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Atlantis Transactions in Geometry

Johan Gielis
Paolo Emilio Ricci
Ilia Tavkhelidze
Editors

Modeling in Mathematics

Proceedings of the Second Tbilisi-Salerno Workshop on Modeling in Mathematics

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Volume 2

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Introduction

The second volume of the Atlantis Transactions in Geometry series is a collection of papers presented at the Second Tbilisi-Salerno Workshop on Modeling in Mathematics (Tbilisi, March 16–18, 2015). This workshop resulted from a close and long standing cooperation between the Iv. Javakhishvili Tbilisi State University and the University of Salerno. The organizing committee consisted of A. Di Nola, R. Grigolia, R. Botschorishvili, J. Gielis, R. Koplatadze, T. Tadumadze, I. Tavkhelidze, M. Transirico, T. Chelidze, and R. Liparteliani. The event was cosponsored by both universities, two grants of the Shota Rustaveli National Science Foundation and the Georgian International Society of Cardiomyopathy (Georgia), The University of Antwerp, and The Simon Stevin Institute of Geometry (Belgium).

In this volume the core is on geometric modeling, expressed in geometrical, logical or analytical language, or even a combination of Boolean logic and geometry. Various chapters have a direct connection to natural phenomena, including the modeling of electromagnetic pulse propagation in biological tissues, Multi Modal Epistemic Lukasiewicz logic in immune systems, fusion in flowers, and evolution equations. Other chapters provide fundamental methods describing natural shapes and phenomena, which are fully geometric or have a close connection to geometrical or operational methods. The chapters are written in styles and language that should be accessible for a very wide audience with a geometric focus.

Gauss already stressed that the "*Geometric method will be indispensable in the early study of young people, to prevent one-sidedness and to give to the understanding a lineliness and directness, which is much less developed and—occasionally—rather jeopardized by the analytical method*". During this workshop, for his many great contributions to geometry and mathematics, the second Simon Stevin Prize for Geometry was awarded to Prof. Paolo Emilio Ricci for his fundamental contributions to mathematics in many fields, including mathematical physics, orthogonal polynomials, special functions, numerical analysis, approximation theory, and geometry. His contributions in any of these fields are fundamental, with new concepts, new methods, and new discoveries [1]. Special mention is made of his open and very inspiring style of cooperation and collaboration with colleagues worldwide, of which his coauthorship in many chapters in this volume is proof of this.

At the end of the twentieth century André Weil [2] wrote: "*Whatever the truth of the matter, mathematics in our century would not have made such impressive progress without the geometric sense of Elie Cartan, Heinz Hopf, Chern and a very few more. It seems safe to predict that such men will always be needed if mathematics is to go on as before*". It is safe to add Prof. Paolo Emilio Ricci to Weil's list of eminent geometers, to which also Prof. Bang-Yen Chen belongs as the first recipient of the Simon Stevin Prize for Geometry [3]. Simon Stevin himself was a major figure in such lists [4].

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Fractional–Calculus–Based FDTD Algorithm for Ultra–Wideband Electromagnetic Pulse Propagation in Complex Layered Havriliak–Negami Media

Diego Caratelli, Luciano Mescia and Pietro Bia

Abstract A novel finite–difference time–domain algorithm for modeling ultra–wideband electromagnetic pulse propagation in layered multi–relaxed Havriliak–Negami media is presented. The proposed scheme is based on a general, yet computationally efficient, series representation of the fractional derivative operator associated with the permittivity function describing the frequency dispersion properties of the dielectric material. Dedicated uniaxial perfectly matched layer boundary conditions are derived and implemented in combination with the basic time–marching scheme. Moreover, a total field/scattered field formulation is adopted in order to analyze the material response under plane–wave excitation. Compared to alternative numerical methodologies available in the scientific literature, the proposed technique features a significantly enhanced robustness and accuracy which are essential for solving complex electromagnetic propagation problems typically encountered in bio–engineering applications.

1 Introduction

During the last decade, pulsed electric fields (*PEFs*) have been playing a key role in a number of new research activities in bioelectrics, a new interdisciplinary field which combine knowledge of electromagnetic principles and theory, modeling and

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simulations, physics, material science, cell biology, and medicine. The main goal of this discipline is the study of the interaction between electromagnetic fields and biological tissues aimed at the investigation of nanopulse bioeffects for human safety as well as for at use of ultrashort pulses in biomedical and biotechnological applications [1–5].

Current applications of *PEF* are primarily based on reversible or irreversible electroporation, that is the process by which the permeability to drugs, molecules, and genetic material of the plasma membrane of a biological cell is affected. This phenomenon can result either permanent permeabilization of cancer cells or the destabilization of the cell membranes and intracellular components useful to trigger cellular mechanism leading to cellular death [6–8]. As a result, electroporation based therapies and treatments can be used to achieve selective killing of cancer cells, tissue ablation, gene therapy and *DNA* based vaccination. In particular, in the cancer therapy *PEFs* have been defined for the treatment of easily accessible cutaneous and subcutaneous tumor nodules, prostate cancer, fibrosarcoma. This approach has demonstrated remarkable potential for the treatment of solid tumors without hyperthermia or delivering drugs or genes [3–5, 9]. Other therapeutic applications include coronary and peripheral vascular disease, activating platelets, plasmids transfection, immune responses enhancement, tissue imaging [3]. Moreover, the application of this new technology could have a great impact on molecular biology, by promoting the understanding of molecular mechanisms of cells.

The efficiency of *PEF* treatment depends on the electric field distribution within the treated tissue. In fact, the cellular death mechanism is strongly affected by pulse parameters such as amplitude, duration, number of pulses and repetition frequency. However, *PEF* exposure could result in side effects such as tissue damage, conformational changes in macromolecules, alteration of the biochemical reaction rates, membrane characteristics and temperature levels [10]. Therefore, in order to predict the effect of exposures and assess possible outcomes it is very important to know the local electric field distribution inside the exposed tissue. In many applicative cases, the electromagnetic field cannot be easily measured. To this aim, theoretical models are invaluable tools to better understand the involved mechanisms as well as to evaluate and optimize treatment modalities and to develop disease–specific or even patient–specific protocols.

The electric field distribution excited in biological media mainly depends on the electric properties of tissues. But the lack of data and accurate models, over broad frequency ranges, has been so far an obstacle for both theoretical and experimental studies. In fact, the complexity of the structure and composition of biological matter produces anomalies in the dynamic dielectric properties resulting in a strong dispersion of dielectric susceptibility. This dispersion, can be explained by considering that the disordered nature and microstructure of the systems yield a multiple relaxation times. As a result, the time-domain response is generally non–symmetric and markedly different from that of dielectric media modeled by the simple Debye equation. Therefore, it is important to define empirical models for each organ, in a wide frequency range, for studies regarding the interaction between electromagnetic wave and biological bodies, especially for *PEF* excitation.

The dielectric properties of biological tissues result from the interaction of electromagnetic energy with the tissue constituents at the cellular and molecular level. This process is strongly affected by the bound water content. The frequency variation of the dielectric properties of tissues with high water content can be easily described by the Debye relation. This kind of response is obtained for an assembly of identical dipoles yielding a loss of energy proportional to the electric field frequency. However, it is well known that the dielectric properties of many biological materials display α, $-\beta$, $-\gamma$ and $-\delta$ dispersion types attributed to a different polarization mechanism [11]. As a consequence, an accurate representation of the experimental dielectric response in frequency domain usually cannot be described by a simple exponential expression with a single relaxation time (Debye model). To this end, a number of empirical relationships including Cole-Cole (*CC*), Cole-Davidson (*CD*) and Havriliak-Negami (*HN*) equations have been proposed in order to fit such types of dielectric spectra. The Cole–Cole model is generally chosen to describe the relative complex permittivity of many types of biological tissues over wide frequency ranges. However, *HN* representation includes both *CC* and *CD* models and provides an extended model flexibility enabling a better parametrization of the arbitrary dispersive media properties.

The accurate modeling of electromagnetic field propagation in the mentioned dispersive materials is essential for gaining a deeper insight into the physical mechanisms affecting the interaction between pulsed electric fields (*PEFs*) and biological media. Finite–difference time–domain (*FDTD*) method has been widely used in electromagnetic modeling due to its straightforward implementation and ability to model a broad range of exposure conditions [12, 13]. Since *CC*, *CD*, and *HN* dispersion functions include fractional powers of the angular frequency, suitable mathematical models adequately describing the response of such complex dispersive media have to be embedded in the core of the *FDTD* algorithm [14–19].

Recently, a novel *FDTD* methodology for modeling Havriliak–Negami (*HN*) media has been presented by the authors in [1]. Said formulation is based on the optimal truncation of the binomial series related to the *HN* fractional derivative operator, in accordance with the Riemann–Liouville theory. Typically, the aforementioned truncated series approach provides a very good approximation of both real and imaginary parts of *HN* permittivity functions, and numerous test cases discussed in [1, 2] demonstrate that the proposed scheme is reliable and accurate over broad frequency ranges. However, further investigations have highlighted some numerical inaccuracies wherein specific *HN* materials have to be modeled over ultra–wide bands, at angular frequencies $\omega \gg 1/\tau$, τ denoting the characteristic relaxation time of the medium [20, 21]. In order to overcome these limitations, the authors have extended the previously presented *FDTD* scheme by implementing a more general series representation of the *HN* fractional derivative operator in order to account for multiple relaxation times and ohmic losses occurring in the considered biological medium. The enhanced accuracy of the modified *FDTD* procedure has been assessed by several test cases involving complex stratified *HN* media, and compared against a fully analytical modeling approach.

2 Mathematical Formulation

The dielectric properties of biological tissues are determined by the interaction of the electromagnetic energy with the tissue constituents at cellular and molecular level. As a result, the permittivity and electrical conductivity vary from tissue to tissue and depend on the working frequency. In order to accurately model the electromagnetic wave propagation over broad frequency ranges, suitable analytical models of the dielectric properties are needed. In particular, the macroscopic characteristics of general dispersive media can be modeled by using the following multi–relaxation *HN* relationship:

$$\varepsilon_r(\omega) = \varepsilon_{r_\infty} + \sum_{l=1}^{N} \frac{\varepsilon_{r_{s,l}} - \varepsilon_{r_\infty}}{\left[1 + (j\omega\tau_l)^{\alpha_l}\right]^{\beta_l}} - j\frac{\sigma}{\omega\varepsilon_0}, \tag{1}$$

where σ is the static ionic conductivity, ε_{r_∞} is the asymptotic relative permittivity for $\omega\tau \to +\infty$, τ_l and $\varepsilon_{r_{s,l}}$ denote the l–th relaxation time and static relative permittivity (for $\omega\tau \to 0^+$) respectively, and $0 < \alpha_l,\ \beta_l < 1$ are heuristically derived model fitting parameters for $l = 1, 2, \ldots, N$, with N being the maximum number of relaxation processes occurring in the considered media. In (1), as usual, $\omega = 2\pi f$ is the angular frequency, and ε_0 denotes the permittivity of free space.

In the proposed *FDTD* scheme, the following approximated expansion is adopted in place of the truncated binomial series presented in [1]:

$$\underbrace{\left[1 + (j\omega\tau_l)^{\alpha_l}\right]^{\beta_l}}_{F(j\omega)} \simeq \underbrace{\sum_{n=0}^{K_l} \chi_{n,l}\,(j\omega\tau_l)^{\zeta_{n,l}}}_{F^a(j\omega)}, \tag{2}$$

where the parameters $\zeta_{n,l}$ and $\chi_{n,l}$ are assumed to satisfy the inequalities $|\chi_{n,l}| < a$ and $0 < \zeta_{n,l} < b$, with a and b denoting assigned positive real numbers.

Let $K_{\max}$ be the maximum expansion order in (2), and δ be a given small positive threshold to be used for controlling the accuracy of the approximation. In this way, the parameters K_l, $\zeta_{n,l}$, and $\chi_{n,l}$ ($l = 1, 2, \ldots, N$) can be evaluated as follows:

1. Initialize $K_l = 1$, and set the working frequency range $\omega_{\min} < \omega < \omega_{\max}$;
2. Calculate $\chi_{n,l}$ and $\zeta_{n,l}$ by using the Nelder–Mead algorithm [22];
3. Evaluate the relative error function

$$e_r = \sqrt{\frac{\int_{\omega_{\min}}^{\omega_{\max}} |F(j\omega) - F^a(j\omega)|^2 d\omega}{\int_{\omega_{\min}}^{\omega_{\max}} |F(j\omega)|^2 d\omega}}. \tag{3}$$

4. If $e_r \leq \delta$ or $K_l = K_{\max}$, the algorithm stops, else update the expansions orders as $K_l = K_l + 1$, and go to step 2.

The evaluation of the electromagnetic field distribution excited within the multi–layered dielectric material under analysis can be then performed by using the *FDTD* scheme proposed in [1], that has been here further extended in order to take the ohmic losses as well as the multi–relaxation response of the medium into account.

Let us consider a non-magnetic dispersive medium with complex relative permittivity described by (1). Under such assumption, the differential version of the Ampere's law in time domain, within said material, can be written as:

$$\nabla \times \mathbf{H} = \varepsilon_0 \varepsilon_{r_\infty} \partial_t \mathbf{E} + \sigma \mathbf{E} + \sum_{l=1}^{N} \mathbf{J}_l, \tag{4}$$

with ∂_t denoting the partial derivative operator with respect to time, and where the auxiliary displacement current density terms $\mathbf{J}_l$ ($l = 1, 2, \ldots, N$) have been introduced. It is straightforward to find out that the k–th term ($1 \leq k \leq N$) is such to satisfy the equation:

$$\mathrm{D}_t^{\alpha_k, \beta_k} \mathbf{J}_k = \varepsilon_0 \Delta \varepsilon_{r_k} \partial_t \mathbf{E}, \tag{5}$$

involving the fractional derivative operator $\mathrm{D}_t^{\alpha_k, \beta_k} = \mathcal{F}^{-1} \left\{ \left[1 + (j\omega\tau_k)^{\alpha_k} \right]^{\beta_k} \right\} = \left(1 + \tau_k^{\alpha_k} \mathrm{D}_t^{\alpha_k} \right)^{\beta_k}$ as defined in [1]. In (5), for the sake of brevity, the scalar quantities $\Delta\varepsilon_{r_k} = \varepsilon_{r_{s,k}} - \varepsilon_{r_\infty}$ have been used.

Upon substituting (5) in (4), and applying a second–order accurate finite–difference scheme, one readily obtains, at the time instant $t = m\Delta t$:

$$(\nabla \times \mathbf{H})|^m - \frac{\varepsilon_{r_\infty}}{\Delta \varepsilon_{r_k}} \left(\mathrm{D}_t^{\alpha_k, \beta_k} \mathbf{J}_k \right) \Big|^m = \sum_{l=1}^{N} \mathbf{J}_l|^m + \sigma \, \mathbf{E}|^m, \tag{6}$$

where the vector terms appearing on the right–hand side of the equation are evaluated by means of the semi–implicit approximation:

$$\left. \begin{Bmatrix} \mathbf{J}_l \\ \mathbf{E} \end{Bmatrix} \right|^m = \frac{1}{2} \left(\left. \begin{Bmatrix} \mathbf{J}_l \\ \mathbf{E} \end{Bmatrix} \right|^{m-\frac{1}{2}} + \left. \begin{Bmatrix} \mathbf{J}_l \\ \mathbf{E} \end{Bmatrix} \right|^{m+\frac{1}{2}} \right). \tag{7}$$

In a similar way, from Eq. (5) it follows that:

$$\mathbf{E}|^{m+\frac{1}{2}} = \mathbf{E}|^{m-\frac{1}{2}} + \frac{\Delta t}{\varepsilon_0 \Delta \varepsilon_{r_k}} \left(\mathrm{D}_t^{\alpha_k, \beta_k} \mathbf{J}_k \right) \Big|^m, \tag{8}$$

where:

$$\mathrm{D}_t^{\alpha_k, \beta_k} \mathbf{J}_k \simeq \sum_{n=0}^{K_k} \chi_{n,k} \tau_k^{\zeta_{n,k}} \mathrm{D}_t^{\zeta_{n,k}} \mathbf{J}_k, \tag{9}$$

Let $\nu_{n,k}$ be the integer number such that $\nu_{n,k}-1 \leqslant \zeta_{n,k} \leqslant \nu_{n,k}$. So, applying the Riemann–Liouville definition of fractional derivative, the following equation is derived:

$$\mathrm{D}_t^{\zeta_{n,k}} \mathbf{J}_k(t) = \frac{\mathrm{d}^{\nu_{n,k}}}{\mathrm{d}t^{\nu_{n,k}}} \int_0^t \frac{(t-u)^{\nu_{n,k}-\zeta_{n,k}-1}}{\Gamma\left(\nu_{n,k}-\zeta_{n,k}\right)} \mathbf{J}_k(u)\,\mathrm{d}u. \tag{10}$$

By setting:

$$\mathbf{I}_{n,k}(t) = \int_0^t (t-u)^{\nu_{n,k}-\zeta_{n,k}-1}\, \mathbf{J}_k(u)\,\mathrm{d}u, \tag{11}$$

and applying a central finite difference approximation with time step Δt, one can readily obtain, at the general time instant $t = m\Delta t$:

$$\begin{aligned} \mathbf{I}_{n,k}\big|^m &\simeq \sum_{p=0}^{m-1} \mathbf{J}_k|^{m-p-\frac{1}{2}} \int_{p\Delta t}^{(p+1)\Delta t} u^{\nu_{n,k}-\zeta_{n,k}-1}\mathrm{d}u \\ &= \frac{\Delta t^{\nu_{n,k}-\zeta_{n,k}}}{\nu_{n,k}-\zeta_{n,k}} \sum_{p=0}^{m-1} \left[(p+1)^{\nu_{n,k}-\zeta_{n,k}} - p^{\nu_{n,k}-\zeta_{n,k}}\right] \mathbf{J}_k|^{m-p-\frac{1}{2}}\,. \end{aligned} \tag{12}$$

By using the following expansion [23]:

$$(p+1)^{\nu_{n,k}-\zeta_{n,k}} - p^{\nu_{n,k}-\zeta_{n,k}} \simeq \sum_{q=1}^{Q_{n,k}} a_{n,k,q} e^{-b_{n,k,q}p}, \tag{13}$$

with the order $Q_{n,k}$ and the coefficients $a_{n,k,q}$ and $b_{n,k,q}$ being suitably chosen in order to minimize the mean square error, and upon setting:

$$\mathbf{\Psi}_{n,k,q}\big|^m = \sum_{p=0}^{m-1} a_{n,k,q} e^{-b_{n,k,q}p}\, \mathbf{J}_k|^{m-p-\frac{1}{2}} = a_{n,k,q}\, \mathbf{J}_k|^{m-\frac{1}{2}} + e^{-b_{n,k,q}}\, \mathbf{\Psi}_{n,k,q}\big|^{m-1}, \tag{14}$$

equation (12) can be rewritten as:

$$\mathbf{I}_{n,k}\big|^m \simeq \frac{\Delta t^{\nu_{n,k}-\zeta_{n,k}}}{\nu_{n,k}-\zeta_{n,k}} \left(S_{n,k}\, \mathbf{J}_k|^{m-\frac{1}{2}} + \sum_{q=1}^{Q_{n,k}} e^{-b_{n,k,q}}\, \mathbf{\Psi}_{n,k,q}\big|^{m-1} \right), \tag{15}$$

where:

$$S_{n,k} = \sum_{q=1}^{Q_{n,k}} a_{n,k,q}. \tag{16}$$

In (10), the time derivative of $\mathbf{I}_{n,k}$ calculated at the time instant $t = m\Delta t$ can be approximated by means of the expression:

$$\left.\frac{\mathrm{d}^{\nu_{n,k}}\mathbf{I}_{n,k}}{\mathrm{d}t^{\nu_{n,k}}}\right|^{m} \simeq \frac{1}{(\Delta t)^{\nu_{n,k}}}\sum_{p=0}^{\nu_{n,k}}(-1)^p\binom{\nu_{n,k}}{p}\,\mathbf{I}_{n,k}\big|^{m-p+1}$$
$$= \frac{\Delta t^{-\zeta_{n,k}}}{\nu_{n,k}-\zeta_{n,k}}\left\{S_{n,k}\left[\mathbf{J}_k|^{m+\frac{1}{2}} + \sum_{p=1}^{\nu_{n,k}}(-1)^p\binom{\nu_{n,k}}{p}\mathbf{J}_k|^{m-p+\frac{1}{2}}\right]\right.$$
$$\left. + \sum_{p=1}^{\nu_{n,k}}(-1)^p\binom{\nu_{n,k}}{p}\left(\sum_{q=1}^{Q_{n,k}} e^{-b_{n,k,q}}\,\boldsymbol{\Psi}_{n,k,q}\big|^{m-p}\right)\right\}. \tag{17}$$

In this way, after some algebra, it is not difficult to show that:

$$\left(\mathrm{D}_t^{\alpha_k,\beta_k}\mathbf{J}_k\right)\Big|^m \simeq \sum_{n=0}^{K_k}\frac{\chi_{n,k}}{\left(\nu_{n,k}-\zeta_{n,k}\right)!}\left(\frac{\tau_k}{\Delta t}\right)^{\zeta_{n,k}}\sum_{p=0}^{\nu_{n,k}}\left[A_{n,k,p}\,\mathbf{J}_k|^{m-p+\frac{1}{2}}\right.$$
$$\left. + \sum_{q=1}^{Q_{n,k}} B_{n,k,p,q}\,\boldsymbol{\Psi}_{n,k,q}\big|^{m-p}\right], \tag{18}$$

with:

$$\begin{Bmatrix} A_{n,k,p} \\ B_{n,k,p,q}\end{Bmatrix} = (-1)^p\binom{\nu_{n,k}}{p}\begin{Bmatrix} S_{n,k} \\ e^{-b_{n,k,q}}\end{Bmatrix}, \tag{19}$$

Finally, by combining (6) with (7), (8), and (18), one can readily obtain:

$$\left[\left(\varepsilon_{r_\infty}+\frac{\sigma\Delta t}{2\varepsilon_0}\right)\frac{C_k}{\Delta\varepsilon_{r_k}}+\frac{1}{2}\right]\mathbf{J}_k|^{m+\frac{1}{2}} + \frac{1}{2}\sum_{l=1,l\neq k}^{N}\mathbf{J}_l|^{m+\frac{1}{2}} =$$
$$= (\nabla\times\mathbf{H})|^m - \sigma\mathbf{E}|^{m-\frac{1}{2}} - \frac{1}{2}\sum_{l=1}^{N}\mathbf{J}_l|^{m-\frac{1}{2}} - \left(\varepsilon_{r_\infty}+\frac{\sigma\Delta t}{2\varepsilon_0}\right)$$
$$\cdot\frac{1}{\Delta\varepsilon_{r_k}}\sum_{n=0}^{K_k}\frac{\chi_{n,k}}{\left(\nu_{n,k}-\zeta_{n,k}\right)!}\left(\frac{\tau_k}{\Delta t}\right)^{\zeta_{n,k}}\left[\sum_{p=1}^{\nu_{n,k}}A_{n,k,p}\,\mathbf{J}_k|^{m-p+\frac{1}{2}}\right.$$
$$\left. + \sum_{p=0}^{\nu_{n,k}}\sum_{q=1}^{Q_{n,k}} B_{n,k,p,q}\,\boldsymbol{\Psi}_{n,k,q}\big|^{m-p}\right] = \boldsymbol{\eta}_k\big|^m, \tag{20}$$

where:

$$C_k = \sum_{n=0}^{K_k} A_{n,k,0}\frac{\chi_{n,k}}{\nu_{n,k}-\zeta_{n,k}}\left(\frac{\tau_k}{\Delta t}\right)^{\zeta_{n,k}}, \tag{21}$$

for $k = 1, 2, \ldots, N$. It is apparent from (20) that in the presented formulation, contrary to the methodology in [1], the evaluation of the displacement current density entails solving a symmetric system of N linear equations, this reflecting the multi–relaxation characteristics of the dielectric material under analysis. As a matter of fact, Eq. (19) can be recast in the more compact matrix form:

$$\underbrace{\left[\frac{1}{2}\,\underline{\mathbf{U}}+\left(\varepsilon_{r_\infty}+\frac{\sigma\,\Delta t}{2\varepsilon_0}\right)\underline{\mathbf{D}}\right]}_{\underline{\mathbf{T}}}\cdot\mathbf{J}|^{m+\frac{1}{2}}=\boldsymbol{\eta}|^{m}\,, \tag{22}$$

with $\underline{\mathbf{U}}$ being the unit matrix of order N, and $\underline{\mathbf{D}}=\mathrm{diag}\,\{D_1, D_2, \ldots, D_N\}$ the diagonal matrix with nonzero entries $D_k = C_k/\Delta\varepsilon_{r_k}$. In (22), $\mathbf{J}|^{m+\frac{1}{2}}$ denotes the vector of the unknown current densities at the time instant $t=\left(m+\frac{1}{2}\right)\Delta t$, namely:

$$\mathbf{J}|^{m+\frac{1}{2}}=\begin{bmatrix}\mathbf{J}_1|^{m+\frac{1}{2}}\\ \mathbf{J}_2|^{m+\frac{1}{2}}\\ \vdots\\ \mathbf{J}_N|^{m+\frac{1}{2}}\end{bmatrix}. \tag{23}$$

Similarly, the column vector $\boldsymbol{\eta}|^{m}$ is built up by arraying the auxiliary electromagnetic field quantities $\boldsymbol{\eta}_k\big|^{m}$ $(k=1,2,\ldots,N)$ appearing on the right–hand side of (20). It is worth noting that the inverse of the coefficient matrix $\underline{\mathbf{T}}$ of the linear system (22) can be conveniently computed only one time before the time–marching scheme is initiated. In this way, in comparison to the *FDTD* procedure described in [1], the algorithmic implementation of the technique proposed in this research study actually results in a reduced additional computational cost of $O\left(N^2\right)$ floating–point operations useful to determine the solution of (20) as:

$$\mathbf{J}|^{m+\frac{1}{2}}=\underline{\mathbf{T}}^{-1}\cdot\boldsymbol{\eta}|^{m}\,. \tag{24}$$

Once the current density terms $\mathbf{J}_l|^{m+\frac{1}{2}}$ $(l=1,2,\ldots,N)$ are evaluated, the electric field distribution within the considered dielectric medium can be derived from (6) as:

$$\mathbf{E}|^{m+\frac{1}{2}}=\frac{2\varepsilon_0\varepsilon_{r_\infty}-\sigma\,\Delta t}{2\varepsilon_0\varepsilon_{r_\infty}+\sigma\,\Delta t}\,\mathbf{E}|^{m-\frac{1}{2}}+\frac{2\Delta t}{2\varepsilon_0\varepsilon_{r_\infty}+\sigma\,\Delta t}\Bigg[(\nabla\times\mathbf{H})|^{m} -\frac{1}{2}\sum_{l=1}^{N}\left(\mathbf{J}_l|^{m-\frac{1}{2}}+\mathbf{J}_l|^{m+\frac{1}{2}}\right)\Bigg], \tag{25}$$

where judicious use of (7) has been made. Finally, by carrying out a second–order accurate finite–difference approximation of the Faraday's law in the time domain, the following update equation for the magnetic field is readily obtained:

$$\mathbf{H}|^{m+1} = \mathbf{H}|^{m} - \frac{\Delta t}{\mu_0} \left(\nabla \times \mathbf{E}\right)|^{m+\frac{1}{2}}, \tag{26}$$

with μ_0 denoting the magnetic permeability of free space.

In order to truncate the *FDTD* computational domain and solve electromagnetic problems with open boundaries, dedicated uniaxial perfectly matched layer (*UPML*) conditions [24] have to be derived and implemented numerically accounting for the electrical conductivity and the multi–relaxation characteristics of the *HN* medium under analysis. To this end, let us first introduce the auxiliary electric field vector **e** as:

$$\mathbf{e} = \left(\kappa_z + \frac{\sigma_z}{j\omega\varepsilon_0}\right)\mathbf{E}, \tag{27}$$

with κ_z, σ_z denoting the *UPML* material parameters in accordance with the complex coordinate stretching approach [12]:

$$\kappa_z(z) = \begin{cases} 1, & z \notin \text{UPML} \\ 1 + (\kappa_{\text{MAX}} - 1)\left(\dfrac{z - z^*_{\text{UPML}}}{d_{\text{UPML}}}\right)^m, & z \in \text{UPML} \end{cases} \tag{28}$$

$$\sigma_z(z) = \begin{cases} 0, & z \notin \text{UPML} \\ \sigma_{\text{MAX}}\left(\dfrac{z - z^*_{\text{UPML}}}{d_{\text{UPML}}}\right)^m, & z \in \text{UPML} \end{cases} \tag{29}$$

In (28)–(29), z^*_{UPML} and d_{UPML} denote, respectively, the coordinate of the *UPML* interface and the relevant thickness. In particular, σ_{MAX} is the maximum value assumed by the conductivity at the truncation of the *UPML* region $\left(z = z^*_{\text{UPML}} + d_{\text{UPML}}\right)$ and κ_{MAX} is a real coefficient which is selected heuristically in order to enhance the absorption of electromagnetic waves within the *UPML* region and, in this way, minimize the spurious reflection level in the solution domain.

Multiplying both sides of (27) by $j\omega$ and transforming into the time domain immediately yields:

$$\partial_t \mathbf{e} = \kappa_z \partial_t \mathbf{E} + \frac{\sigma_z}{\varepsilon_0}\mathbf{E}. \tag{30}$$

In this way, it is not difficult to find out that the Ampere's law can be written, within the *UPML* region, as:

$$\nabla \times \mathbf{H} = \varepsilon_0 \varepsilon_{r_\infty} \partial_t \mathbf{e} + \sigma \mathbf{e} + \sum_{l=1}^{N} \mathbf{j}_l, \tag{31}$$

where the $l-$th displacement current density term satisfies the fractional derivative equation:

$$\mathrm{D}_t^{\alpha_l,\beta_l} \mathbf{j}_l = \varepsilon_0 \Delta\varepsilon_{r_l} \partial_t \mathbf{e}. \tag{32}$$