmidt–Turkel FDTD scheme for non-magnetised cold plasma

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A fourth-order finite-difference time-domain (FDTD) scheme is proposed for the solution of Maxwell's equations in cold plasma (Drude medium), based on the multistage method of Jameson, Schmidt and Turkel, which was originally introduced in the framework of fluid dynamics. First, the system of governing differential equations is formed as a general first-order, operator-based approach, and then a four-stage algorithm is established. The accuracy of the method is verified in benchmark problems compared with analytical solutions and with the conventional second-order FDTD algorithm.

Introduction: Computational electromagnetics (CEM) has evolved into an indispensable tool for the modelling of devices and structures spanning from microwave to optical frequencies. The finite-difference time-domain (FDTD) method is considered as a versatile and robust method in CEM due to its simplicity and efficiency [1, 2]. The conventional FDTD method is a non-dissipative scheme with second-order accuracy both in space and time, which inevitably leads to accumulated numerical dispersion errors, especially in long-time simulations and/or large computational domains.

In this context, high-order (HO) FDTD techniques constitute promising alternatives to the second-order FDTD method, as they are more accurate thanks to the reduced grid anisotropy and dispersion errors [1, 3, 4]. The HO methods were initially proposed for simple dielectrics with constant electric permittivity and magnetic susceptibility (non-dispersive media) varying only in space. Subsequently, HO techniques were extended to account for complex materials, including dispersive media with frequency-dependent constitutive parameters. For instance, HO schemes have been proposed for the modelling of lossy [5, 6] and dispersive media [7–11] and, recently, for the study of non-linear optical media [12] and metamaterials [13].

Runge–Kutta (RK) schemes are a family of multistage numerical techniques, which are widely used for the solution of differential equations in various fields. Although RK methods provide high accuracy, they involve large computational effort and increased memory requirements. To overcome such problems, Jameson, Schmidt and Turkel (JST) introduced back in 1981 a more efficient scheme with fewer intermediate variables and reduced computations per time step. This original JST scheme was proposed for the study of aerodynamical problems and computational fluid dynamics. Recently, its application has been extended to Maxwell's equations in non-dispersive media [14].

In this work, we apply the JST methodology in a fourth-order HO-FDTD scheme for dispersive media, namely cold plasma described by the Drude model. We formulate the governing equations in the medium as a system of first-order differential equations and we propose a novel numerical scheme based on the JST algorithm while preserving the fourth-order accuracy of the corresponding RK scheme. The spatial derivatives are evaluated using central fourth-order approximations except for the boundaries where one-sided approximations are utilised. Initially, we demonstrate the fourth-order convergence rate of the proposed technique in a resonating cavity problem. In addition, the accuracy of the proposed scheme with respect to the standard second-order FDTD method is investigated in the case of broadband wave propagation in Drude media. A direct comparison with the analytical solution reveals its superiority, which is significantly more pronounced at high frequencies or long propagation distances.

Formulation: The governing field equations in non-magnetised cold plasma (Drude medium) in the absence of sources are

$$\nabla\times\boldsymbol{E} = -\mu_0\frac{\partial \boldsymbol{H}}{\partial t} \tag{1a}$$

$$\nabla\times\boldsymbol{H} = \varepsilon_\infty\varepsilon_0\frac{\partial \boldsymbol{E}}{\partial t} + \boldsymbol{J} \tag{1b}$$

$$\frac{\partial \boldsymbol{J}}{\partial t} + \gamma\boldsymbol{J} = \varepsilon_0\omega_p^2\boldsymbol{E}, \tag{1c}$$

where ω_p is the plasma frequency, γ is the electron-neutral collision frequency and ε_∞ the relative permittivity at infinite frequency. The relative electric permittivity of the medium is described by

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{j\omega\gamma - \omega^2}. \tag{2}$$

The governing equations (1a–c) can be recast as the following general first-order system:

$$\frac{\partial \boldsymbol{U}}{\partial t} = \mathcal{L}(\boldsymbol{U}), \quad \text{with } \boldsymbol{U} = \begin{pmatrix}\boldsymbol{E}\\ \boldsymbol{H}\\ \boldsymbol{J}\end{pmatrix}, \tag{3}$$

where $\mathcal{L}$ represents the operator

$$\mathcal{L} = \begin{pmatrix} 0 & \dfrac{1}{\varepsilon_0\varepsilon_\infty}\nabla\times & -\dfrac{1}{\varepsilon_0\varepsilon_\infty} \\ -\dfrac{1}{\mu_0}\nabla\times & 0 & 0 \\ \varepsilon_0\omega_p^2 & 0 & -\gamma \end{pmatrix}. \tag{4}$$

The system of (3) can be solved using the classical explicit fourth-order RK method (RK4) as follows:

$$\boldsymbol{U}^{(1)} = \boldsymbol{U}^n + \frac{\Delta t}{2}\mathcal{L}(\boldsymbol{U}^n) \tag{5}$$

$$\boldsymbol{U}^{(2)} = \boldsymbol{U}^n + \frac{\Delta t}{2}\mathcal{L}(\boldsymbol{U}^{(1)}) \tag{6}$$

$$\boldsymbol{U}^{(3)} = \boldsymbol{U}^n + \Delta t\mathcal{L}(\boldsymbol{U}^{(2)}) \tag{7}$$

$$\boldsymbol{U}^{n+1} = \frac{1}{3}(-\boldsymbol{U}^n + \boldsymbol{U}^{(1)} + 2\boldsymbol{U}^{(2)} + \boldsymbol{U}^{(3)}) + \frac{\Delta t}{6}\mathcal{L}(\boldsymbol{U}^{(3)}), \tag{8}$$

which features fourth-order accuracy in both linear and non-linear problems. In the case of linear problems, the more efficient JST scheme can be applied

$$\boldsymbol{U}^{(1)} = \boldsymbol{U}^n + \frac{\Delta t}{4}\mathcal{L}(\boldsymbol{U}^n) \tag{9a}$$

$$\boldsymbol{U}^{(2)} = \boldsymbol{U}^n + \frac{\Delta t}{3}\mathcal{L}(\boldsymbol{U}^{(1)}) \tag{9b}$$

$$\boldsymbol{U}^{(3)} = \boldsymbol{U}^n + \frac{\Delta t}{2}\mathcal{L}(\boldsymbol{U}^{(2)}) \tag{9c}$$

$$\boldsymbol{U}^{n+1} = \boldsymbol{U}^n + \Delta t\mathcal{L}(\boldsymbol{U}^{(3)}). \tag{9d}$$

This scheme eliminates the need to store the intermediate variables. The update equations of E_x, H_y and J_x for the first stage of the algorithm are given by

$$E_x^{(1)} = E_x^n + \frac{\Delta t}{4\varepsilon_0\varepsilon_\infty}\left(\frac{\delta_y H_z^n}{\Delta y} - \frac{\delta_z H_y^n}{\Delta z} - J_x^n\right) \tag{10}$$

$$H_y^{(1)} = H_y^n + \frac{\Delta t}{4\mu_0}\left(\frac{\delta_x E_z^n}{\Delta x} - \frac{\delta_z E_x^n}{\Delta z}\right) \tag{11}$$

$$J_x^{(1)} = J_x^n + \frac{\Delta t}{4}\left(\varepsilon_0\omega_p^2 E_x^n - \gamma J_x^n\right). \tag{12}$$

The remaining update equations can be found in a similar fashion. The spatial derivatives $\partial/\partial\beta$, with $\beta = x, y, z$, are invoked by the central, fourth-order spatial operator

$$\frac{\delta_\beta f_i}{\Delta\beta} = \frac{1}{24\Delta\beta}\left(f_{i-3/2} - 27f_{i-1/2} + 27f_{i+1/2} - f_{i+3/2}\right), \tag{13}$$

where the index i corresponds to the spatial variable β and the coefficients are calculated by an analytical expression [8]. It is noted that the fields are staggered according to the Yee scheme in space, but not in time.

One-sided approximations of the derivatives are employed at the boundaries of the computational domain [3]. Assuming that the computational domain is terminated with the electric field, the spatial derivative of the magnetic field at the first grid point next to the boundary is approximated by

$$\delta_\beta H_{\beta,1} = \frac{1}{24}(-23H_{\beta,1/2} + 21H_{\beta,3/2} + 3H_{\beta,5/2} - H_{\beta,7/2}), \quad (14)$$

while the derivative of the electric field half cell next to the boundary is approximated by

$$\delta_\beta E_{\beta,1/2} = \frac{1}{24}(-22E_{\beta,0} + 17E_{\beta,1} + 9E_{\beta,2} - 5E_{\beta,3} + E_{\beta,4}). \quad (15)$$

The above derivative approximations are third- and fourth-order, respectively and were obtained using Taylor expansions.

Numerical results and discussion: To check the accuracy of the proposed technique, we present a number of benchmark simulations using the proposed formulation in comparison with the second-order technique [15], namely the FDTD(2,2) scheme, and analytical solutions. As a first example, we consider the case of modes resonating in a one-dimensional cavity composed of a Drude medium, whose electric field is given by

$$E_x(z,t) = E_0 \sin\left(\pi m \frac{z}{L}\right) e^{s_m t}, \quad (16)$$

where L is the length of the cavity, m the mode order, corresponding to the integer number of half-wavelengths in the cavity, and s_m is a complex number to be determined. The partial differential equation yielding the electric field in the cavity is

$$\frac{1}{\mu_0}\frac{\partial^3 E_x}{\partial z^2 \partial t} - \varepsilon_0\varepsilon_\infty \frac{\partial^3 E_x}{\partial t^3} + \frac{\gamma}{\mu_0}\frac{\partial^2 E_x}{\partial z^2} - \varepsilon_0\varepsilon_\infty \gamma \frac{\partial^2 E_x}{\partial t^2} - \varepsilon_0 \omega_p^2 \frac{\partial E_x}{\partial t} = 0. \quad (17)$$

By substituting the solution for E_x of (16) in (17), the following dispersion relation is obtained:

$$s_m^3 + \gamma s_m^2 + \left[c_\infty^2\left(\frac{\pi m}{L}\right)^2 + \frac{\omega_p^2}{\varepsilon_\infty}\right] s_m + \gamma c_\infty^2 \left(\frac{\pi m}{L}\right)^2 = 0, \quad (18)$$

where $c_\infty = 1/\sqrt{\mu_0 \varepsilon_0 \varepsilon_\infty}$. Our goal is to demonstrate the convergence rate of the accuracy of the proposed scheme with respect to the analytical solution. For simplicity, we set $\mu_0 = 1$ and $\varepsilon_0 = 1$. The parameters of the Drude medium are selected as $\varepsilon_\infty = 1$, $\omega_p = 3$ and $\gamma = 10$. In the numerical computations we use the initial conditions for the fields E_x, H_y and J_x as functions of z obtained from the analytical solutions at zero time, taking into account that the magnetic field is staggered in space. We also choose $L = 2\pi$, $m = 10$ and run simulations for $t = 20$ with a varying spatial discretisation step Δz and a corresponding time step $\Delta t = 0.4\Delta z$. We calculate the L_2 error norm defined as

$$L_2 = \sqrt{\Delta t \Delta z \sum_n \sum_i (e_i^n)^2} \quad (19)$$

where e_i^n is the difference of the numerical solution from the exact one at the nth time step and at position $i\Delta z$ in space. Fig. 1*a* illustrates the electric field in the cavity at time $t = 20$ for grid size $\Delta z = L/(N_z - 1)$ with $N_z = 101$. It is observed that the solution of the proposed scheme, namely the (4,4) method, almost perfectly overlaps with the analytical one, whereas the (2,2) method leads to an evident deviation. The fourth-order accuracy of the proposed method in comparison to its second-order counterpart is demonstrated in Fig. 1*b* by calculating the L_2 error as a function of the spatial discretisation step.

We next investigate a wave propagation problem inside a Drude medium. A hard source is imposed at the left boundary of the computational domain in each stage of the scheme to simulate a plane wave propagating along the positive z-direction. The source is a modulated Gaussian source with spectral content in the region 5–100 GHz. The total simulation time is properly chosen before the wave reaches the right boundary. The parameters of the Drude medium are $\varepsilon_\infty = 1$, $\omega_p = 2\pi 30 \times 10^9$ rad/s and $\gamma = 0.1\,\omega_p$. The cell size is $\Delta z = 0.1$ mm and the selected time step is $\Delta t = 0.13342$ ps. The electric field is recorded at a distance 1 m away from the source, which corresponds to 333 wavelengths of the smallest excited wavelength. The analytical solution in the frequency domain of a wave propagating in a dispersive medium along the $+z$-direction is $E(\omega, z) = E_0 e^{-z(a+jb)}$, with

$$a = -\frac{\omega}{c_0}\Im m\{\sqrt{\varepsilon(\omega)}\}, \quad b = \frac{\omega}{c_0}\Re e\{\sqrt{\varepsilon(\omega)}\}, \quad (20)$$

where c_0 is the velocity of light in vacuum. The time-domain solution of the proposed and reference FDTD schemes with respect to the exact solution is presented in Fig. 2. It is observed that the (4,4) scheme shows a significantly inferior numerical dispersion error.

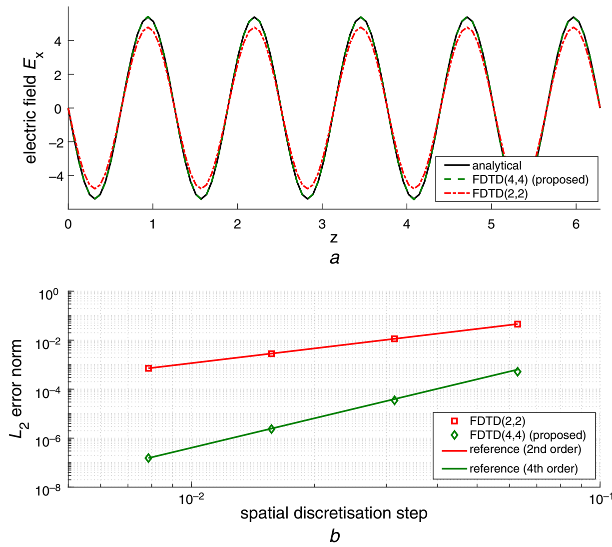

Fig. 1 *Electric fields and convergence rates*

a Electric field in the investigated cavity computed using the proposed (4,4) and the conventional (2,2) FDTD method versus analytical solution
b Convergence rate for the proposed and the reference method for various grid sizes demonstrating an accuracy of fourth and second order, respectively

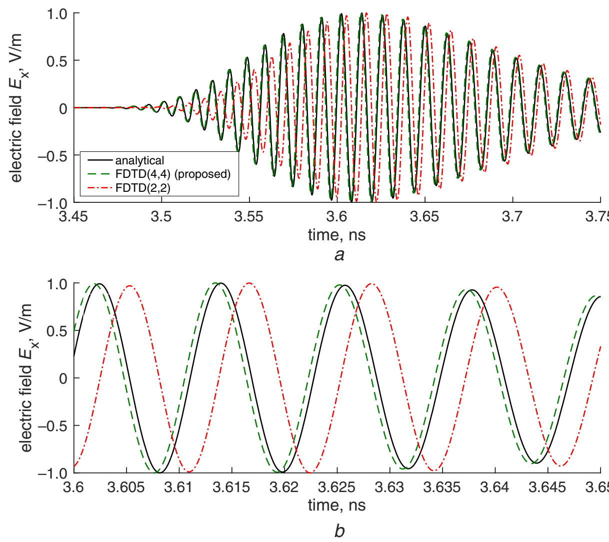

Fig. 2 *Electric fields*

a Time-domain solution of the E_x component of a wave propagating in a Drude medium computed using the reference (2,2) and the proposed (4,4) FDTD method with respect to the analytical solution
b A zoomed part of the signals from 3.6 to 3.65 ns

Last, we consider the previous problem with a cell size $\Delta z = 0.2$ mm and $\Delta t = 0.4\Delta z/c_0$ and record the electric field at two positions separated by a distance d. A transfer function T is calculated by dividing the Fourier-transformed spectra of the recorded signals $T(\omega, d) = E(\omega, z_0 + d)/E(\omega, z_0)$, where z_0 is a reference point in space. The transfer function is obtained also analytically as $T(\omega, d) = e^{-d(a+jb)}$, where a and b are defined in (20). The parameters z_0 and d are chosen as $z_0 = 0.2$ m and $d = 0.3$ m. Fig. 3*a* shows the real part of the transfer function in the spectral region from 40 to 90 GHz, as provided by the analytical solution and calculated by the proposed (4,4) and the reference (2,2) FDTD method. It is observed that both numerical methods provide similar results at low frequencies but the solution of the second-order scheme deviates at high frequencies. This discrepancy is clearly demonstrated in Fig. 3*b*, which focuses on the high frequency part of the considered spectrum.

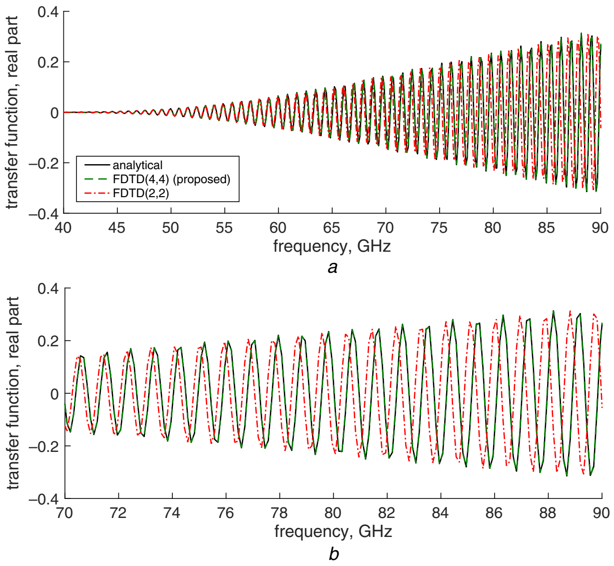

Fig. 3 *Real part of transfer function*

a Real part of the transfer function calculated by the analytical, the proposed and the conventional second-order FDTD scheme as a function of frequency
b A zoomed part in the spectral region from 70 to 90 GHz

Conclusion: An accurate fourth-order FDTD scheme for the study of wave propagation in cold plasma is introduced. The proposed method belongs to the multi-stage techniques, thus avoiding the use of previous time steps of the fields while simultaneously reducing the intermediate variables when compared to the classical fourth-order RK scheme. The accuracy and robustness of the proposed technique, especially at high frequencies, long-distance and/or prolonged time simulations, is verified in a series of examples benchmarked against analytical solutions and the standard second-order FDTD method.

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One or more of the Figures in this Letter are available in colour online.

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References

1 Taflove, A.: 'Advances in computational electrodynamics: the finite-difference time-domain method' (Artech House, Norwood, MA, USA, 1998)
2 Prokopidis, K.P., and Zografopoulos, D.C.: 'A unified FDTD/PML scheme based on critical points for accurate studies of plasmonic structures', *J. Lightwave Technol.*, 2013, **31**, (15), pp. 2467–2476
3 Yefet, A., and Petropoulos, P.G.: 'A staggered fourth-order accurate explicit finite difference scheme for the time-domain Maxwell's equations', *J. Comput. Phys.*, 2001, **168**, (2), pp. 286–315
4 Hesthaven, J.S.: 'High-order accurate methods in time-domain computational electromagnetics: a review', *Adv. Imag. Elect. Phys.*, 2003, **127**, (1), pp. 59–123
5 Prokopidis, K.P., and Tsiboukis, T.D.: 'Higher-order FDTD(2,4) scheme for accurate simulations in lossy dielectrics', *Electron. Lett.*, 2003, **39**, (11), pp. 835–836
6 Zygiridis, T.T., and Tsiboukis, T.D.: 'Improved finite-difference time-domain algorithm based on error control for lossy materials', *IEEE Trans. Microw Theory Techn.*, 2008, **56**, (6), pp. 1440–1445
7 Young, J.L.: 'A higher order FDTD method for EM propagation in a collisionless cold plasma', *IEEE Trans. Antennas Propagat*, 1996, **44**, (9), pp. 1283–1289
8 Prokopidis, K.P., Kosmidou, E.P., and Tsiboukis, T.D.: 'An FDTD algorithm for wave propagation in dispersive media using higher-order schemes', *J. Electromagnet. Wave*, 2004, **18**, (9), pp. 1171–1194
9 Bokil, V.A., and Gibson, N.L.: 'Analysis of spatial high-order finite difference methods for Maxwell's equations in dispersive media', *IMA J. Numer. Anal.*, 2012, **32**, (3), pp. 926–956
10 Jenkinson, M.J., and Banks, J.W.: 'High-order accurate FDTD schemes for dispersive Maxwell's equations in second-order form using recursive convolutions', *J. Comput. Appl. Math.*, 2018, **336**, pp. 192–218
11 Angel, J.B., Banks, J.W., Henshaw, W.D., *et al.*: 'A high-order accurate scheme for Maxwell's equations with a generalized dispersive material model', *J. Comput. Phys.*, 2019, **378**, pp. 411–444
12 Bokil, V.A., Cheng, Y., Jiang, Y., *et al.*: 'High spatial order energy stable FDTD methods for Maxwell's equations in nonlinear optical media in one dimension', *J. Sci. Comput.*, 2018, **77**, (1), pp. 330–371
13 Sakkaplangkul, P., Bokil, V.A., and Carvalho, C.: 'A fully fourth order accurate energy stable finite difference method for Maxwell's equations in metamaterials', *IEEE J. Multiscale Multiphys. Comput. Tech.*, 2019, **4**, pp. 260–268
14 Fathy, A., Wang, C., Wilson, J., *et al.*: 'A fourth order difference scheme for Maxwell equations on Yee grid', *J. Hyperbolic Differ. Equ.*, 2008, **5**, (3), pp. 613–642
15 Joseph, R.M., Hagness, S.C., and Taflove, A.: 'Direct time integration of Maxwell's equations in linear dispersive media with absorption for scattering and propagation of femtosecond electromagnetic pulses', *Opt. Lett.*, 1991, **16**, (18), pp. 1412–1414