A 3D Nonlinear Maxwell's Equations Solver Based On A Hybrid Numerical Method

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Abstract

In this paper we explore the possibility for solving the 3D Maxwell's equations in the presence of nonlinear and/or inhomogeneous material response. We propose using a hybrid approach which combines a boundary integral representation with a domain-based method. This hybrid approach has previously been successfully applied to 1D linear and nonlinear transient wave scattering problems. The basic idea of the approach is to propagate the Maxwell's equations inside the scattering objects forward in time by using a domain-based method, while a boundary integral representation of the electromagnetic field is used to supply the domain-based method with the required surface values. Thus no grids outside the scattering objects are needed and this greatly reduces the computational cost and complexity.

1 Introduction

Boundary Element method (BEM), as a tool for solving scattering problems, has several attractive features. First and foremost, BEM is well suited to treating scattering problems in unbounded domains because the boundary integral equations are located on the surfaces of the scattering objects and thus one whole dimension is taken out of the problem. Secondly, the scattering objects are usually defined by sharp material boundaries and thus a domain-based method must seek to resolve the fast variation in the corresponding solutions generated by the boundaries. This is a well known problem in the most popular domain-based method for electromagnetic scattering, the Finite Difference Time Domain method(FDTD) [1–3]. This method like all domain-based methods must also struggle with reducing wave reflection from the boundary of the finite computational box which is added in order to discretize the outside domain. This problem has been more or less solved by using perfectly matched layers [4, 5], but the solution comes with additional cost and complexity. While the BEM takes this radiation condition into account automatically.

However BEM has some drawbacks too. Firstly, singularities always appear during the deriving of the boundary equations from the PDEs. How to accurately calculate these integrals with singularities is an issue of the subject especially for irregular scattering objects. While the domain-based method is much simpler to implement. Secondly, the derivation of the BEM relies on Green's functions which is only defined for linear systems of PDEs. For some applications where the nonlinearity dominates, the BEM cannot be derived. However for the applications where the nonlinearity can be discarded, a computational approach based on Green's functions is feasible. Scattering of electromagnetic waves, where nonlinearities only come into play at very high field intensities, is such an area. Thirdly, the time-domain integral equations are retarded and there is large memory requirement. Also the matrix resulted from the BEM is dense and nonsymmetrical, thus it is usually not easy to solve. However the major obstacle that has prevented BEM from being popular is the late time instabilities. Although the sources of these instabilities are not fully recognized, many remedies have been made to improve the stabilities of BEM schemes for time dependent electromagnetics [6–12].

Our work has not been aimed at joining in or improving on any of the efforts pursued by these research groups. Our major aim has been to generalize boundary approaches to electromagnetic scattering for cases where the scattering objects have an inhomogeneous and/or nonlinear response. Most work in the area of time dependent BEM has been focused on metallic objects with linear response whose dimensions are large with respect to the wave length, antennas is a major example of the kind of structure one has been interested in. The kind of problem we have in mind is scattering from very small objects, from micron to nanometer scale, objects who might have engineered inhomogeneities in their structure and strong, also engineered, nonlinear response. At this scale, the standard simplifying assumption of disregarding the inside of the scattering objects and modeling them using surface charges and currents, is not applicable. The skin depth at this microscopic scale can easily be as large as the scattering objects themselves, which is a marked difference to what is true for macroscopic antenna theory. For this reason, and also because of the complex inner structure of these microscopic scattering objects, a different approach is needed. The traditional BEM can not be used here.

Our approach is based on the same integral representation of the electromagnetic field [13] as the traditional BEM, however, we use the integral representation in a way that is different from what one does in BEM. We solve the Maxwell's equations on the inside of each scattering object, as an initial boundary value problem, and use the integral identities to supply the boundary values needed in order to make the initial boundary value problem for Maxwell, well posed. This kind of approach for solving electromagnetic scattering problems was first proposed in 1972 by E. Wolf and D. N. Pattanyak [14] in the context of stationary linear scattering and was based on the Ewald-Oseen optical extinction theorem. For this reason we call this particular way of reformulating the electromagnetic scattering problem for the Ewald Oseen Scattering(EOS) formulation. This reformulation can be applied to any kind of wave scattering situation. It has previously been applied to two toy models of 1D linear and nonlinear transient wave scattering by the authors [15] where the EOS formulations work perfectly well with high accuracy and low computational load and without any instabilities, even at very late times.

In section 2 we show some of the details of the derivation of our EOS formulation for Maxwell's equations and in section 3 we discuss some tests we have run on our numerical implementation of the EOS formulation of Maxwell's equations. In this paper we do not describe the numerical implementational details, like how we handle the singular integrals and issues of numerical stability.

These, mainly very technical considerations, would cloud the main message of the current paper, which is that our EOS formulation of scattering problems works. The technical details pertaining to our choise of implementation, some of which are probably relevant for most numerical implementations of the EOS formulation, will be reported elsewhere in a paper soon to appear [16]. Here we will just note that, just like for the 1D case, the internal numerical scheme, Lax-Wendroff for our case, determines a stability interval for the time step. The difference is that, in the 1D case, the stability interval is purely determined by the internal numerical scheme while in 3D case, there is another lower limit of the stability interval determined by the integral part of the scheme. We also find that the late time instability is highly depended on the features of the scattering materials. Section 4 summarizes what we have achieved and discuss extensions of our work that could be of interest to pursue.

2 EOS formulations of the 3D Maxwell's equations

In this paper, we investigate an electromagnetic scattering problem described by the 3D Maxwell's equations

$$\begin{aligned} \nabla \times \mathbf{E} + \partial_t \mathbf{B} &= 0, \\ \nabla \times \mathbf{H} - \partial_t \mathbf{D} &= \mathbf{J}, \\ \nabla \cdot \mathbf{D} &= \rho, \\ \nabla \cdot \mathbf{B} &= 0, \end{aligned}$$

where $\mathbf{J}$ and ρ are the current density and the charge density of free charges. Bound charges and currents determine $\mathbf{D}$ and $\mathbf{H}$ as functionals of $\mathbf{E}$ and $\mathbf{B}$,

$$\begin{aligned} \mathbf{D} &= \mathbf{D}[\mathbf{E}, \mathbf{B}], \\ \mathbf{H} &= \mathbf{H}[\mathbf{E}, \mathbf{B}]. \end{aligned}$$

In the simplest situation, where the response from the bound charges and currents is linear, isotropic, homogeneous and instantaneous, we have

$$\mathbf{D} = \varepsilon \mathbf{E}, \;\; \mathbf{H} = \frac{1}{\mu}\mathbf{B},$$

where $\sqrt{\frac{1}{\varepsilon\mu}} = c$ is the speed of light in the material. For this particular situation, we have

$$\begin{aligned} \nabla \times \mathbf{E} + \partial_{\mathbf{t}} \mathbf{B} &= 0, \\ \nabla \times \mathbf{B} - \frac{1}{c^2}\partial_t \mathbf{E} &= \mu \mathbf{J}, \\ \nabla \cdot \mathbf{E} &= \frac{1}{\varepsilon}\rho, \\ \nabla \cdot \mathbf{B} &= 0. \end{aligned} \tag{2.1}$$

We now rewrite the Maxwell's equations into a form that is a suitable starting point for our EOS formulation of the elctromagnetic wave scattering problem.

First, observe that

$$\begin{aligned} \partial_t \nabla \cdot \mathbf{B} &= 0, \\ \partial_t \nabla \cdot \mathbf{E} &= -\frac{1}{\varepsilon} \nabla \cdot \mathbf{J}. \end{aligned} \tag{2.2}$$

Equations (2.1) and (2.2) lead to

$$\partial_t (\nabla \cdot \mathbf{E} - \frac{1}{\varepsilon} \rho) = -\frac{1}{\varepsilon} (\partial_t \rho + \nabla \cdot \mathbf{J}). \tag{2.3}$$

All fields we consider will be driven by the source that will operate for some finite time interval. This means that at some time in the past $t = t_0$, we have

$$\begin{aligned} \nabla \cdot \mathbf{B}(\mathbf{x}, t_0) &= 0, \\ \nabla \cdot \mathbf{E}(\mathbf{x}, t_0) &= \frac{1}{\varepsilon} \rho(\mathbf{x}, t_0) = 0, \end{aligned}$$

and this together with (2.2) and (2.3) imply that for any t

$$\nabla \cdot \mathbf{B}(\mathbf{x}, t) = 0$$

holds true. If we now use the equation of charge conservation

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0$$

then

$$\nabla \cdot \mathbf{E}(\mathbf{x}, t) = \frac{1}{\varepsilon} \rho(\mathbf{x}, t)$$

also holds true at all time. Taking these considerations into account, Maxwell's equations can be written in the following equivalent form

$$\nabla \times \mathbf{E} + \partial_t \mathbf{B} = 0, \tag{2.4a}$$

$$\nabla \times \mathbf{B} - \frac{1}{c^2} \partial_t \mathbf{E} = \mu \mathbf{J}, \tag{2.4b}$$

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0. \tag{2.4c}$$

In order to complete the model, we must supply an equation of motion for the current $\mathbf{J}$

$$\partial_t \mathbf{J} = F[\mathbf{J}, \rho, \mathbf{E}, \mathbf{B}].$$

The specific form for the functional F is determined by what kind of material response we are considering. In order for the system to lead to an efficient numerical method it is important that the sources $\rho, \mathbf{J}$ are confined to some small region. In this paper, in order to be specific, we look at the case of a small metallic object interacting with light. We are not seeking to make a detailed computational investigation of this system, but is rather focused on testing our computational approach with respect to implementational complexity and numerical stability. For this reason we choose the following simple nonlinear model for the metal response of such a system

$$\partial_t \mathbf{J} = (\alpha - \beta \rho) \mathbf{E} - \gamma \mathbf{J}, \tag{2.5}$$

where α, β and γ are constants.

Following the usual approach, it is easy to show that the electric field satisfy the following equation

$$\frac{1}{c^2}\partial_{tt}\mathbf{E} - \nabla^2\mathbf{E} = -\frac{1}{\varepsilon}\nabla\rho - \mu\partial_t\mathbf{J}. \tag{2.6}$$

Each vector component of equation (2.6) is an inhomogeneous wave equation. Let's suppose the scattering object is confined in a compact homogeneous domain denoted by V_1 while the light source is located in an unbounded domain outside the object which is denoted by V_0. μ, ε are the magnetic permeability and the electric permittivity with their values μ_1, ε_1 inside and μ_0, ε_0 outside respectively. c represents the speed of light, with value c_1 inside and c_0 outside the scattering object V_1. The sources $\mathbf{J_0}$ and ρ_0 are given and $\mathbf{J_1}$, ρ_1 are the response sources generated by the metallic object interacting with the light field.

We are now ready to start the construction of the EOS formulations of this scattering problem.

Applying the integral relation for the wave equation (A.6) derived in Appendix A on equation (2.6) in domain V_0 and V_1 respectively, we get

$$\begin{aligned}\mathbf{E}_j(\mathbf{x},t) = &-\int_{V_j} \mathrm{d}V' h_j(\mathbf{x}',\mathbf{x})\{\mu_j\partial_{t'}\mathbf{J}_j + \frac{1}{\varepsilon_j}\nabla'\rho_j\}(\mathbf{x}',T)\\ &\mp\int_S \mathrm{d}S'\{h_j(\mathbf{x}',\mathbf{x})(\partial_{\mathbf{n}'}\mathbf{E}_j)(\mathbf{x}',T) - \partial_{\mathbf{n}'}h_j(\mathbf{x}',\mathbf{x})\mathbf{E}_j(\mathbf{x}',T)\\ &+\frac{1}{c_j}h_j(\mathbf{x}',\mathbf{x})\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|(\partial_{t'}\mathbf{E}_j)(\mathbf{x}',T)\},\end{aligned} \tag{2.7}$$

where

$$h_j(\mathbf{x}',\mathbf{x}) = \frac{c_j}{4\pi|\mathbf{x}'-\mathbf{x}|},$$

with $j=0$ representing the outside domain V_0 and $j=1$ representing the inside domain V_1. Here $\mathbf{x}\in V_j$ and $\mathbf{n'}$ is the unit normal to the boundary, S of V_1, at the point $\mathbf{x}'\in S$, pointing out of the domain V_1. The upper sign applies to the case $j=0$ and the lower sign for the case $j=1$. The same convention applies to all the following expressions in this section.

After a series of algebraic manipulations, starting with (2.7), we obtain

$$\begin{aligned}&\mathbf{E}_j(\mathbf{x},t) = -\partial_t\frac{\mu_j}{4\pi}\int_{V_j}\mathrm{d}V'\frac{\mathbf{J}_j(\mathbf{x}',T)}{|\mathbf{x}'-\mathbf{x}|} - \nabla\frac{1}{4\pi\varepsilon_j}\int_{V_j}\mathrm{d}V'\frac{\rho_j(\mathbf{x}',T)}{|\mathbf{x}'-\mathbf{x}|}\\ &\mp\partial_t[\frac{1}{4\pi}\int_S \mathrm{d}S'\{\frac{1}{c_j|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\times\mathbf{E}_j(\mathbf{x}',T))\times\nabla'|\mathbf{x}'-\mathbf{x}|\\ &+\frac{1}{c_j|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\cdot\mathbf{E}_j(\mathbf{x}',T))\nabla'|\mathbf{x}'-\mathbf{x}| + \frac{1}{|\mathbf{x}'-\mathbf{x}|}\mathbf{n}'\times\mathbf{B}_j(\mathbf{x}',T)\}]\\ &\pm\frac{1}{4\pi}\int_S \mathrm{d}S'\{(\mathbf{n}'\times\mathbf{E}_j(\mathbf{x}',T))\times\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\\ &+(\mathbf{n}'\cdot\mathbf{E}_j(\mathbf{x}',T))\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\}.\end{aligned} \tag{2.8}$$

These manipulations are detailed in Appendix B.
Like the electric field, the magnetic field also satisfies a wave equation

$$\frac{1}{c^2}\partial_{tt}\mathbf{B} - \nabla^2\mathbf{B} = \mu\nabla\times\mathbf{J}. \tag{2.9}$$

After a set of algebraic manipulations, similar to the ones we did for the electric field, we obtain

$$
\begin{aligned}
&\mathbf{B}_j(\mathbf{x},t) = \nabla\times\frac{\mu_j}{4\pi}\int_{V_j}\mathrm{d}V'\frac{\mathbf{J}_j(\mathbf{x}',T)}{|\mathbf{x}'-\mathbf{x}|}\\
&+\partial_t[\frac{1}{4\pi}\int_S \mathrm{d}S'\{\frac{1}{c_j|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\times\mathbf{B}_j(\mathbf{x}',T))\times\nabla'|\mathbf{x}'-\mathbf{x}|\\
&\mp\frac{1}{c_j|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\cdot\mathbf{B}_j(\mathbf{x}',T))\nabla'|\mathbf{x}'-\mathbf{x}| - \frac{1}{c_j^2}\frac{1}{|\mathbf{x}'-\mathbf{x}|}\mathbf{n}'\times\mathbf{E}_j(\mathbf{x}',T)\}]\\
&\pm\frac{1}{4\pi}\int_S \mathrm{d}S'\{(\mathbf{n}'\times\mathbf{B}_j(x',T))\times\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\\
&+(\mathbf{n}'\cdot\mathbf{B}_j(\mathbf{x}',T))\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\}.
\end{aligned}
\tag{2.10}
$$

The identities (2.8) and (2.10), for the electric and magnetic field, are our version of the general integral identities for the electromagnetic field derived by D.S.Jones [13]. In addition to these two identities we get, in a very similar way, two additional integral identities [16],

$$
\begin{aligned}
&0 = -\partial_t\frac{\mu_{1-j}}{4\pi}\int_{V_{1-j}}\mathrm{d}V'\frac{\mathbf{J}_{1-j}(\mathbf{x}',T)}{|\mathbf{x}'-\mathbf{x}|} - \nabla\frac{1}{4\pi\varepsilon_{1-j}}\int_{V_{1-j}}\mathrm{d}V'\frac{\rho_{1-j}(\mathbf{x}',T)}{|\mathbf{x}'-\mathbf{x}|}\\
&\pm\partial_t[\frac{1}{4\pi}\int_S \mathrm{d}S'\{\frac{1}{c_{1-j}|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\times\mathbf{E}_{1-j}(\mathbf{x}',T))\times\nabla'|\mathbf{x}'-\mathbf{x}|\\
&+\frac{1}{c_{1-j}|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\cdot\mathbf{E}_{1-j}(\mathbf{x}',T))\nabla'|\mathbf{x}'-\mathbf{x}| + \frac{1}{|\mathbf{x}'-\mathbf{x}|}\mathbf{n}'\times\mathbf{B}_{1-j}(\mathbf{x}',T)\}]\\
&\mp\frac{1}{4\pi}\int_S \mathrm{d}S'\{(\mathbf{n}'\times\mathbf{E}_{1-j}(\mathbf{x}',T))\times\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\\
&+(\mathbf{n}'\cdot\mathbf{E}_{1-j}(\mathbf{x}',T))\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\},
\end{aligned}
\tag{2.11}
$$

and

$$
\begin{aligned}
&0 = \nabla\times\frac{\mu_{1-j}}{4\pi}\int_{V_{1-j}}\mathrm{d}V'\frac{\mathbf{J}_{1-j}(\mathbf{x}',T)}{|\mathbf{x}'-\mathbf{x}|}\\
&\pm\partial_t[\frac{1}{4\pi}\int_S \mathrm{d}S'\{\frac{1}{c_{1-j}|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\times\mathbf{B}_{1-j}(\mathbf{x}',T))\times\nabla'|\mathbf{x}'-\mathbf{x}|\\
&+\frac{1}{c_{1-j}|\mathbf{x}'-\mathbf{x}|}(\mathbf{n}'\cdot\mathbf{B}_{1-j}(\mathbf{x}',T))\nabla'|\mathbf{x}'-\mathbf{x}| - \frac{1}{c_{1-j}^2}\frac{1}{|\mathbf{x}'-\mathbf{x}|}\mathbf{n}'\times\mathbf{E}_{1-j}(\mathbf{x}',T)\}]\\
&\mp\frac{1}{4\pi}\int_S \mathrm{d}S'\{(\mathbf{n}'\times\mathbf{B}_{1-j}(x',T))\times\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\\
&+(\mathbf{n}'\cdot\mathbf{B}_{1-j}(\mathbf{x}',T))\nabla'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\},
\end{aligned}
\tag{2.12}
$$

for $\mathbf{x}\in V_j,\ j=0,1$. In the above expressions,

$$\mathbf{E}_j(\mathbf{x}',t) = \lim_{\mathbf{x}\to\mathbf{x}'}\mathbf{E}_j(\mathbf{x},t)$$

and

$$\mathbf{B}_j(\mathbf{x}',t) = \lim_{\mathbf{x}\to\mathbf{x}'} \mathbf{B}_j(\mathbf{x},t),$$

where $\mathbf{x} \in V_j$, $j = 0, 1$. In the end, we have a full set of the integral identities of the inside and the outside fields expressed by (2.8), (2.10), (2.11) and (2.12) which can be written compactly as

$$\begin{aligned}
\mathbf{E}_1 &= M_1(\mathbf{n}' \times \mathbf{E}_1, \mathbf{n}' \cdot \mathbf{E}_1, \mathbf{n}' \times \mathbf{B}_1), \\
0 &= M_0(\mathbf{n}' \times \mathbf{E}_0, \mathbf{n}' \cdot \mathbf{E}_0, \mathbf{n}' \times \mathbf{B}_0), \\
\mathbf{B}_1 &= N_1(\mathbf{n}' \times \mathbf{B}_1, \mathbf{n}' \cdot \mathbf{B}_1, \mathbf{n}' \times \mathbf{E}_1), \\
0 &= N_0(\mathbf{n}' \times \mathbf{B}_0, \mathbf{n}' \cdot \mathbf{B}_0, \mathbf{n}' \times \mathbf{E}_0),
\end{aligned} \tag{2.13}$$

for $\mathbf{x} \in V_1$ and

$$\begin{aligned}
\mathbf{E}_0 &= M_0(\mathbf{n}' \times \mathbf{E}_0, \mathbf{n}' \cdot \mathbf{E}_0, \mathbf{n}' \times \mathbf{B}_0), \\
0 &= M_1(\mathbf{n}' \times \mathbf{E}_1, \mathbf{n}' \cdot \mathbf{E}_1, \mathbf{n}' \times \mathbf{B}_1), \\
\mathbf{B}_0 &= N_0(\mathbf{n}' \times \mathbf{B}_0, \mathbf{n}' \cdot \mathbf{B}_0, \mathbf{n}' \times \mathbf{E}_0), \\
0 &= N_1(\mathbf{n}' \times \mathbf{B}_1, \mathbf{n}' \cdot \mathbf{B}_1, \mathbf{n}' \times \mathbf{E}_1,
\end{aligned} \tag{2.14}$$

for $\mathbf{x} \in V_0$.

We will now derive the boundary integral identities of (2.4) by letting $\mathbf{x}$ approach the surface from the inside and the outside of the scattering object V_1, separately. We observe that, in this limit, strong singularities only appear in the last term of the integrals in (2.13) and (2.14). Hence we are faced with a singular term which takes the form of

$$\begin{aligned}
\mathbf{I} &= \lim_{\epsilon\to 0} \int_{S_\epsilon} \mathrm{d}S' \{ (\mathbf{n}' \times \mathbf{A}(\mathbf{x}',T)) \times \nabla' \frac{1}{|\mathbf{x}'-\mathbf{x}|} + (\mathbf{n}' \cdot \mathbf{A}(\mathbf{x}',T)) \nabla' \frac{1}{|\mathbf{x}'-\mathbf{x}|} \} \\
&= \lim_{\epsilon\to 0} \int_{S_\epsilon} \mathrm{d}S' \{ (\frac{\mathbf{x}'-\mathbf{x}}{|\mathbf{x}'-\mathbf{x}|^3} \cdot \mathbf{A}) \mathbf{n}' - (\frac{\mathbf{x}'-\mathbf{x}}{|\mathbf{x}'-\mathbf{x}|^3} \cdot \mathbf{n}') \mathbf{A} - (\mathbf{n}' \cdot \mathbf{A}) \frac{\mathbf{x}'-\mathbf{x}}{|\mathbf{x}'-\mathbf{x}|^3} \},
\end{aligned} \tag{2.15}$$

where $\mathbf{A}(\mathbf{x}',T)$ is a vector function with $\mathbf{x}'$ located on the surface S_ϵ which is an small disk of radius ϵ. If we let $\mathbf{x}$ approach a surface point $\boldsymbol{\xi}$, from the inside of V_1, along a direction

$$\mathbf{x} - \boldsymbol{\xi} = \epsilon \mathbf{a} = -\epsilon\alpha\mathbf{n} - \epsilon\boldsymbol{\beta},$$

where $\mathbf{n}$ is the unit normal vector pointing out of V_1, at the point $\boldsymbol{\xi}$, and $\boldsymbol{\beta}$ is a unit vector along the direction $\mathbf{x}' - \boldsymbol{\xi}$, tangential to S, at the same point $\boldsymbol{\xi}$, we have

$$\lim_{\epsilon\to 0} \int_{S_\epsilon} \frac{\mathbf{x}'-\mathbf{x}}{|\mathbf{x}'-\mathbf{x}|^3} \, \mathrm{d}S = \lim_{\epsilon\to 0} \int_{S_\epsilon} \frac{\boldsymbol{\eta} + \epsilon\alpha\mathbf{n}}{|\boldsymbol{\eta} + \epsilon\alpha\mathbf{n}|^3} \, \mathrm{d}S, \tag{2.16}$$

where $\eta = \mathbf{x}' - \boldsymbol{\xi} + \epsilon\boldsymbol{\beta}$. Using spherical coordinates, (2.16) turns into

$$\lim_{\epsilon\to 0} \int_0^{2\pi} \int_0^{\epsilon} \rho \frac{(\rho\cos\theta, \rho\sin\theta, \epsilon\alpha)}{(\rho^2 + (\epsilon\alpha)^2)^{\frac{3}{2}}} \, \mathrm{d}\theta \, \mathrm{d}\rho = \chi\mathbf{n},$$

where $\chi = 2\pi\alpha(1 - \frac{1}{\sqrt{\alpha^2+1}})$. Similarly, if $\mathbf{x}$ approaches $\boldsymbol{\xi}$ from outside of V_1, we have,

$$\lim_{\epsilon\to 0}\int_{S_\epsilon} \frac{\mathbf{x}'-\mathbf{x}}{|\mathbf{x}'-\mathbf{x}|^3}\,\mathrm{d}S = -\chi\mathbf{n}.$$

So in the end,

$$\begin{aligned} I_+ &= \chi\mathbf{A}, \\ I_- &= -\chi\mathbf{A}, \end{aligned}$$

where I_+ and I_- denote the limit of equation (2.15) by letting $\mathbf{x}$ approach S_ϵ from the inside and the outside of V_1 respectively. After taking these inside and outside limits, we get the following set of equations

$$\begin{aligned} \mathbf{E}_+ &= M_1(\mathbf{n}'\times\mathbf{E}_+, \mathbf{n}'\cdot\mathbf{E}_+, \mathbf{n}'\times\mathbf{B}_+) + \chi\mathbf{E}_+, \\ 0 &= M_0(\mathbf{n}'\times\mathbf{E}_-, \mathbf{n}'\cdot\mathbf{E}_-, \mathbf{n}'\times\mathbf{B}_-) - \chi\mathbf{E}_-, \\ \mathbf{E}_- &= M_0(\mathbf{n}'\times\mathbf{E}_-, \mathbf{n}'\cdot\mathbf{E}_-, \mathbf{n}'\times\mathbf{B}_-) + \chi\mathbf{E}_-, \\ 0 &= M_1(\mathbf{n}'\times\mathbf{E}_+, \mathbf{n}'\cdot\mathbf{E}_+, \mathbf{n}'\times\mathbf{B}_+) - \chi\mathbf{E}_+, \end{aligned} \tag{2.17}$$

where $\mathbf{E}_+$ is the limit of $\mathbf{E_1}$ with $\mathbf{x}$ approaching the surface from the inside of the object while $\mathbf{E}_-$ is the limit of $\mathbf{E_0}$ with $\mathbf{x}$ approaching the surface from the outside of the object. These equations, because of the limits taken, contains singular integrals that must be interpreted as Cauchy principal integrals. Adding the first two equations of (2.17) gives us

$$\begin{aligned} \mathbf{E}_+ &= M_1(\mathbf{n}'\times\mathbf{E}_+, \mathbf{n}'\cdot\mathbf{E}_+, \mathbf{n}'\times\mathbf{B}_+) + M_0(\mathbf{n}'\times\mathbf{E}_-, \mathbf{n}'\cdot\mathbf{E}_-, \mathbf{n}'\times\mathbf{B}_-) \\ &\quad + \chi\mathbf{E}_+ - \chi\mathbf{E}_-, \end{aligned} \tag{2.18}$$

and adding the last two equations of (2.17) gives us

$$\begin{aligned} \mathbf{E}_- &= M_0(\mathbf{n}'\times\mathbf{E}_-, \mathbf{n}'\cdot\mathbf{E}_-, \mathbf{n}'\times\mathbf{B}_-) + M_1(\mathbf{n}'\times\mathbf{E}_+, \mathbf{n}'\cdot\mathbf{E}_+, \mathbf{n}'\times\mathbf{B}_+) \\ &\quad + \chi\mathbf{E}_- - \chi\mathbf{E}_+. \end{aligned} \tag{2.19}$$

Repeating the derivations we just did for the electric field, give us, in a similar way, the following set of equations for the magnetic field

$$\begin{aligned} \mathbf{B}_+ &= N_1(\mathbf{n}'\times\mathbf{B}_+, \mathbf{n}'\cdot\mathbf{B}_+, \mathbf{n}'\times\mathbf{E}_+) + N_0(\mathbf{n}'\times\mathbf{B}_-, \mathbf{n}'\cdot\mathbf{B}_-, \mathbf{n}'\times\mathbf{E}_-) \\ &\quad + \chi\mathbf{B}_+ - \chi\mathbf{B}_-, \end{aligned} \tag{2.20}$$

$$\begin{aligned} \mathbf{B}_- &= N_0(\mathbf{n}'\times\mathbf{B}_-, \mathbf{n}'\cdot\mathbf{B}_-, \mathbf{n}'\times\mathbf{E}_-) + N_1(\mathbf{n}'\times\mathbf{B}_+, \mathbf{n}'\cdot\mathbf{B}_+, \mathbf{n}'\times\mathbf{E}_+) \\ &\quad + \chi\mathbf{B}_- - \chi\mathbf{B}_+, \end{aligned} \tag{2.21}$$

where $\mathbf{B}_+$ is the limit of $\mathbf{B_1}$ with $\mathbf{x}$ approaching the surface from the inside of the object while $\mathbf{B}_-$ is the limit of $\mathbf{B_0}$ with $\mathbf{x}$ approaching the surface from the outside of the object. Also in these equations the singular integrals that occur must be interpreted as Cauchy principal value integrals. So far, we have two outer equations for the outer limit fields $\mathbf{E}_-$, $\mathbf{B}_-$ and two inner equations for the inner limit fields $\mathbf{E}_+$, $\mathbf{B}_+$. We also have the usual electromagnetic boundary conditions at the surface S which separate regions with different susceptibilities and permittivities

$$\begin{aligned}
\mathbf{n}' \times \mathbf{E}_+ &= \mathbf{n}' \times \mathbf{E}_-, \\
\mathbf{n}' \times \mathbf{B}_+ &= \frac{u_1}{u_0}\mathbf{n}' \times \mathbf{B}_-, \\
\mathbf{n}' \cdot \mathbf{B}_+ &= \mathbf{n}' \cdot \mathbf{B}_-, \\
\mathbf{n}' \cdot \mathbf{E}_+ &= \frac{\varepsilon_0}{\varepsilon_1}\mathbf{n}' \cdot \mathbf{E}_-.
\end{aligned}$$

It might appear that we have more equations than we need here. The very same problem was encountered earlier while deriving the EOS formulation for two 1D toy models [15]. It appears as if we can use the two outer equations to solve for $\mathbf{E}_-$ and $\mathbf{B}_-$ and then use the boundary conditions to find $\mathbf{E}_+$ and $\mathbf{B}_+$. But these field values inside the scattering object cannot in general be consistent with the field values derived directly from the two inner equations for $\mathbf{E}_+$ and $\mathbf{B}_+$. For example, if there is a source inside of V_1 and no source outside of V_1, the first approach would give vanishing electric and magnetic field whereas the second approach certainly would not. On the other hand, for a given source, the Maxwell equations has a unique solution, which by construction also satisfy all the integral identities.

In order to understand what the problem is, and how to fix it, we must just realize that, from an abstract point of view, we have the following formal situation

$$\begin{aligned}
A\mathbf{X} &= \mathbf{b}, \\
B\mathbf{X} &= \mathbf{c},
\end{aligned} \tag{2.22}$$

where A and B are singular but where we know that (2.22) has a unique solution.

In this situation, let us assume that $\alpha A + B$ is nonsingular for some choice of α. Any solution of (2.22) is a solution of

$$(\alpha A + B)\mathbf{X} = \alpha\mathbf{b} + \mathbf{c}, \tag{2.23}$$

and since $\alpha A + B$ is nonsingular the unique solution of the singular system (2.22) must in fact be the unique solution of the nonsingular system (2.23). We know that the solution of Maxwell is unique for a given source, so since the integral equations are equivalent to Maxwell, our four integral equations for the two unknown fields on S must have a unique solution. This happens only if they are singular. Thus in our situation, we can simply add (2.18) and (2.19), which gives

$$\begin{aligned}
\mathbf{E}_+ + \mathbf{E}_- = 2(&M_1(\mathbf{n}' \times \mathbf{E}_+, \mathbf{n}' \cdot \mathbf{E}_+, \mathbf{n}' \times \mathbf{B}_+) \\
&+ M_0(\mathbf{n}' \times \mathbf{E}_-, \mathbf{n}' \cdot \mathbf{E}_-, \mathbf{n}' \times \mathbf{B}_-)),
\end{aligned} \tag{2.24}$$

and add (2.20) and (2.21), which gives

$$\begin{aligned}
\mathbf{B}_+ + \mathbf{B}_- = 2(&N_1(\mathbf{n}' \times \mathbf{B}_+, \mathbf{n}' \cdot \mathbf{B}_+, \mathbf{n}' \times \mathbf{E}_+) \\
&+ N_0(\mathbf{n}' \times \mathbf{B}_-, \mathbf{n}' \cdot \mathbf{B}_-, \mathbf{n}' \times \mathbf{E}_-)).
\end{aligned} \tag{2.25}$$

Observe that for any vector $\mathbf{A}$, the following identities hold true

$$\begin{aligned}
\mathbf{n} \times (\mathbf{n} \times \mathbf{A}) &= (\mathbf{n} \cdot \mathbf{A})\mathbf{n} - (\mathbf{n} \cdot \mathbf{n})\mathbf{A}, \\
\mathbf{A} &= (\mathbf{n} \cdot \mathbf{A})\mathbf{n} - \mathbf{n} \times (\mathbf{n} \times \mathbf{A}).
\end{aligned} \tag{2.26}$$

Performing (2.26) on (2.24) and (2.25) we obtain the following final boundary integral identities

$$(I + \frac{1}{2}(\frac{\varepsilon_1}{\varepsilon_0} - 1)\mathbf{n}\ \mathbf{n})\mathbf{E}_+(\mathbf{x}, t) = \mathbf{I}_e + \mathbf{O}_e + \mathbf{B}_e, \tag{2.27a}$$

$$(I + \frac{1}{2}(1 - \frac{\mu_0}{\mu_1})\mathbf{n}\ \mathbf{n})\mathbf{B}_+(\mathbf{x}, t) = \mathbf{I}_b + \mathbf{O}_b + \mathbf{B}_b, \tag{2.27b}$$

where $\mathbf{x} \in S$, $\mathbf{n}$ is the unit normal vector pointing out of V_1 at the point $\mathbf{x}$, I is the identity matrix and

$$\mathbf{I}_e = -\partial_t \frac{\mu_1}{4\pi} \int_{V_1} \mathrm{d}V' \frac{\mathbf{J}_1(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|} - \frac{1}{4\pi\varepsilon_1} \nabla \int_{V_1} \mathrm{d}V' \frac{\rho_1(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|}, \tag{2.28}$$

$$\mathbf{O}_e = -\partial_t \frac{\mu_0}{4\pi} \int_{V_0} \mathrm{d}V' \frac{\mathbf{J}_0(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|} - \nabla \frac{1}{4\pi\varepsilon_0} \int_{V_0} \mathrm{d}V' \frac{\rho_0(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|}, \tag{2.29}$$

$$\begin{aligned} \mathbf{B}_e = & \frac{1}{4\pi} \partial_t \int_S \mathrm{d}S^{'} \{ (\frac{1}{c_1} - \frac{1}{c_0}) \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\mathbf{n}^{'} \times \mathbf{E}_+(\mathbf{x}', T)) \times \nabla' |\mathbf{x}' - \mathbf{x}| \\ & + (\frac{1}{c_1} - \frac{\varepsilon_1}{\varepsilon_0 c_0}) \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\mathbf{n}^{'} \cdot \mathbf{E}_+(\mathbf{x}', T)) \nabla' |\mathbf{x}' - \mathbf{x}| \\ & + (1 - \frac{\mu_0}{\mu_1}) \frac{1}{|\mathbf{x}' - \mathbf{x}|} \mathbf{n}^{'} \times \mathbf{B}_+(\mathbf{x}', T) \} \\ & - \frac{1}{4\pi} \int_S \mathrm{d}S^{'} ((1 - \frac{\varepsilon_1}{\varepsilon_0}) (\mathbf{n}^{'} \cdot \mathbf{E}_+(\mathbf{x}', T)) \nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|}), \end{aligned} \tag{2.30}$$

$$\mathbf{I}_b = \nabla \times \frac{\mu_1}{4\pi} \int_{V_1} \mathrm{d}V' \frac{\mathbf{J}_1(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|}, \tag{2.31}$$

$$\mathbf{O}_b = \nabla \times \frac{\mu_0}{4\pi} \int_{V_0} \mathrm{d}V' \frac{\mathbf{J}_0(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|}, \tag{2.32}$$

$$\begin{aligned} \mathbf{B}_b = & \frac{1}{4\pi} \partial_t \int_S \mathrm{d}S^{'} \{ (\frac{1}{c_1} - \frac{\mu_0}{\mu_1 c_0}) \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\mathbf{n}^{'} \times \mathbf{B}_+(\mathbf{x}', T)) \times \nabla' |\mathbf{x}' - \mathbf{x}| \\ & + (\frac{1}{c_1} - \frac{1}{c_0}) \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\mathbf{n}^{'} \cdot \mathbf{B}_+(\mathbf{x}', T)) \nabla' |\mathbf{x}' - \mathbf{x}| \\ & + (\frac{1}{c_0^2} - \frac{1}{c_1^2}) \frac{1}{|\mathbf{x}' - \mathbf{x}|} \mathbf{n}^{'} \times \mathbf{E}_+(\mathbf{x}', T) \} \\ & - \frac{1}{4\pi} \int_S \mathrm{d}S^{'} \{ (1 - \frac{u_0}{u_1}) (\mathbf{n}^{'} \times \mathbf{B}_+(\mathbf{x}', T)) \times \nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|} \}. \end{aligned} \tag{2.33}$$

Note that $\mathbf{O}_e$ and $\mathbf{O}_b$ are fields on the surfaces generated by the source in the absence of the scattering objects. Equations (2.4) and (2.5) together with the boundary integral identities (2.27a) and (2.27b) compose the EOS formulations of our model.

3 Artificial source test and numerical implementation

The motivation, for introducing the EOS formulation for Maxwell's equations, is a numerical one. The technical issues occuring for the numerical implementation discussed in this paper, will be part of any numerical implementation of our scheme, which in general will involve multiple, arbitrarily shaped, scattering objects, that include linear and nonlinear optical response. We expect however, that the general nature of these issues will reveal themselves already in the simplest possible setting, where we have one scattering object of rectangular shape. The numerical implementation consists of a domain method for the model (2.4) and (2.5), determining the evolution of the fields inside the scattering object, and a scheme for updating the boundary values of the fields using the integral identities (2.27a) and (2.27b). For the internal domain method we choose to use a combination of Lax-Wendroff on (2.4) and modified Euler's method on (2.5), this is similar to what we did for the simple 1D case [15], previously. For the boundary part of the scheme we use the mid-point rule to the nonsingular integrals appearing in (2.27). The treatment of the singular integrals is technical and rather lengthy and will therefore be reported elsewhere [17]. Here it is enough to note that we calculate the singular integrals by reducing them to a singular core, which we calculate exactly, and nonsingular surface and line integrals, that we calculate numerically. The reductions proceed through a nontrivial use of well known integral identities.

For the inside of the scattering object we will use a rectangular grid. This grid is however not uniform close to the boundary. This is because the grid has to support both the discrete approximations to the partial derivatives and discrete approximations to the integrals, used to update the boundary values based on the current and previous internal values of the fields. The fact that in our scheme the boundary values are dynamical variables, enforce some special difference rules that applies close to the boundary. This is an extra complication for our scheme, but they are manageable, and will be part of any scheme that implements the EOS formulation introduced in this paper. Details are given in [17].

What we do in this section is to report on some tests that we have run on our scheme. A usual approach to testing of numerical implementations involve finding exact special solutions corresponding to special source functions. In this section we do not use this approach, but rather use an artificial source test to verify the correctness of our EOS formulations. The basic idea behind the artificial source test, of some numerical scheme designed for a system of PDEs, $\mathscr{L}\psi = 0$, is to slightly modify the system by adding an arbitrary source to all the equations in the system, creating a new modified system $\mathscr{L}\psi = g$. This modification typically lead to minimal modifications to the numerical scheme, where most of the effort and complexity are usually spent on the derivatives and nonlinear terms. For the equations, however, the presence of the sources change the situation completely. This is because the presence of the added sources implies that *any* function is a solution to the equations for *some* choice of sources. Thus we can pick a function ψ_0 and insert it into the model and calculate the source function $g_0 = \mathscr{L}\psi_0$ so that our chosen function is a solution to the extended equation. Finally we run the numerical scheme with the calculated source function and compare the numerical solution with the exact solution ψ_0.

A modified model of (2.4) and (2.5) with artificial sources is generally constructed by

$$
\begin{aligned}
&\partial_t \mathbf{B} + \nabla \times \mathbf{E} = \boldsymbol{\varphi}_1,\\
&\frac{1}{c_1^2}\partial_t \mathbf{E} - \nabla \times \mathbf{B} = -\mu_1 \mathbf{J} + \boldsymbol{\varphi}_2,\\
&\nabla \cdot \mathbf{E} = \frac{1}{\varepsilon_1}\rho + \varphi_3,\\
&\nabla \cdot \mathbf{B} = \boldsymbol{\varphi}_4,\\
&\partial_t \mathbf{J} = (\alpha - \beta\rho)\mathbf{E} - \gamma \mathbf{J} + \boldsymbol{\varphi}_5,
\end{aligned}
$$

where $\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \boldsymbol{\varphi}_4$ and $\boldsymbol{\varphi}_5$ are a set of vector functions and φ_3 is a scale function. Observe that

$$\nabla \cdot (\nabla \times \mathbf{E}) + \nabla \cdot \partial_t \mathbf{B} = \nabla \cdot \boldsymbol{\varphi}_1,$$

and this yields

$$\partial_t \boldsymbol{\varphi}_4 = \nabla \cdot \boldsymbol{\varphi}_1.$$

Based on this we suppose $\boldsymbol{\varphi}_1 = 0$ and $\boldsymbol{\varphi}_4 = 0$ which can simplify the choice of the exact solutions. We also observe that if φ_2 and φ_3 are set to be both 0, then the continuity equation

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0$$

is automatically satisfied. So in the end, the source extended model is given by

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0, \tag{3.1a}$$

$$\frac{1}{c_1^2}\partial_t \mathbf{E} - \nabla \times \mathbf{B} = -\mu_1 \mathbf{J}, \tag{3.1b}$$

$$\nabla \cdot \mathbf{E} = \frac{1}{\varepsilon_1}\rho, \tag{3.1c}$$

$$\partial_t \mathbf{J} = (\alpha - \beta\rho)\mathbf{E} - \gamma \mathbf{J} + \boldsymbol{\varphi}. \tag{3.1d}$$

For model (3.1), any choice of $\tilde{\mathbf{E}}, \tilde{\mathbf{B}}$ can be a solution if the artificial source is given by

$$\boldsymbol{\varphi} = \partial_t \tilde{\mathbf{J}} - (\alpha - \beta\tilde{\rho})\tilde{\mathbf{E}} - \gamma \tilde{\mathbf{J}},$$

where $\tilde{\mathbf{J}}$ and $\tilde{\rho}$ are given respectively by

$$
\begin{aligned}
&\tilde{\mathbf{J}} = \frac{1}{\mu_1}(\nabla \times \tilde{\mathbf{B}} - \frac{1}{c_1^2}\partial_t \tilde{\mathbf{E}}),\\
&\tilde{\rho} = \varepsilon_1 \nabla \cdot \tilde{\mathbf{E}}.
\end{aligned}
$$

Due to (3.1a), we can simply choose a vector function $\boldsymbol{\phi}$, such that

$$
\begin{aligned}
&\tilde{\mathbf{E}} = -\partial_t \boldsymbol{\phi},\\
&\tilde{\mathbf{B}} = \nabla \times \boldsymbol{\phi}.
\end{aligned}
\tag{3.2}
$$

Figure 3.1 shows the comparison between the numerical implementations and the exact solutions where we have used

$$\boldsymbol{\phi} = (\arctan(b^2 t^2) e^{-\alpha_1 (x - x_o + y - y_o + z - z_o + \beta_1 (t - t_a))^2}, 0, 0).$$

Values of the parameters are listed below the figure. From figure it is evident that the agreement between the exact solution and the numerical solution is excellent.

For a general case where the electromagnetic fields inside the object are produced by the outside source, we set up the outside source $\mathbf{J}_0$ and ρ_0 to be a combination of a bump function in time and a delta function in space which is easily integrated in space. In order to satisfy the continuity equation

$$\partial_t \rho_0 + \nabla \cdot \mathbf{J}_0 = 0,$$

we can choose a vector function $\boldsymbol{\varphi}$ such that

$$\begin{aligned} \mathbf{J}_0 &= -\partial_t \boldsymbol{\varphi}, \\ \rho_0 &= \nabla \cdot \boldsymbol{\varphi}. \end{aligned} \tag{3.3}$$

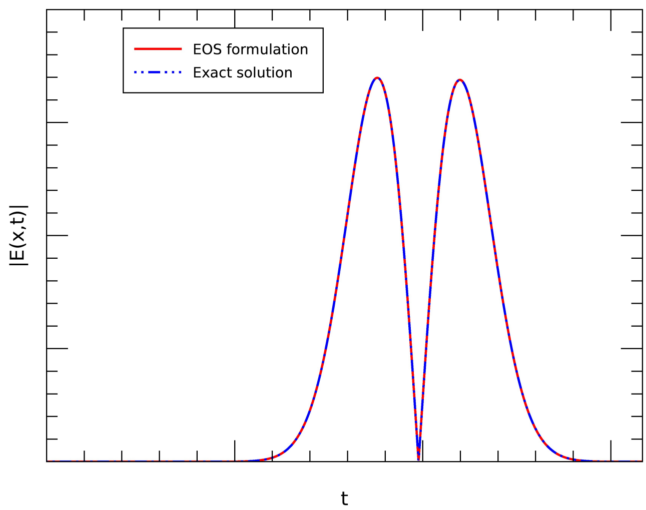


Figure 3.1: Artificial source test: $|\mathbf{E}(\mathbf{x}, t)|$. Intensity of electric field at a specific point at different times. $b = 1.0, \alpha_1 = 40, \beta_1 = 1.0, x_o = 0.0, y_o = 0.0, z_o = 0.0, t_a = 1.0, c_0 = 1.0, \mu_0 = 1.0, \varepsilon_0 = 1.0, c_1 = 0.82, \mu_1 = 1.0, \varepsilon_1 = 1.5, \tau = 0.45, \alpha = 1.0, \beta = 0.01, \gamma = 0.01$.

Figure 3.2 shows the intensity of the electric field on a surface in yz plane at different times. Values of parameters used are shown below the figure. The figure shows a pulse of light passing through the plane, which is what we would expect from the nature of our chosen source. For figure 3.2 , we have chosen

$$\boldsymbol{\varphi} = (\varphi, 0, 0),$$

where

$$\varphi(\mathbf{x}, t) = \begin{cases} \delta(\mathbf{x} - \mathbf{x}_0) e^{\frac{1}{(t-t_0)^2 - 1}} & t \in [t_0 - 1, t_0 + 1], \\ 0 & t \notin [t_0 - 1, t_0 + 1], \end{cases}$$

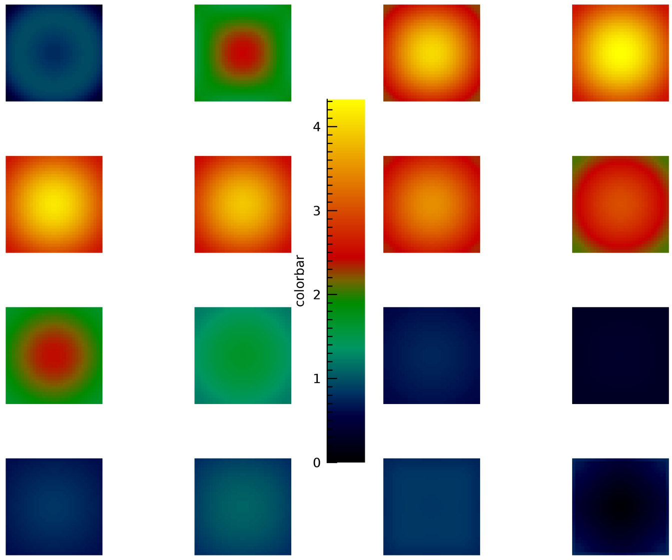


Figure 3.2: The intensity of the electric field on a specific surface in yz plane at different times. $t_0 = 1.5, x_0 = -0.3, y_0 = 0.0, z_0 = 0.0, c_0 = 1.0, \mu_0 = 1.0, \varepsilon_0 = 1.0, c_1 = 0.82, \mu_1 = 1.0, \varepsilon_1 = 1.5, \tau = 0.45, \alpha = 0.1, \beta = 0.01, \gamma = 2$.

with $\mathbf{x}_0 = (x_0, y_0, z_0)$.

Our numerical scheme, being explicit, is not unconditionally stable. There is however a stable range, $\tau_1 < \tau < \tau_2$, for the time step Δt

$$\Delta t = \frac{\tau}{c_1} Min\{\Delta x, \Delta y, \Delta z\},$$

where τ_1 and τ_2 determine the lower and upper boundaries of the stability range for the sceheme. We have carefully investigated the source of the upper and lower bound of the range and how the width of the stability range depends on material parameters. It is not appropriate to include these fairly techincal numerical investigations here, a full discussion will be presented elsewhere in [17]. Here it is enough to note that the source of the lower stability bound is the numerical implementation of the boundary part of the algoritm, and the source of the upper bound is the numerical implementation of the domain part of the algorithm, for our case this is a combination of Lax-Wendroff for the electromagnetic fields, and modified Euler for the current .

4 Conclusions

In this paper we have showed that our EOS formulation of electromagnetic scattering can be accurately and stably implemented using one particular choice of numerical scheme for the inside of the objects and for the integral representation of the boundary values required by the inside scheme. For a stable numerical solution, the time step needs to be confined in some range, where we have found that this range is not only determined by the internal domain-base method due to the non-uniform grids but also determined by the boundary integral representations. Discussions on how the internal non-uniform grids and the boundary integral representation effect the time stable range is reported in [15] which will be published elsewhere. It is worth stressing that the existence of the stability range and its width depends not only on the material parameters but certainly on choices made for the numerical implementation of the boundary part and domain part of the algorithm. In principle, any numerical scheme can be used for the domain part of the algorithm, also the extremely well established FDTD method. It would be interesting to see how this method would perform with respect to stability. There is also the question of going fully implicit, both for the boundary part and the domain part of the algorithm. One would think that this would have a chance of producing an unconditionally stable algorithm for our EOS formulation for Maxwell's equations.

Appendices

A The integral identity for a 3D wave equation

We will start by considering a wave equation in 3D

$$\frac{1}{c^2}\partial_{tt}\varphi(\mathbf{x},t) - \nabla^2\varphi(\mathbf{x},t) = \rho(\mathbf{x},t), \tag{A.1}$$

where $\mathbf{x} = (x, y, z)$, c is the propagation speed and

$$\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2.$$

Let $D \times T$ be a given space-time domain. We will assume that the source $\rho(\mathbf{x},t)$ is entirely contained in $D \times T$. The operator

$$\mathcal{L} = \frac{1}{c^2}\partial_{tt} - \nabla^2$$

is formally self adjoint. Observe that for any pair of functions defined in $D \times T$ we have

$$\begin{aligned}
&\mathcal{L}\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\mathcal{L}\psi(\mathbf{x},t)\\
&= \frac{1}{c^2}\partial_t(\partial_t\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\partial_t\psi(\mathbf{x},t))\\
&- \nabla\cdot(\nabla\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\nabla\psi(\mathbf{x},t)),
\end{aligned}$$

so

$$\begin{aligned}
&\int_{D\times T}\{\mathcal{L}\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\mathcal{L}\psi(\mathbf{x},t)\}\,\mathrm{d}V\,\mathrm{d}t\\
&= \frac{1}{c^2}\int_{D_2}\{\partial_t\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\partial_t\psi(\mathbf{x},t)\}\,\mathrm{d}V\\
&- \frac{1}{c^2}\int_{D_1}\{\partial_t\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\partial_t\psi(\mathbf{x},t)\}\,\mathrm{d}V\\
&- \int_{S\times T}\{\partial_{\mathbf{n}}\varphi(\mathbf{x},t)\psi(\mathbf{x},t) - \varphi(\mathbf{x},t)\partial_{\mathbf{n}}\psi(\mathbf{x},t)\}\,\mathrm{d}S\,\mathrm{d}t.
\end{aligned} \tag{A.2}$$

This is the fundamental integral identity for the wave equation in 3D. Next we will need the advanced Green's function for $\mathcal{L}$ which is given by

$$G(\mathbf{x}, t, \mathbf{x}', t') = Q(\mathbf{x} - \mathbf{x}', t - t'),$$

where $Q(\mathbf{y}, s)$ satisfies

$$\frac{1}{c^2}\partial_{ss}Q(\mathbf{y}, s) - \nabla^2 Q(\mathbf{y}, s) = \delta(\mathbf{y})\delta(s), \qquad s < 0, \tag{A.3}$$

and

$$Q(\mathbf{y}, s) = 0, \qquad s > 0.$$

Because of translational invariance, we can take the Fourier transform of (A.3) and get

$$[-(\frac{\omega}{c})^2 + \zeta^2]\hat{Q}(\xi, \omega) = 1, \qquad \zeta = |\xi|,$$

$$\hat{Q}(\xi, \omega) = \frac{1}{D(\xi, \omega)}, \tag{A.4}$$

where

$$D(\xi, \omega) = -(\frac{\omega}{c})^2 + \zeta^2.$$

Applying the inverse Fourier transform on (A.4) gives

$$Q(\mathbf{y}, s) = \frac{1}{16\pi^4}\int q(\xi, s)e^{i\xi\cdot\mathbf{y}}\, \mathrm{d}\xi,$$

where

$$q(\xi, s) = \int_{C_\varepsilon} \frac{e^{-izs}}{D(\xi, z)}\, \mathrm{d}z,$$

and C_ε is a contour slightly below the real axis. Observe that the integrand has simple poles at $z = \pm c\zeta$, so if $s > 0$, we must close the contour in the lower half-plane. By Cauchy,

$$q(\xi, s) = 0.$$

If $s < 0$, we must now close the contour in the upper half plane and Cauchy's theorem gives

$$q(\xi, s) = \frac{c\pi i}{\zeta}[e^{isc\zeta} - e^{-isc\zeta}],$$

and

$$\frac{1}{16\pi^4}\int \mathrm{d}\xi\ \frac{c\pi i}{\zeta}e^{isc\zeta}e^{i\xi\cdot\mathbf{y}} = \frac{c}{8\pi^2 r}[\int_0^\infty \mathrm{d}\zeta\ e^{i(r+sc)\zeta} - \int_0^\infty \mathrm{d}\zeta\ e^{-i(r-sc)\zeta}],$$

where $r = |\mathbf{y}|$. Similarly,

$$-\frac{1}{16\pi^4}\int \mathrm{d}\xi\frac{c\pi i}{\zeta}e^{-isc\zeta}e^{i\xi\cdot\mathbf{y}} = \frac{-c}{8\pi^2 r}[\int_0^\infty \mathrm{d}\zeta\ e^{i(r-sc)\zeta} - \int_0^\infty \mathrm{d}\zeta\ e^{-i(r+sc)\zeta}].$$

In the end,

$$Q(\mathbf{y}, s) = \frac{c}{4\pi r}[\delta(r + sc) - \delta(r - sc)].$$

Since if $s < 0$, $\delta(r - sc) = 0$, finally

$$Q(\mathbf{y}, s) = \frac{1}{4\pi r}\delta(s + \frac{r}{c}).$$

Thus our advanced Green's function is

$$G(\mathbf{x}, t, \mathbf{x}', t') = \begin{cases} 0 & \text{if } t > t' \\ \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}\delta(t - t' + \frac{|\mathbf{x}-\mathbf{x}'|}{c}), & \text{if } t < t'. \end{cases} \tag{A.5}$$

We now apply (A.5) to the fundamental integral identity (A.2). Let $\varphi(\mathbf{x}, t)$ be a solution to the wave equation (A.1)

$$\mathcal{L}\varphi(\mathbf{x}, t) = \rho(\mathbf{x}, t),$$

then for any $(\mathbf{x}, t) \in D \times T$, we have

$$\begin{aligned}
&\int_{D\times T} \mathrm{d}V' \,\mathrm{d}t' \{\mathcal{L}\varphi(\mathbf{x}', t')G(\mathbf{x}', t', \mathbf{x}, t) - \varphi(\mathbf{x}', t')\mathcal{L}G(\mathbf{x}', t', \mathbf{x}, t)\} \\
&= \frac{1}{c^2}\int_{D_2} \mathrm{d}V' \{\partial_{t'}\varphi(\mathbf{x}', t')G(\mathbf{x}', t', \mathbf{x}, t) - \varphi(\mathbf{x}', t')\partial_{t'}G(\mathbf{x}', t', \mathbf{x}, t)\}|_{t'=t_2} \\
&- \frac{1}{c^2}\int_{D_1} \mathrm{d}V' \{\partial_{t'}\varphi(\mathbf{x}', t')G(\mathbf{x}', t', \mathbf{x}, t) - \varphi(\mathbf{x}', t')\partial_{t'}G(\mathbf{x}', t', \mathbf{x}, t)\}|_{t'=t_1} \\
&- \int_{S\times T} \mathrm{d}S' \,\mathrm{d}t' \{\partial_{\mathbf{n}'}\varphi(\mathbf{x}', t')G(\mathbf{x}', t', \mathbf{x}, t) - \varphi(\mathbf{x}', t')\partial_{\mathbf{n}'}G(\mathbf{x}', t', \mathbf{x}, t)\}.
\end{aligned}$$

Since $t_2 > t$, for the advance Green's function

$$G(\mathbf{x}', t', \mathbf{x}, t)|_{t'=t_2} = 0.$$

And since the field is entirely driven by the source

$$\varphi(\mathbf{x}, t_1) = 0,$$

we get

$$\begin{aligned}
\varphi(\mathbf{x}, t) = &\int_{D\times T} \mathrm{d}V' \,\mathrm{d}t' \rho(\mathbf{x}', t')G(\mathbf{x}', t', \mathbf{x}, t) \\
&+ \int_{S\times T} \mathrm{d}S' \,\mathrm{d}t' \{\partial_{\mathbf{n}'}\varphi(\mathbf{x}', t')G(\mathbf{x}', t', \mathbf{x}, t) - \varphi(\mathbf{x}', t')\partial_{\mathbf{n}'}G(\mathbf{x}', t', \mathbf{x}, t)\}.
\end{aligned}$$

and

$$G(\mathbf{x}', t', \mathbf{x}, t) = h(\mathbf{x}', \mathbf{x})\theta(t - t')\delta(|\mathbf{x}' - \mathbf{x}| + c(t' - t)),$$

where

$$h(\mathbf{x}', \mathbf{x}) = \frac{c}{4\pi|\mathbf{x}' - \mathbf{x}|}.$$

Since

$$\begin{aligned}
\partial_{\mathbf{n}'}G(\mathbf{x}', t', \mathbf{x}, t) &= \theta(t - t')\partial_{\mathbf{n}'}h(\mathbf{x}', \mathbf{x})\delta(|\mathbf{x}' - \mathbf{x}| + c(t' - t)) \\
&+ \theta(t - t')h(\mathbf{x}', \mathbf{x})\partial_{\mathbf{n}'}\delta(|\mathbf{x}' - \mathbf{x}| + c(t' - t)),
\end{aligned}$$

and

$$\partial_{\mathbf{n}'}\delta(|\mathbf{x}'-\mathbf{x}|+c(t'-t)) = \frac{1}{c}\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|\partial_{t'}\delta(|\mathbf{x}'-\mathbf{x}|+c(t'-t)),$$

we thus have

$$\int_{D\times T} \mathrm{d}V'\,\mathrm{d}t'\rho(\mathbf{x}',t')G(\mathbf{x}',t',\mathbf{x},t) = \int_D \mathrm{d}V' h(\mathbf{x}',\mathbf{x})\rho(\mathbf{x}',T),$$

where

$$T = T(t,\mathbf{x}',\mathbf{x}) = t - \frac{1}{c}|\mathbf{x}'-\mathbf{x}|.$$

From

$$\int_{S\times T} \mathrm{d}S'\,\mathrm{d}t'\partial_{\mathbf{n}'}\varphi(\mathbf{x}',t')G(\mathbf{x}',t',\mathbf{x},t) = \int_S \mathrm{d}S' h(\mathbf{x}',\mathbf{x})(\partial_{\mathbf{n}'}\varphi)(\mathbf{x}',T),$$

and

$$\begin{aligned}&-\int_{S\times T} \mathrm{d}S'\,\mathrm{d}t'\varphi(\mathbf{x}',t')\partial_{\mathbf{n}'}G(\mathbf{x}',t',\mathbf{x},t)\\ &= -\int_S \mathrm{d}S'\partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\varphi(\mathbf{x}',T) + \int_S \mathrm{d}S'\frac{1}{c}h(\mathbf{x}',\mathbf{x})\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|(\partial_{t'}\varphi)(\mathbf{x}',T).\end{aligned}$$

finally we get

$$\begin{aligned}\varphi(\mathbf{x},t) = \int_D \mathrm{d}V' h(\mathbf{x}',\mathbf{x})\rho(\mathbf{x}',T) + \int_S \mathrm{d}S'\{h(\mathbf{x}',\mathbf{x})(\partial_{\mathbf{n}'}\varphi)(\mathbf{x}',T)\\ - \partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\varphi(\mathbf{x}',T) + \frac{h(\mathbf{x}',\mathbf{x})}{c}\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|(\partial_{t'}\varphi)(\mathbf{x}',T)\}.\end{aligned} \tag{A.6}$$

This is the integral identity for an operator defining a 3D wave equation and it holds for any solution of the scalar 3D wave equation.

B The integral identity of the electric wave equation

Here we do some calculations to derive (2.8) from (2.7). For the writing in simplicity, we write $\mathbf{E}, \mathbf{J}, \rho, c, \mu, \epsilon$ instead of $\mathbf{E}_j, \mathbf{J}_j, \rho_j, c_j, \mu_j, \epsilon_j$, $j = 0, 1$ respectively here. Observe first that

$$\begin{aligned}\partial_{\mathbf{n}'}(\mathbf{E}(\mathbf{x}',T)) = (\mathbf{n}'\cdot\nabla')(\mathbf{E}(\mathbf{x}',T)) = ((\mathbf{n}'\cdot\nabla')\mathbf{E})(\mathbf{x}',T)\\ + (\partial_{t'}E)(\mathbf{x}',T)(-\frac{1}{c}(\mathbf{n}'\cdot\nabla')|\mathbf{x}'-\mathbf{x}|),\end{aligned}$$

so,

$$\begin{aligned}
\mathbf{E}(\mathbf{x},t) = &-\int_D \mathrm{d}V' h(\mathbf{x}',\mathbf{x})\{\mu\partial_{t'}\mathbf{J} + \frac{1}{\varepsilon}\nabla'\rho\}(\mathbf{x}',T) \\
&+ \int_S \mathrm{d}S'\{h(\mathbf{x}',\mathbf{x})\partial_{\mathbf{n}'}(\mathbf{E}(\mathbf{x}',T)) + \frac{1}{c}h(\mathbf{x}',\mathbf{x})(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}| \\
&- \partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\mathbf{E}(\mathbf{x}',T) + \frac{1}{c}h(\mathbf{x}',\mathbf{x})(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|\} \\
&+ \int_S \mathrm{d}S'\{h(\mathbf{x}',\mathbf{x})\partial_{\mathbf{n}'}(\mathbf{E}(\mathbf{x}',T)) - \partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\mathbf{E}(\mathbf{x}',T) \\
&+ \frac{2}{c}h(\mathbf{x}',\mathbf{x})(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|\}.
\end{aligned} \tag{B.1}$$

We are going to rework the first term in the integral (B.1). Observe that for a vector field $\mathbf{a}$ and a scalar f we have,

$$\begin{aligned}
(\mathbf{n}\cdot\nabla)(f\mathbf{a}) &= (\mathbf{n}\cdot\nabla f)\mathbf{a} + f(\mathbf{n}\cdot\nabla)\mathbf{a}, \\
\nabla\cdot(f\mathbf{a}) &= \nabla f\cdot\mathbf{a} + f\nabla\cdot\mathbf{a}, \\
\nabla\times(f\mathbf{a}) &= \nabla f\times\mathbf{a} + f\nabla\times\mathbf{a},
\end{aligned}$$

so,

$$\mathbf{n}\times(\nabla\times(f\mathbf{a})) = \nabla f(\mathbf{n}\cdot\mathbf{a}) - \mathbf{a}(\mathbf{n}\cdot\nabla f) + f\mathbf{n}\times(\nabla\times\mathbf{a}).$$

Further,

$$\begin{aligned}
&(\mathbf{n}\cdot\nabla)(f\mathbf{a}) + \mathbf{n}\times(\nabla\times(f\mathbf{a})) - n\nabla\cdot(f\mathbf{a}) \\
&= f(\mathbf{n}\cdot\nabla)\mathbf{a} + (\mathbf{n}\times\nabla f)\times\mathbf{a} + f\mathbf{n}\times(\nabla\times\mathbf{a}) - f\mathbf{n}\nabla\cdot\mathbf{a}.
\end{aligned}$$

so if we let $f = h(\mathbf{x}',\mathbf{x})$ and $\mathbf{a} = \mathbf{E}(\mathbf{x}',T)$, we thus have

$$\begin{aligned}
&\int_S \mathrm{d}S' h(\mathbf{x}',\mathbf{x})\partial_{\mathbf{n}'}(\mathbf{E}(\mathbf{x}',T)) \\
&= \int_S \mathrm{d}S'\{-(\mathbf{n}'\times\nabla' h(\mathbf{x}',\mathbf{x}))\times\mathbf{E}(\mathbf{x}',T) \\
&- h(\mathbf{x}',\mathbf{x})\mathbf{n}'\times(\nabla'\times(\mathbf{E}(\mathbf{x}',T))) \\
&+ h(\mathbf{x}',\mathbf{x})\mathbf{n}'\nabla'\cdot(\mathbf{E}(\mathbf{x}',T))\}.
\end{aligned} \tag{B.2}$$

Inserting (B.2) into (B.1) leads to

$$\begin{aligned}
\mathbf{E}(\mathbf{x},t) = &-\int_D \mathrm{d}V' h(\mathbf{x}',\mathbf{x})\{\mu\partial_{t'}J + \frac{1}{\varepsilon}\nabla'\rho\}(\mathbf{x},T) \\
&+ \int_S \mathrm{d}S'\{h(\mathbf{x}',\mathbf{x})\mathbf{n}'\nabla'\cdot(\mathbf{E}(\mathbf{x}',T)) - (\mathbf{n}'\times\nabla' h(\mathbf{x}',\mathbf{x}))\times\mathbf{E}(\mathbf{x}',T) \\
&- h(\mathbf{x}',\mathbf{x})\mathbf{n}'\times(\nabla'\times(\mathbf{E}(\mathbf{x}',T))) - \partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\mathbf{E}(\mathbf{x}',T) \\
&+ \frac{2}{c}h(\mathbf{x}',\mathbf{x})(\partial_{t'}\mathbf{E})(\mathbf{x},T)\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|\}.
\end{aligned}$$

Since

$$\begin{aligned}
\nabla'(\mathbf{E}(\mathbf{x}',T)) &= (\nabla'\cdot\mathbf{E})(\mathbf{x}',T) - \frac{1}{c}(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\cdot\nabla'|\mathbf{x}'-\mathbf{x}|, \\
\nabla'\times(\mathbf{E}(\mathbf{x}',T)) &= (\nabla'\times\mathbf{E})(\mathbf{x}',T) + \frac{1}{c}(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\times\nabla'|\mathbf{x}'-\mathbf{x}|,
\end{aligned}$$

in the end, (B.1) can be written in the following form

$$\begin{aligned}\mathbf{E}(\mathbf{x},t) = &-\int_D \mathrm{d}V' h(\mathbf{x}',\mathbf{x})\{\mu\partial_{t'}\mathbf{J} + \frac{1}{\varepsilon}\nabla'\rho\}(\mathbf{x}',T)\\ &+\int_S \mathrm{d}S'\{h(\mathbf{x}',\mathbf{x})\mathbf{n}'(\nabla'\cdot\mathbf{E})(\mathbf{x}',T)\\ &-\frac{1}{c}h(\mathbf{x}',\mathbf{x})\mathbf{n}'(\partial_{\mathbf{t}'}\mathbf{E})(\mathbf{x}',\mathbf{T})\cdot\nabla'|\mathbf{x}'-\mathbf{x}|)\\ &-(\mathbf{n}'\times\nabla' h(\mathbf{x}',\mathbf{x}))\times\mathbf{E}(\mathbf{x}',T) - h(\mathbf{x}',\mathbf{x})\mathbf{n}'\times(\nabla'\times\mathbf{E})(\mathbf{x}',T)\\ &-\frac{1}{c}h(\mathbf{x}',\mathbf{x})\mathbf{n}'\times((\partial_{t'}\mathbf{E})(\mathbf{x}',T)\times\nabla'|\mathbf{x}'-\mathbf{x}|)\\ &-\partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\mathbf{E}(\mathbf{x}',T) + \frac{2}{c}h(\mathbf{x}',\mathbf{x})(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|\}.\end{aligned}$$

Notice that

$$(\mathbf{n}\times\mathbf{a})\times\nabla f - (\mathbf{n}\times\nabla f)\times\mathbf{a} = (\mathbf{n}\cdot\nabla f)\mathbf{a} - (\mathbf{n}\cdot\mathbf{a})\nabla f,$$

and

$$-(\mathbf{n}\times\nabla f)\times\mathbf{a} - (\mathbf{n}\cdot\nabla f)\mathbf{a} = -(\mathbf{n}\times\mathbf{a})\times\nabla f - (\mathbf{n}\cdot\mathbf{a})\nabla f,$$

and performing them on h and $\mathbf{E}$ gives

$$\begin{aligned}&-(\mathbf{n}'\times\nabla' h(\mathbf{x}',\mathbf{x}))\times\mathbf{E}(\mathbf{x}',T) - \partial_{\mathbf{n}'}h(\mathbf{x}',\mathbf{x})\mathbf{E}(\mathbf{x}',T)\\ &= -(\mathbf{n}'\times\mathbf{E}(\mathbf{x}',T))\times\nabla' h(\mathbf{x}',\mathbf{x}) - (\mathbf{n}'\cdot\mathbf{E}(\mathbf{x}',T))\nabla' h(\mathbf{x}',\mathbf{x}).\end{aligned}$$

In addition

$$\begin{aligned}&(\mathbf{n}\times\mathbf{a})\times\nabla f + \mathbf{n}\times(\mathbf{a}\times\nabla f)\\ &= 2(\mathbf{n}\cdot\nabla f)\mathbf{a} - (\mathbf{a}\cdot\nabla f)\mathbf{n} - (\mathbf{n}\cdot\mathbf{a})\nabla f,\end{aligned}$$

and

$$\begin{aligned}&-(\mathbf{a}\cdot\nabla f)\mathbf{n} - \mathbf{n}\times(\mathbf{a}\times\nabla f) + 2(\mathbf{n}\cdot\nabla f)\mathbf{a}\\ &= (\mathbf{n}\times\mathbf{a})\times\nabla f + (\mathbf{n}\cdot\mathbf{a})\nabla f,\end{aligned}$$

give

$$\begin{aligned}&-\mathbf{n}'((\partial_{t'}\mathbf{E})(\mathbf{x}',T)\cdot\nabla'|\mathbf{x}'-\mathbf{x}|) - \mathbf{n}'\times((\partial_{t'}\mathbf{E})(\mathbf{x},T)\times\nabla'|\mathbf{x}'-\mathbf{x}|)\\ &+2\partial_{\mathbf{n}'}|\mathbf{x}'-\mathbf{x}|(\partial_{t'}\mathbf{E})(\mathbf{x}',T)\\ &= (\mathbf{n}'\times(\partial_{t'}\mathbf{E})(\mathbf{x}',T))\times\nabla'|\mathbf{x}'-\mathbf{x}| + (\mathbf{n}'\cdot(\partial_{t'}\mathbf{E})(\mathbf{x}',T))\nabla'|\mathbf{x}'-\mathbf{x}|.\end{aligned}$$

Thus

$$\begin{aligned}\mathbf{E}(\mathbf{x},t) = &-\int_D \mathrm{d}V' h(\mathbf{x}',\mathbf{x})\{\mu\partial_{t'}\mathbf{J} + \frac{1}{\varepsilon}\nabla'\rho\}(\mathbf{x}',T)\\ &+\int_S \mathrm{d}S'\{h(\mathbf{x}',\mathbf{x})\mathbf{n}'(\nabla'\cdot\mathbf{E})(\mathbf{x}',T) - (\mathbf{n}'\times E(\mathbf{x}',T))\times\nabla' h(\mathbf{x}',\mathbf{x})\\ &-(\mathbf{n}'\cdot E(\mathbf{x}',T))\nabla' h(\mathbf{x}',\mathbf{x}) + \frac{1}{c}h(\mathbf{x}',\mathbf{x})(\mathbf{n}'\times(\partial_{t'}\mathbf{E})(\mathbf{x}',T))\times\nabla'|\mathbf{x}'-\mathbf{x}|\\ &+\frac{1}{c}h(\mathbf{x}',\mathbf{x})(\mathbf{n}'\cdot(\partial_{t'}\mathbf{E})(\mathbf{x}',T))\nabla'|\mathbf{x}'-\mathbf{x}| - h(\mathbf{x}',\mathbf{x})\mathbf{n}'\times(\nabla'\times\mathbf{E})(\mathbf{x}',T)\}.\end{aligned}$$

Using the special form of the divergence theorem, we have

$$\begin{aligned}
&\int_S \mathrm{d}S' h(\mathbf{x}', \mathbf{x})\mathbf{n}'(\nabla' \cdot \mathbf{E})(\mathbf{x}', T) \\
&= \int_D \mathrm{d}V' h(\mathbf{x}', \mathbf{x})\frac{1}{\varepsilon}(\nabla'\rho)(\mathbf{x}', T) - \int_{D}, \mathrm{d}V' h(\mathbf{x}', \mathbf{x})\frac{1}{\varepsilon}\nabla\rho(\mathbf{x}', T) \\
&+ \int_D \mathrm{d}V' \frac{1}{\varepsilon}\rho(\mathbf{x}', T)\nabla' h(\mathbf{x}', \mathbf{x}),
\end{aligned}$$

where

$$\nabla' h(\mathbf{x}', \mathbf{x}) = \frac{1}{4\pi}\nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|} = -\nabla h(\mathbf{x}', \mathbf{x}).$$

Together with

$$(\partial_{t'}\mathbf{J})(\mathbf{x}', T) = \partial_t(\mathbf{J}(\mathbf{x}', T)),$$

we finally get

$$\begin{aligned}
&\mathbf{E}(\mathbf{x}, t) = -\partial_t \frac{\mu}{4\pi}\int_D \mathrm{d}V' \frac{\mathbf{J}(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|} - \nabla\frac{1}{4\pi\varepsilon}\int_D \mathrm{d}V' \frac{\rho(\mathbf{x}', T)}{|\mathbf{x}' - \mathbf{x}|} \\
&+ \partial_t[\frac{1}{4\pi}\int_S \mathrm{d}S' \{\frac{1}{c|\mathbf{x}' - \mathbf{x}|}(\mathbf{n}' \times \mathbf{E}(\mathbf{x}', T)) \times \nabla'|\mathbf{x}' - \mathbf{x}| \\
&+ \frac{1}{c|\mathbf{x}' - \mathbf{x}|}(\mathbf{n}' \cdot \mathbf{E}(\mathbf{x}', T))\nabla'|\mathbf{x}' - \mathbf{x}| + \frac{1}{|\mathbf{x}' - \mathbf{x}|}\mathbf{n}' \times \mathbf{B}(\mathbf{x}', T)\}] \\
&- \frac{1}{4\pi}\int_S \mathrm{d}S' \{(\mathbf{n}' \times \mathbf{E}(\mathbf{x}', T)) \times \nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|} \\
&+ (\mathbf{n}' \cdot \mathbf{E}(\mathbf{x}', T))\nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|}\}.
\end{aligned}$$

This is the integral identity of the electric wave equation (2.6).

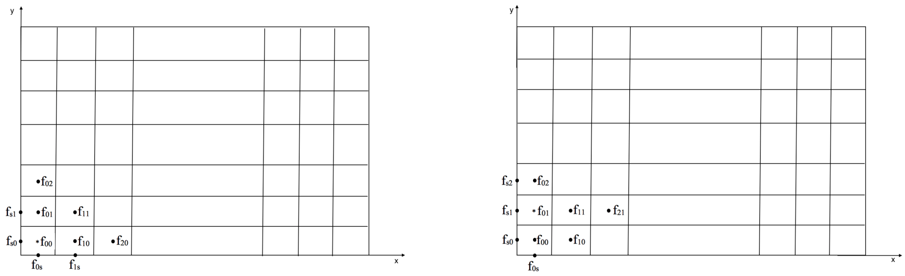
C The first order, the second order and the mixed space derivatives

Here we illustrate a general rule. Suppose we have a three variable function $f(x, y, z)$ defined on grids (D.1). In order to get a second order accuracy, we apply the polynomials in two variables of degree 3 which is expressed by

$$\begin{aligned}
f(x, y, z) = f(x_i, y_i, z_k) &+ \zeta_1\delta x + \zeta_2\delta x^2 + \zeta_3\delta x^3 + \zeta_4\delta x\delta y + \zeta_5\delta x^2\delta y \\
&+ \zeta_6\delta x\delta y^2 + \zeta_7\delta y + \zeta_8\delta y^2 + \zeta_9\delta y^3,
\end{aligned}$$

where $\delta x = x - x_i$, $\delta y = y - y_i$ and

$$\begin{aligned}
\zeta_1 &= \frac{\partial f(x_i, y_j, z_k)}{\partial x}, & \zeta_2 &= \frac{\partial^2 f(x_i, y_j, z_k)}{\partial x^2}, & \zeta_3 &= \frac{\partial^3 f(x_i, y_j, z_k)}{\partial x^3}, \\
\zeta_4 &= \frac{\partial^2 f(x_i, y_j, z_k)}{\partial x\partial y}, & \zeta_5 &= \frac{\partial^3 f(x_i, y_j, z_k)}{\partial x^2\partial y}, & \zeta_6 &= \frac{\partial^3 f(x_i, y_j, z_k)}{\partial x\partial y^2}, \\
\zeta_7 &= \frac{\partial f(x_i, y_j, z_k)}{\partial y}, & \zeta_8 &= \frac{\partial^2 f(x_i, y_j, z_k)}{\partial y^2}, & \zeta_9 &= \frac{\partial^3 f(x_i, y_j, z_k)}{\partial y^3}.
\end{aligned}$$



(a) $i = 0, j = 0$ (b) $i = 0, j = 1$

Figure C.1: Two examples of the involved grid points for calculating the space derivatives of e_p and b_p, $p = 1, 2, 3$.

Except for $f(x_i, y_j, z_k)$, we always need 9 extra grid points that are closest to (x_i, y_j, z_k) in order to get the expressions of $\zeta_1, \zeta_2, \cdots, \zeta_9$. We'll see that these expressions vary depending on the locations of i and j. For example, if $i = 0, j = 0$, the involved grid points are $f_{s,0}$, $f_{0,0}$, $f_{1,0}$, $f_{2,0}$, $f_{0,s}$, $f_{1,s}$, $f_{s,1}$, $f_{0,1}$, $f_{1,1}$ and $f_{0,2}$ while if $i = 0, j = 1$, the involved grid points are $f_{s,0}$, $f_{0,0}$, $f_{1,0}$, $f_{0,s}$, $f_{s,1}$, $f_{0,1}$, $f_{1,1}$, $f_{2,1}$, $f_{s,2}$ and $f_{0,2}$ where

$$f_{s,j} = \begin{cases} f(x_a, y_j, z_k) & i = 0 \\ f(x_b, y_j, z_k) & i = N_x - 1 \end{cases}$$

$$f_{i,s} = \begin{cases} f(x_i, y_a, z_k) & j = 0 \\ f(x_i, y_b, z_k) & j = N_y - 1 \end{cases}$$

$$f_{i,j} = f(x_i, y_j, z_k),$$

and so on. Figure C.1 illustrates two examples of the involved grid points. Finally if $i = 0$ or $i = N_x - 1$ we have

$$\frac{\partial f(x_i, y_j, z_k)}{\partial x} = \pm(f_{s,j},\ f_{i,j},\ f_{i\pm1,j},\ f_{i\pm2,j}\ ) \cdot W_1,$$

$$\frac{\partial^2 f(x_i, y_j, z_k)}{\partial x^2} = (f_{s,j},\ f_{i,j},\ f_{i\pm1,j},\ f_{i\pm2,j}\ ) \cdot W_2,$$

$$\frac{\partial^2 f(x_i, y_j, z_k)}{\partial x \partial y} =$$

$$\begin{cases} \pm(\ f_{s,j},\ f_{s,j+1},\ f_{i,s},\ f_{i,j},\ f_{i,j+1},\ f_{i\pm1,s},\ f_{i\pm1,j},\ f_{i\pm1,j+1}\ ) \cdot W_3 & j = 0 \\ \mp(\ f_{s,j},\ f_{s,j-1},\ f_{i,s},\ f_{i,j},\ f_{i,j-1},\ f_{i\pm1,s},\ f_{i\pm1,j},\ f_{i\pm1,j-1}\ ) \cdot W_3 & j = N_y - 1 \\ \pm(\ f_{s,j-1}, f_{s,j}, f_{s,j+1}, f_{i,j}, f_{i,j+1}, f_{i\pm1,j-1}, f_{i\pm1,j}\ ) \cdot W_4 & 0 < j < \frac{N_y}{2} \\ \mp(\ f_{s,j+1}, f_{s,j}, f_{s,j-1}, f_{i,j}, f_{i,j-1}, f_{i\pm1,j+1}, f_{i\pm1,j}\ ) \cdot W_4 & \frac{N_y}{2} <= j < N_y - 1 \end{cases}$$

It takes the upper sign for $i = 0$ and the nether sign for $i = N_x - 1$.
If $0 < i < N_x - 1$, we have

$$\begin{aligned}
\frac{\partial f(x_i, y_j, z_k)}{\partial x} &= \left(f_{i-1,j},\ f_{i+1,j} \right) \cdot W_5, \\
\frac{\partial^2 f(x_i, y_j, z_k)}{\partial x^2} &= \left(f_{i-1,j},\ f_{i,j},\ f_{i+1,j} \right) \cdot W_6, \\
\frac{\partial^2 f(x_i, y_j, z_k)}{\partial x \partial y} &=
\end{aligned}$$

$$\begin{cases}
\pm\left(f_{i\mp 1,s},\ f_{i,s},\ f_{i,j},\ f_{i\pm 1,s},\ f_{i\pm 1,j},\ f_{i\mp 1,j+1},\ f_{i,j+1} \right) \cdot W_4 & j = 0 \\
\mp\left(f_{i\mp 1,s},\ f_{i,s},\ f_{i,j},\ f_{i\pm 1,s},\ f_{i\pm 1,j},\ f_{i\mp 1,j-1},\ f_{i,j-1} \right) \cdot W_4 & j = N_y - 1 \\
\left(f_{i+1,j+1},\ f_{i+1,j-1},\ f_{i-1,j+1},\ f_{i-1,j-1} \right) \cdot W_7 & 0 < j < N_y - 1
\end{cases}$$

It takes the upper sign for $0 < i < N_x - 2$ and the nether sign for $i = N_x - 2$.
In the above expressions, $W_i, W_2, \cdots, W_7$ are vectors expressed by

$$W_1 = \frac{1}{30\ \Delta x} \begin{pmatrix} -32 \\ 15 \\ 20 \\ -3 \end{pmatrix}, \qquad W_2 = \frac{1}{(\Delta x)^2} \begin{pmatrix} 3.2 \\ -5 \\ 2 \\ -0.2 \end{pmatrix},$$

$$W_3 = \frac{1}{3\ \Delta x \Delta y} \begin{pmatrix} 4 \\ -4 \\ 4 \\ -9 \\ 5 \\ -4 \\ 5 \\ -1 \end{pmatrix}, \qquad W_4 = \frac{1}{3\ \Delta x \Delta y} \begin{pmatrix} 1 \\ 2 \\ -3 \\ -3 \\ 3 \\ -1 \\ 1 \end{pmatrix},$$

$$W_5 = \frac{1}{2\ \Delta x} \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \qquad W_6 = \frac{1}{(\Delta x)^2} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix},$$

$$W_7 = \frac{1}{4\,\Delta x \Delta y} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}.$$

These rules apply to all space derivatives of $e_1, e_2, e_3, b_1, b_2, b_3$.

D Numerical discretizations of the EOS formulations

In this section, we present the numerical discretizations of the EOS formulations of the model described by the 3D maxwell equations where the scattering object is confined in $V_1 = [x_a, x_b] \times [y_a, y_b] \times [z_a, z_b]$. Similarly as in the 1D toy models [15], for a second order accuracy solutions, we perform the Lax-Wendroff method on (2.4) and the modified Euler's method on (2.5) and we use the mid-point rules to the integrals in (2.27). Based on this, we discretize the space domain by the following non-uniform grids in V_1,

$$\begin{aligned} x_i &= x_a + (i+0.5)\Delta x, \qquad & i = 0,1,2,\cdots N_x - 1, \\ y_j &= y_a + (j+0.5)\Delta y, \qquad & j = 0,1,2,\cdots N_y - 1, \\ z_k &= z_a + (k+0.5)\Delta z, \qquad & k = 0,1,2,\cdots N_z - 1, \end{aligned} \tag{D.1}$$

with

$$\begin{aligned} \Delta x &= \frac{x_b - x_a}{N_x}, \\ \Delta y &= \frac{y_b - y_a}{N_y}, \\ \Delta z &= \frac{z_b - z_a}{N_z}, \end{aligned}$$

where N_x, N_y and N_z are positive integer numbers. The time step is designated to be

$$t_n = n\Delta t,\ n = 0,1,2\cdots,$$

where

$$\Delta t = \frac{\tau}{c_1} Min\{\Delta x, \Delta y, \Delta z\}$$

and $0 < \tau < 1$ for an explicit numerical method. If we write the vector fields using notations

$$\begin{aligned} \mathbf{E}_1 &= (e_1, e_2, e_3), \\ \mathbf{B}_1 &= (b_1, b_2, b_3), \\ \mathbf{J}_1 &= (j_1, j_2, j_3), \\ F_1 &= F(e_1, j_1), \\ F_2 &= F(e_2, j_2), \\ F_3 &= F(e_3, j_3), \end{aligned}$$

then (2.4) and (2.5) can be expanded into the following formulas

$$\partial_t e_1 = c_1^2 (\frac{\partial b_3}{\partial y} - \frac{\partial b_2}{\partial z} - \mu_1 j_1), \tag{D.2}$$

$$\partial_t e_2 = c_1^2 (\frac{\partial b_1}{\partial z} - \frac{\partial b_3}{\partial x} - \mu_1 j_2), \tag{D.3}$$

$$\partial_t e_3 = c_1^2 (\frac{\partial b_2}{\partial x} - \frac{\partial b_1}{\partial y} - \mu j_3), \tag{D.4}$$

$$\partial_t b_1 = \frac{\partial e_2}{\partial z} - \frac{\partial e_3}{\partial y}, \tag{D.5}$$

$$\partial_t b_2 = \frac{\partial e_3}{\partial x} - \frac{\partial e_1}{\partial z}, \tag{D.6}$$

$$\partial_t b_3 = \frac{\partial e_1}{\partial y} - \frac{\partial e_2}{\partial x}, \tag{D.7}$$

$$\partial_t \rho_1 = -(\frac{\partial j_1}{\partial x} + \frac{\partial j_2}{\partial y} + \frac{\partial j_3}{\partial z}), \tag{D.8}$$

$$\partial_t j_1 = (\alpha - \beta\rho_1)e_1 - \gamma j_1 = F_1, \tag{D.9}$$

$$\partial_t j_2 = (\alpha - \beta\rho_1)e_2 - \gamma j_2 = F_2, \tag{D.10}$$

$$\partial_t j_3 = (\alpha - \beta\rho_1)e_3 - \gamma j_3 = F_3. \tag{D.11}$$

Now we take a look at the solutions at the grid point (x_i, y_j, z_k) at time t_n. From Taylor series we have the following solutions to (D.2) - (D.8),

$$\phi^{n+1}_{i,j,k} = \phi^n_{i,j,k} + \Delta t(\frac{\partial \phi}{\partial t})^n_{i,j,k} + \frac{1}{2}(\Delta t)^2(\frac{\partial^2 \phi}{\partial t^2})^n_{i,j,k}, \tag{D.12}$$

where ϕ represents $e_1, e_2, e_3, b_1, b_2, b_3, \rho_1$ and

$$(\frac{\partial e_1}{\partial t})^n_{i,j,k} = c_1^2[\frac{\partial b_3}{\partial y} - \frac{\partial b_2}{\partial z} - \mu_1 j_1]^n_{i,j,k}$$

$$(\frac{\partial e_2}{\partial t})^n_{i,j,k} = c_1^2[\frac{\partial b_1}{\partial z} - \frac{\partial b_3}{\partial x} - \mu_1 j_2]^n_{i,j,k}$$

$$(\frac{\partial e_3}{\partial t})^n_{i,j,k} = c_1^2[\frac{\partial b_2}{\partial x} - \frac{\partial b_1}{\partial y} - \mu_1 j_3]^n_{i,j,k}$$

$$(\frac{\partial b_1}{\partial t})^n_{i,j,k} = (\frac{\partial e_2}{\partial z} - \frac{\partial e_3}{\partial y})^n_{i,j,k},$$

$$(\frac{\partial b_2}{\partial t})^n_{i,j,k} = (\frac{\partial e_3}{\partial x} - \frac{\partial e_1}{\partial z})^n_{i,j,k},$$

$$(\frac{\partial b_3}{\partial t})^n_{i,j,k} = (\frac{\partial e_1}{\partial y} - \frac{\partial e_2}{\partial x})^n_{i,j,k},$$

$$(\frac{\partial \rho_1}{\partial t})^n_{i,j,k} = -(\frac{\partial j_1}{\partial x} + \frac{\partial j_2}{\partial y} + \frac{\partial j_3}{\partial z})^n_{i,j,k}$$

and

$$(\frac{\partial^2 e_1}{\partial t^2})^n_{i,j,k} = c_1^2[\frac{\partial^2 e_1}{\partial y^2} - \frac{\partial}{\partial y}\frac{\partial e_2}{\partial x} - \frac{\partial}{\partial z}\frac{\partial e_3}{\partial x} + \frac{\partial^2 e_1}{\partial z^2} - \mu_1 F_1]^n_{i,j,k},$$

$$(\frac{\partial^2 e_2}{\partial t^2})^n_{i,j,k} = c_1^2[\frac{\partial^2 e_2}{\partial z^2} - \frac{\partial}{\partial z}\frac{\partial e_3}{\partial y} - \frac{\partial}{\partial x}\frac{\partial e_1}{\partial y} + \frac{\partial^2 e_2}{\partial x^2} - \mu_1 F_2]^n_{i,j,k},$$

$$(\frac{\partial^2 e_3}{\partial t^2})^n_{i,j,k} = c_1^2[\frac{\partial^2 e_3}{\partial x^2} - \frac{\partial}{\partial x}\frac{\partial e_1}{\partial z} - \frac{\partial}{\partial y}\frac{\partial e_2}{\partial z} + \frac{\partial^2 e_3}{\partial y^2} - \mu_1 F_3]^n_{i,j,k},$$

$$(\frac{\partial^2 b_1}{\partial t^2})^n_{i,j,k} = c_1^2[\frac{\partial^2 b_1}{\partial y^2} - \frac{\partial}{\partial y}\frac{\partial b_2}{\partial x} - \frac{\partial}{\partial z}\frac{\partial b_3}{\partial x} + \frac{\partial^2 b_1}{\partial z^2} + \mu_1(\frac{\partial j_3}{\partial y} - \frac{\partial j_2}{\partial z})]^n_{i,j,k},$$

$$(\frac{\partial^2 b_2}{\partial t^2})^n_{i,j,k} = c_1^2[\frac{\partial^2 b_2}{\partial z^2} - \frac{\partial}{\partial z}\frac{\partial b_3}{\partial y} - \frac{\partial}{\partial x}\frac{\partial b_1}{\partial y} + \frac{\partial^2 b_2}{\partial x^2} + \mu_1(\frac{\partial j_1}{\partial z} - \frac{\partial j_3}{\partial x})]^n_{i,j,k},$$

$$(\frac{\partial^2 b_3}{\partial t^2})^n_{i,j,k} = c_1^2[\frac{\partial^2 b_3}{\partial x^2} - \frac{\partial}{\partial x}\frac{\partial b_1}{\partial z} - \frac{\partial}{\partial y}\frac{\partial b_2}{\partial z} + \frac{\partial^2 b_3}{\partial y^2} + \mu_1(\frac{\partial j_2}{\partial x} - \frac{\partial j_1}{\partial y})]^n_{i,j,k},$$

$$(\frac{\partial^2 \rho_1}{\partial t^2})^n_{i,j,k} = -[\frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z}]^n_{i,j,k}.$$

For equations (D.9)-(D.11), the modified Euler's method is performed which gives

$$
\begin{aligned}
(\bar{j_p})^{n+1}_{i,j,k} &= (j_p)^n_{i,j,k} + \Delta t \cdot F((e_p)^n_{i,j,k}, (j_p)^n_{i,j,k}),\\
(j_p)^{n+1}_{i,j,k} &= \frac{1}{2}((j_p)^n_{i,j,k} + (\bar{j_p})^{n+1}_{i,j,k} + \Delta t \cdot F((e_p)^{n+1}_{i,j,k}, (\bar{j_p})^{n+1}_{i,j,k})),
\end{aligned}
\tag{D.13}
$$

where $p = 1, 2, 3$. The electric field and the magnetic field inside the object are aroused by the light sources located outside the scattering object so that the values of them will be effected by the values on the boundary. While the charge density and the current density are entirely induced by the changing electric field and the changing magnetic field inside the object and this generally produces discontinuity of J_1 and ρ_1 on the surface of the object. Due to this, the space derivatives of $\mathbf{E}_1$ and $\mathbf{B}_1$ near the boundary will involve the inside values and also the surface value while the space derivatives of ρ_1, j_p and $F_p, p = 1, 2, 3$ near the boundary will only involve the inside values. Here we only write down the space derivatives with respect to x of them and the same rules are applied to the space derivatives with respect to y and z. Except the internal nodes closest to the surface, the space derivatives are approximated to second order accuracy by the following standard finite difference formulas

$$
\begin{aligned}
(\frac{\partial \phi}{\partial x})^n_{i,j,k} &= \frac{\phi^n_{i+1,j,k} - \phi^n_{i-1,j,k}}{2\,\Delta x},\\
(\frac{\partial^2 \phi}{\partial x^2})^n_{i,j,k} &= \frac{\phi^n_{i+1,j,k} - 2\phi^n_{i,j,k} + \phi^n_{i-1,j,k}}{(\Delta x)^2}, \qquad 0 < i < N_x - 1.
\end{aligned}
$$

For the internal nodes closest to the surface, the following second order accuracy difference rules are applied

$$
\begin{aligned}
(\frac{\partial \phi}{\partial x})^n_{0,j,k} &= \frac{1}{2 \cdot \Delta x}(4\phi^n_{1,j,k} - 3\phi^n_{0,j,k} - \phi^n_{2,j,k}),\\
(\frac{\partial \phi}{\partial x})^n_{N_x-1,j,k} &= -\frac{1}{2 \cdot \Delta x}(4\phi^n_{N_x-2,j,k} - 3\phi^n_{N_x-1,j,k} - \phi^n_{N_x-3,j,k})
\end{aligned}
$$

where $\phi = \rho_1, j_p, F_p$, $p = 1, 2, 3$. For the electric fields $\mathbf{E}_1$ and the magnetic field $\mathbf{B}_1$, we need the space derivatives of both the first order and the second order including the mixed derivatives.

Next step, we need to discretize the boundary integral identities (2.27a) and (2.27b). We take a look at the field values at grid point $\mathbf{x}_p$, $p = 0, 1, 2, \cdots, N_s$ where

$$N_s = 2(N_x N_y + N_x N_z + N_y N_z).$$

The discretized form of (2.28) can be written as

$$
\begin{aligned}
(\mathbf{I}_e)^n_p = &-\frac{1}{4\pi}\sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z}(\mu_1 f_1 \partial_t \mathbf{J}_1(\mathbf{x}_{i,j,k}, T_1) + \frac{1}{\varepsilon_1}\mathbf{f}_3 \rho_1(\mathbf{x}_{i,j,k}, T_1)\\
&+ \frac{1}{\varepsilon_1 c_1}\mathbf{f}_2 \partial_t \rho_1(\mathbf{x}_{i,j,k}, T_1)),
\end{aligned}
$$

where

$$T_1 = t_n - \frac{|\mathbf{x}_{i,j,k} - \mathbf{x}_p|}{c_1},$$

and

$$
\begin{aligned}
f_1 &= \iiint_{V_{i,j,k}} \frac{1}{|\mathbf{x}' - \mathbf{x}_p|} \,\mathrm{d}V, \\
\mathbf{f}_2 &= \iiint_{V_{i,j,k}} \frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}_p|^2} \,\mathrm{d}V, \\
\mathbf{f}_3 &= \iiint_{V_{i,j,k}} \frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}_p|^3} \,\mathrm{d}V,
\end{aligned}
\tag{D.14}
$$

with

$$
V_{i,j,k} = [x_i - \frac{\Delta x}{2}, x_i + \frac{\Delta x}{2}] \times [y_j - \frac{\Delta y}{2}, y_j + \frac{\Delta y}{2}] \times [z_k - \frac{\Delta z}{2}, z_k + \frac{\Delta z}{2}].
$$

Notice that expressions $(D.14)$ are singular when $\mathbf{x_p}$ is located on one of the surfaces of $V_{i,j,k}$. All calculations of the singular integrals, both the singular volume integrals and the singular surface integrals in this paper will be discussed in [16]. It is observed that for vectors $\mathbf{A}$ and $\mathbf{C}$, we have the following identity

$$
\mathbf{A} \times \boldsymbol{\varphi} \times \mathbf{C} = (\mathbf{C} \cdot \mathbf{A})\boldsymbol{\varphi} - (\mathbf{A}\mathbf{C}) \cdot \boldsymbol{\varphi},
$$

and due to

$$
\begin{aligned}
\nabla' |\mathbf{x}' - \mathbf{x}| &= \frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|}, \\
\nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|} &= -\frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|^3},
\end{aligned}
$$

we get the following relationships

$$
\begin{aligned}
& \frac{1}{|\mathbf{x}' - \mathbf{x}|} (\mathbf{n}' \times \mathbf{E}_+(\mathbf{x}', T)) \times \nabla' |\mathbf{x}' - \mathbf{x}| \\
& = (\frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|^2} \cdot \mathbf{n}') \mathbf{E}_+(\mathbf{x}', T) - (\mathbf{n}' \frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|^2}) \cdot \mathbf{E}_+(\mathbf{x}', T), \\
& (\mathbf{n}' \cdot \mathbf{E}_+(\mathbf{x}', T)) \nabla' |\mathbf{x}' - \mathbf{x}| = (\frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|} \mathbf{n}') \cdot \mathbf{E}_+(\mathbf{x}', T), \\
& (\mathbf{n}' \times \mathbf{E}_+(\mathbf{x}', T)) \times \nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|} \\
& = (\mathbf{n}' \frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|^3}) \cdot \mathbf{E}_+(\mathbf{x}', T) - (\frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|^3} \cdot \mathbf{n}') \mathbf{E}_+(\mathbf{x}', T), \\
& (\mathbf{n}' \cdot \mathbf{E}_+(\mathbf{x}', T)) \nabla' \frac{1}{|\mathbf{x}' - \mathbf{x}|} = -(\frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x}' - \mathbf{x}|^3} \mathbf{n}') \cdot \mathbf{E}_+(\mathbf{x}', T).
\end{aligned}
$$

Inserting the above relationships in (2.30), we obtain

$$
\begin{aligned}
(\mathbf{B}_e)_p^n = \frac{1}{4\pi} \sum_{q=0}^{N_s} & (K_1(\mathbf{n}_q \cdot \mathbf{E}_+(\mathbf{x}_q, T_2))\mathbf{g}_3 + K_2(\mathbf{n}_q \times \partial_t \mathbf{E}_+(\mathbf{x}_q, T_2)) \times \mathbf{g}_2 \\
& + K_3(\mathbf{n}_q \cdot \partial_t \mathbf{E}_+(\mathbf{x}_q, T_2))\mathbf{g}_2 + K_4(\mathbf{n}_q \times \partial_t \mathbf{B}_+(\mathbf{x}_q, T_2))),
\end{aligned}
\tag{D.15}
$$

where

$$
T_2 = t_n - \frac{|\mathbf{x}_q - \mathbf{x}_p|}{c_1},
$$

and

$$\begin{aligned}
K_1 &= 1 - \frac{\varepsilon_1}{\varepsilon_0},\\
K_2 &= \frac{1}{c_1} - \frac{1}{c_0},\\
K_3 &= \frac{1}{c_1} - \frac{\varepsilon_1}{c_0\varepsilon_0},\\
K_4 &= (1 - \frac{\mu_0}{\mu_1})g_1,
\end{aligned}$$

with

$$\begin{aligned}
g_1 &= \int_{S_q} \frac{1}{|\mathbf{x}' - \mathbf{x}_p|}\,\mathrm{d}S',\\
\mathbf{g}_2 &= \int_{S_q} \frac{\mathbf{x}' - \mathbf{x}_p}{|\mathbf{x}' - \mathbf{x}_p|^2}\,\mathrm{d}S',\\
\mathbf{g}_3 &= \int_{S_q} \frac{\mathbf{x}' - \mathbf{x}_p}{|\mathbf{x}' - \mathbf{x}_p|^3}\,\mathrm{d}S'.
\end{aligned} \tag{D.16}$$

Similarly, in (2.27b) we obtain

$$(\mathbf{I}_b)_p^n = \frac{u_1}{4\pi}\sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z}(\frac{1}{c_1}\mathbf{f}_2 \times \partial_t\mathbf{J}_1(\mathbf{x}_{i,j,k}, T_1) - \mathbf{J}_1(\mathbf{x}_{i,j,k}, T_1) \times \mathbf{f}_3)),$$

and

$$\begin{aligned}
(\mathbf{B}_b)_p^n = \frac{1}{4\pi}\sum_{q=0}^{N_s}(&K_5(\mathbf{n}_q \times \mathbf{B}_+(\mathbf{x}_q, T_2)) \times \mathbf{g}_3 + K_5(\mathbf{n}_q \times \partial_t\mathbf{B}_+(\mathbf{x}_q, T_2)) \times \mathbf{g}_2\\
&+ K_2(\mathbf{n}_q \cdot \partial_t\mathbf{B}_+(\mathbf{x}_q, T_2))\mathbf{g}_2 + K_6(\mathbf{n}_q \times \partial_t\mathbf{E}_+(\mathbf{x}_q, T_2))),
\end{aligned} \tag{D.17}$$

with

$$\begin{aligned}
K_5 &= \frac{1}{c_1} - \frac{\mu_0}{c_0\mu_1},\\
K_6 &= (\frac{1}{c_0^2} - \frac{1}{c_1^2})g_1.
\end{aligned}$$

It is clear that when the integrating point $\mathbf{x}'$ and the observing point $\mathbf{x}$ are in the same integral grid S_q, which indicates $q = p$, expressions in (D.16) are singular. The calculations of this type of sigular integrals can also be found in [16]. There are so far unknown terms on the right side of the equations of (D.15) and (D.17) due to the time derivatives $\partial_t\mathbf{E}(\mathbf{x}_q, T_2)$ and $\partial_t\mathbf{B}(\mathbf{x}_q, T_2)$ when $p = q$. Moving these unknown terms out of the summation, (D.15) and (D.17) can be compactly written as

$$\begin{aligned}
(\mathbf{B}_e)_p^n &= \sum_{q\neq p}(\mathbf{E}_r)_q + (\mathbf{E}_r)_p,\\
(\mathbf{B}_b)_p^n &= \sum_{q\neq p}(\mathbf{B}_r)_q + (\mathbf{B}_r)_p
\end{aligned}$$

where $\mathbf{E}_r$ and $\mathbf{B}_r$ are respectively the short notations of the right terms of (D.15) and (D.17) that are going to be summed up. For $p = q$, due to symmetric of $\mathbf{x}' - \mathbf{x}$ on S_q, there are

$$\mathbf{g}_2 = 0,$$

and

$$\mathbf{g}_3 = 0.$$

And this yields

$$\begin{aligned}
(\mathbf{E}_r)_p &= \frac{1}{4\pi} K_4 \ \mathbf{n}_p \times \partial_t \mathbf{B}_p^n \\
&= \frac{1}{4\pi} K_4 \ \mathbf{n}_p \times \frac{1}{\Delta t}(\frac{3}{2}\mathbf{B}_p^n - 2\mathbf{B}_p^{n-1} + \frac{1}{2}\mathbf{B}_p^{n-2}). \\
(\mathbf{B}_r)_p &= \frac{1}{4\pi} K_6 \ \mathbf{n}_p \times \partial_t \mathbf{E}_p^n \\
&= \frac{1}{4\pi} K_6 \ \mathbf{n}_p \times \frac{1}{\Delta t}(\frac{3}{2}\mathbf{E}_p^n - 2\mathbf{E}_p^{n-1} + \frac{1}{2}\mathbf{E}_p^{n-2}),
\end{aligned}$$

where we have used the second order polynomial approximation on the time derivatives. After moving unknowns $\mathbf{E}_p^n$ and $\mathbf{B}_p^n$ from the right of the equation to the left, we finally get a solving system

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_p^n \\ \mathbf{B}_p^n \end{pmatrix} = \begin{pmatrix} \mathbf{E}_R \\ \mathbf{B}_R \end{pmatrix}, \tag{D.18}$$

where

$$\begin{aligned}
\mathbf{E}_R &= (\mathbf{I}_e)_p^n + (\mathbf{O}_e)_p^n + \sum_{q \neq p} (\mathbf{E}_r)_q + \frac{1}{4\pi} K_4 \ \mathbf{n}_p \times \frac{1}{\Delta t}(-2\mathbf{B}_p^{n-1} + \frac{1}{2}\mathbf{B}_p^{n-2}), \\
\mathbf{B}_R &= (\mathbf{I}_b)_p^n + (\mathbf{O}_b)_p^n + \sum_{q \neq p} (\mathbf{B}_r)_q + \frac{1}{4\pi} K_6 \ \mathbf{n}_p \times \frac{1}{\Delta t}(-2\mathbf{E}_p^{n-1} + \frac{1}{2}\mathbf{E}_p^{n-2}),
\end{aligned}$$

and $(\mathbf{O}_e)_p^n$ and $(\mathbf{O}_b)_p^n$ are respectively the effect on the surface point x_p at time t_n induced by the outside source which are calculated directly from the sources, and

$$\begin{aligned}
M_{11} &= I + \frac{1}{2}(\frac{\varepsilon_1}{\varepsilon_0} - 1)\mathbf{nn} \\
M_{12} &= -\frac{3}{8\pi\Delta t} K_4 m \\
M_{21} &= -\frac{3}{8\pi\Delta t} K_6 m \\
M_{22} &= I + \frac{1}{2}(1 - \frac{\mu_0}{\mu_1})\mathbf{nn}
\end{aligned}$$

with

$$m = \begin{pmatrix} 0 & -n_2 & n_1 \\ n_2 & 0 & -n_0 \\ -n_1 & n_0 & 0 \end{pmatrix},$$

where n_0, n_1 and n_2 are the three components of the normal field $\mathbf{n}$ at the surface point $\mathbf{x}_p$ and I is a 3×3 identity matrix. Equations (D.12) and (D.13) together with (D.18) are the final discretized form of the EOS formulations of model (2.4) and (2.5).

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