Transient Electromagnetic Analysis of Complex Penetrable Scatterers using Volume Integral Equations

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ABSTRACT

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Simulation tools capable of analyzing electromagnetic (EM) field/wave interactions on complex penetrable scatterers have applications in various areas of engineering ranging from the design of integrated antennas to the subsurface imaging. EM simulation tools operating in the time domain can be formulated to directly solve the Maxwell equations or the integral equations obtained by enforcing fundamental field relations or boundary conditions. Time domain integral equation (TDIE) solvers offer several benefits over differential equation solvers: They require smaller number discretization elements/sampling points (both in space and time). Despite the advantages, TDIE solvers suffer from increased computational cost, stability issues of the time-marching algorithms, and limited applicability to complex scatterers. This thesis is focused on addressing the last two issues associated with time domain volume integral equation (TD-VIE) solvers, as the issue of increased computational cost has been addressed by recently developed acceleration methods. More specifically, four new closely-related, but different marching on-in-time (MOT) algorithms are formulated and implemented to solve the time domain electric and magnetic field volume integral equations (TD-EFVIE and TD-MFVIE). The first algorithm solves the TD-EFVIE to analyze EM wave interactions on high-contrast dielectric scatterers. The stability of this MOT scheme is ensured by using two-sided approximate prolate spherical wave (APSW) functions to discretize the time dependence of the unknown current density as well as an extrapolation scheme to restore the causality of matrix
system resulting from this discretization. The second MOT scheme solves the TD-MFVIE to analyze EM wave interactions on dielectric scatterers. The TD-MFVIE is cast in the form of an ordinary differential equation (ODE) and the unknown magnetic field is expanded using spatial basis functions. The time-dependent coefficients of this expansion are found by integrating the resulting ODE system using a linear multistep method. The third method is formulated and implemented to analyze EM wave interactions on scatterers with Kerr nonlinearity. The former scheme integrates in time a coupled of system of the TD-EFVIE and the nonlinear constitutive relation, which is cast in the form of an ODE system, for the expansion coefficients of the electric field and flux using a linear multistep method. The last method described in this thesis is developed to analyze EM wave interactions on ferrite scatterers.
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Chapter 1

Introduction

Electromagnetic simulation tools for analyzing electromagnetic field/wave interactions on complex scatterers with arbitrary shape have many applications in different areas of engineering ranging from the design of electromagnetic and optical devices and systems [1, 2, 3] to electromagnetic coupling and interference analysis on electrically large platforms [4, 5, 6, 7] and electromagnetic imaging in biomedicine [8, 9, 10] and geophysics [11, 12]. These simulation tools make use of either frequency- or time-domain techniques to solve the Maxwell equations and compute the electromagnetic fields in the problem domain. Frequency-domain techniques model the problem under the assumption of time harmonic excitation (and solution oscillating with the frequency of excitation) and are the most suitable when the analysis is to be carried out over a narrow band of frequencies and the constitutive relations are linear (material properties are not functions of electromagnetic fields). However, when the assumption of linearity is not satisfied or when a broadband analysis is required, time domain techniques are the natural alternative [13, 14, 15].

Time-domain techniques are based on either differential-equation or integral-equation formulation. The most popular differential-equation solvers are finite difference time domain (FDTD) methods [16, 17, 18, 19], where the Maxwell equations are approximated using finite differences (both in space and time) and solved for the unknown samples of fields using time marching. The popularity of FDTD methods can be ascribed to the simplicity of the formulation and the implementation. Time domain finite element method (TD-FEM) is another differential-equation solver [20, 13]. The
unknown fields are expanded using spatial and temporal basis functions, the expansion is inserted into the Maxwell equations, and the resulting equation is converted into a matrix system by testing in space and time. This system is solved for unknown expansion coefficients by time marching, which can be explicit or implicit depending on the type of temporal basis function and time-step size used.

Even though differential equation solvers are popular among the computational electromagnetics (CEM) research community and users of electromagnetic simulation tools, they have several limitations: (i) Unbounded physical domain has to be truncated into a (bounded) computational domain using some artificial boundaries and approximate absorbing conditions (enforced on these boundaries) to imitate field/wave behavior at infinity. The effectiveness of these boundary conditions in reducing reflections from the artificial boundaries is one of the factors that determine the accuracy of the simulation. To make sure that the reflections do not interfere with the “actual” fields, the artificial boundaries have to be introduced at a certain distance from the scatterer. This increases the size of the computational domain, and consequently the amount of computational resources needed for the simulation. (ii) Oftentimes, the time-step size required by a differential-equation solver has to satisfy the Courant condition [21, 19], which gives a relationship between the sizes of the largest time-step allowed and the smallest spatial discretization element.

Time domain integral equation (TDIE) solvers are free from such limitations [22, 23, 24]. TDIE solvers represent the field scattered from an object as spatio-temporal convolutions of the unknown currents/fields induced in the volume or on the surface of the object and the Green function of the background medium where the object resides. Then, an integral equation (in unknown currents/fields) is obtained by enforcing a fundamental field relation or a boundary condition on the scattered field. This approach has several advantages: (i) Only volume/surface of the scatterer is discretized since the unknowns reside on the volume/surface of the scatterer. (ii)
There is no need for approximate absorbing boundary conditions since the Green function implicitly enforces the radiation condition at infinity.

To numerically solve a TDIE, the unknown fields/currents are expanded using spatial and temporal basis functions. This expansion is inserted into the TDIE, and the resulting equation is tested in space and time yielding a lower triangular system of equations. This system can be solved for the unknown expansion coefficients using a marching on-in-time (MOT) scheme. At each time step, a smaller system of equations, termed MOT system in this thesis, is solved for the unknown coefficients of the field/current expansion. The right-hand side of this system consists of the tested incident field and discretized “past” interactions. The “past” interactions are calculated using a spatio-temporal convolution of the Green function with the basis functions weighted with the expansion coefficients obtained in the previous time steps. Based on the time-step size, the discretization, and the testing procedure, the MOT matrix to be inverted can be diagonal or sparse, resulting in an explicit or implicit time stepping scheme, respectively [25, 26, 24, 27].

It should be mentioned here that for a perfect electric conductor or a piecewise homogeneous scatterer, unknown fields/currents are bound to the surface of the conductor or the interface between the two (homogeneous) regions with different material properties. Then the spatio-temporal convolution is computed over a surface. On the other hand, if the scatterer is heterogeneous, the unknown fields/currents are defined in the volume of the scatterer and the spatio-temporal convolution is computed over a volume.

Despite the advantages the TDIE solvers described before, they have not been as popular as the differential-equation solvers. This can be attributed to the late time instabilities and the high computational cost of the classical MOT solution, which is briefly described above. Recent advancements have significantly improved the stability of the MOT schemes. These include the use of implicit time stepping
methods [28], band limited temporal basis functions [29], and space-time Galerkin schemes [30, 31, 32]. Two classes of accelerators have been developed to address the high computational complexity of the MOT schemes: the multilevel plane wave time domain (PWTD) algorithm [33, 34, 35] and the time domain adaptive integral method (TD-AIM) [36, 37, 38]. These algorithms perform a faster evaluation of the transient electromagnetic fields produced by known band-limited sources, using less memory. The PWTD algorithm uses plane wave decompositions and diagonal translation operators to accelerate the computation of transient wave fields. On the other hand, TD-AIM uses blocked fast Fourier transforms to compute the convolution involving the Green function.

In wake of these advancements, the work presented in this thesis is aimed at advancing the MOT-based TDIE solvers for analyzing complex scatterers that are heterogeneous, high-contrast, nonlinear, dispersive, and anisotropic. To this end, several novel MOT schemes are formulated and developed with increasing capabilities for solving time domain volume integral equations (TD-VIEs) enforced on scatterers with increasing complexity in their material properties. These solvers are developed one step at a time but they complement each other in terms of formulation as well as implementation. While moving from one solver to another, bottlenecks are addressed to increase the solver’s applicability.

At the first stages, a stable implicit MOT scheme for solving the time domain electric field volume integral equation (TD-EFVIE) enforced on high-contrast dielectric scatterers is developed. It is well known that high-contrast often results in instability in the MOT solution of the matrix equations resulting from the discretization of the TD-EFVIE [39]. For a stable MOT system, the spatial and temporal discretization has to be performed accurately. It has been observed that Lagrange interpolators, which are usually used by the MOT schemes as temporal basis functions [28], result in inaccurate computation of the matrices, which in return yields an unstable solution.
To overcome this problem, approximate prolate spherical wave (APSW) functions are used as temporal basis functions in expanding the unknown current density. However, since APSW functions are “two-sided” interpolators, i.e., require the knowledge of unknown “future” current samples, the resulting system (in unknown time dependent expansion coefficients) cannot be solved using a traditional MOT scheme. In this thesis, a new extrapolation technique is developed to restore the causality. The extrapolation coefficients are “trained” using decaying and oscillating exponentials, which follow the physical behavior of the fields/currents induced inside a dielectric scatterer. Consequently, the resulting time marching algorithm is significantly more accurate and stable than existing schemes. However, when the contrast of the scatterer is very high, the MOT matrix resulting from the discretization of the TD-EFVIE becomes ill conditioned. This means that the iterative solution of this matrix system, which is required by the implicit MOT scheme at every time step, becomes very slow. Consequently, the overall computation time increases significantly. To address this bottleneck one can solve the time domain magnetic field volume integral equation (TD-MFVIE) instead of the TD-EFVIE. To this end, an (explicit) MOT scheme that calls for the solution of a well-conditioned matrix (regardless of the value of the contrast) is formulated and developed as briefly described next.

Thanks to its second kind nature, the TD-MFVIE can be cast in the form of an ordinary differential equation (ODE), which relate the unknown magnetic field (induced in the scatterer) to its temporal derivative. The magnetic field is expanded using the fully linear curl-conforming basis functions; inserting this expansion in the TD-MFVIE and spatially testing the resulting equation yields a time dependent (semi-discretized) ODE system. A predictor-corrector algorithm, PE(CE)$_n$, is used to integrate this system in time for the coefficients of the unknown expansion. To facilitate the computation of the retarded time integrals, which express...
the scattered magnetic field in terms of the unknown magnetic field on the scatterer, at discrete time steps as required by PE(CE)
m, APSW functions \[29\] are used as interpolators. The resulting time marching algorithm calls for the solution of a system with a (spatial) Gram matrix at the evaluation (E) step. If Galerkin testing is used, the Gram matrix is sparse and well conditioned, and the solution is obtained using an iterative solver. If point testing is used, the Gram matrix consists of four diagonal sub-matrices. Its inverse (which also consists of four diagonal sub-matrices) is computed and stored before the time marching starts. Consequently, the matrix solution required at the evaluation step, is obtained with a simple multiplication of the right-hand side with the inverse of the Gram matrix. The resulting MOT schemes are expected to be more efficient than their implicit counterparts, which call for the inversion of a matrix system that gets denser as the time step size gets larger with decreasing frequency. Additionally, unlike the MOT scheme developed for solving the TD-EFVIE, the efficiency of this new scheme does not degrade as the contrast of the scatterer increases.

The last two stages of the work described in this thesis focus on enabling the application of the two MOT schemes briefly described above to nonlinear and anisotropic scatterers, respectively. However, these are not straightforward tasks, they require coupled solution of TD-VIEs with complex constitutive relations as described next.

First, scatterers with Kerr nonlinearity are considered. Simulation tools that can accurately model the electromagnetic wave/field on this type of scatterers are useful in design of various types of photonic/electromagnetic devices used for higher-harmonic generation, self-wave modulation, self-focusing, and wave mixing \[46\]. To this end, in this work, an explicit MOT scheme for solving the TD-EFVIE enforced on Kerr nonlinear scatterers is proposed. The formulation and implementation steps of this solver follow those of the TD-EFVIE and TD-MFVIE solvers described above while it accounts for the material nonlinearity by enforcing the constitutive relation between
the electric field intensity and flux density as an auxiliary equation. This equation relation and the TD-EFVIE are discretized together by expanding the electric field intensity and flux density, separately. The coupled system of equations are tested in space, and the resulting system is integrated in time for the unknown expansion coefficients using a linear multistep PE(CE)^m method \[47\]. The explicitness of the MOT scheme allows for incorporation of the nonlinearities as simple discretized function evaluations on the right-hand side of the system. An implicit counterpart would require an expensive Newton like nonlinear solver at every time step to perform similar analysis. Next, scatterers made of ferrite materials are considered. Magnetization inside a ferrite can be controlled using an external DC bias, resulting in a tunable permeability that is generally dispersive and anisotropic. Henceforth, ferrites form building blocks in the design of reconfigurable microwave devices such as like circulators, isolators, phase shifters, and patch antennas \[48, 49, 50\]. Electromagnetic analysis of ferrite-based devices requires solution of the coupled system of Maxwell equations and the Landau-Lifshitz-Gilbert (LLG) equation \[51, 52, 53\], that models the nonlinear dynamics of magnetization inside ferrite materials. To this end, in this work, an explicit MOT scheme for solving the coupled system of the LLG equation and the TD-MFVIE. Similar to the explicit MOT scheme for solving the TD-EFVIE enforced on Kerr nonlinear scatterers, the LLG and the TD-MFVIE are discretized together by expanding magnetic field intensity and the flux density, separately. The coupled system of equations is tested in space, and the resulting matrix system is cast in the form of an ODE system. The coefficients of the unknown expansion coefficients of the field intensity and flux density are obtained by integrating this ODE system by a linear multistep PE(CE)^m method \[47\].

Rest of this thesis is organized as follow. Chapter 2 describes the implicit MOT-TD-EFVIE solver that provides stable results with high-contrast scatterers. Chapter 3 present two explicit MOT-TD-MFVIE solvers, whose efficiency do not degrade even
when the contrast increases. Chapter 4 describes an explicit MOT-TD-EFVIE solver developed for analyzing scattering from scatterers with Kerr nonlinearity. Chapter 5 present the explicit MOT-TD-MFVIE solver used for studying wave interactions on magnetized ferrites. Finally, Chapter 6 concludes the thesis with directions for future research.
Chapter 2

A Time Domain Electric Field Volume Integral Equation Solver for Analyzing High-Contrast Scatterers

2.1 Introduction

In time domain electric field volume integral equation (TD-EFVIE) [39], the scattered electric field is represented as a spatio-temporal convolution of the unknown electric flux density induced inside the scatterer with the Green function of the background medium. Then, the TD-EFVIE is constructed by setting the summation of the incident and scattered electric fields to the total electric field, which is represented in terms of the electric flux density, on the volumetric support of the scatterer.

To numerically solve the TD-EFVIE, first, the unknown electric flux density is expanded in terms of spatial and temporal basis functions. Inserting this expansion into the TD-EFVIE and testing the resulting equation at discrete times yield a lower triangular system of equations that is solved by the marching on-in-time (MOT) scheme. At each time step, a smaller system of equations, termed MOT system here, is solved for the unknown coefficients of the flux expansion. The right-hand side of this system consists of the tested incident field and discretized spatio-temporal convolution of the “past” electric flux density (represented in terms of spatio-temporal basis functions weighted with the expansion coefficients computed at the previous time steps) and the Green function.

To obtain an accurate and stable solution by time marching, the MOT matrices must be computed accurately [54]. The Lagrange polynomials (LP) [28 55 56],
which are used as temporal basis functions/interpolators to enable the computation of retarded-time integrals in the scattered electric field representation, provide reasonable accuracy, but are not band-limited and introduce out-of-band errors that eventually ignite instabilities in the MOT solution [29, 57]. Additionally, they have discontinuous derivatives that may introduce additional numerical errors when quadrature rules are used to compute the convolution integrals [41, 31]. These problems have been alleviated using “exact” integration techniques [58, 59, 60, 61, 62, 63, 64, 65, 66] to partially avoid quadrature rules, separable approximations to spatio-temporal convolutions [41, 31] to avoid discontinuities in integration domains, and band-limited approximate prolate spherical wave (APSW) functions with continuous derivatives [67] to replace LP based temporal basis functions [29, 57]. For a given temporal duration, APSW functions have the minimum bandwidth, which significantly increases the accuracy of the interpolation. However, APSW interpolators are “two-sided”, i.e., they require samples of the function to left and right of the data point being interpolated. Consequently, when they are used as temporal basis functions during time marching, they call for “future” samples of currents/fields that are not computed yet, destroying the causality of time marching. MOT scheme’s causality can be restored by extrapolating future samples from past samples that are already computed in the previous time steps.

In [29, 57], a scheme, which computes extrapolation coefficients using temporal samples of sine and cosine functions with discrete frequencies within the bandwidth of excitation, is proposed (i.e., the extrapolation scheme is trained using samples of sine and cosine functions). This scheme assumes that the solution can accurately be represented by pure harmonics, $e^{j\omega t}$, where $\omega$ is the angular frequency, $t$ is the time, and $j = \sqrt{-1}$; and hence it is termed “harmonic function based extrapolation (HE)” in this thesis. As long as this assumption is valid, the HE scheme works well. Indeed, MOT schemes, which use APSW interpolators as temporal basis functions and HE
scheme to restore the causality of time marching, have been shown to yield highly stable solutions when used in solving the time domain surface integral equations [29, 57].

On the other hand, when these HE-enhanced MOT schemes are used in solving the TD-EFVIE, they fail to produce stable results especially for high-contrast dielectric scatterers [68]. This is due to the fact that the temporal behavior of the electromagnetic modes induced inside lossless dielectric scatterers has decaying components as well as oscillating ones [69, p. 697] (i.e., they have complex exponents and can be represented as $e^{-\alpha t + j\omega t}$, where $\alpha$ is a positive real number). This means that the HE scheme can not be used for accurately extrapolating the temporal samples of the fields within the MOT-TD-EFVIE solver, which leads to instability. Additionally, as the contrast of the scatterer increases, the number of modes within the bandwidth of excitation increases. In other words, higher-contrast translates into poorly stable MOT system.

In this chapter, a new extrapolation scheme is used within an MOT-TD-EFVIE solver that uses APSW interpolators as temporal basis functions. This scheme assumes that the MOT solution can be accurately represented in terms of decaying and oscillating exponentials; hence it is termed “complex exponent based extrapolation (CEE)” in this thesis. The coefficients of the CEE scheme are trained using samples of exponentials with exponents on the complex frequency plane. To carry out the sampling in frequency, a semi-disk with radius equal to the maximum frequency of excitation is used [70]. Extrapolation coefficients are computed using the samples with the “most important” complex frequencies located on the semi-disk boundary. These locations are determined by “matrix skeletonization” [71]. This operation is fully error controllable and leads to a highly accurate extrapolation scheme. More importantly, by design, the CEE scheme captures the temporal behavior of the modes induced inside the dielectric scatterers more accurately than the HE scheme (since
it is trained using complex frequencies within the bandwidth of excitation). Indeed, unlike the HE-enhanced TD-EFVIE solver, the proposed MOT scheme maintains its stability even when applied in characterization of transient electromagnetic fields on high-contrast scatterers.

The remainder of this chapter is organized as follows: Section 2.2 describes the proposed MOT-TD-EFVIE solver. Sections 2.2.1, 2.2.2, 2.2.3, 2.2.4, and 2.2.5 respectively, presents the formulation of the TD-EFVIE, expounds the discretization scheme, motivates the choice of temporal basis function and reviews the properties of APSW interpolators, explains short-comings of the HE scheme when applied to the MOT-TD-EFVIE solver, and proposes the CEE scheme to significantly enhance the stability of the MOT-TD-EFVIE solver. Section 2.3 demonstrates the stability and accuracy of the proposed MOT-TD-EFVIE solver, which uses the APSW interpolator and CEE scheme, in characterizing transient electromagnetic wave interactions on high-contrast dielectric scatterers via numerical experiments.
2.2 Formulation

2.2.1 Time Domain Electric Field Volume Integral Equation

Let $V$ denote the support of linear, isotropic, non-magnetic, non-dispersive, lossless, and inhomogeneous dielectric scatterers residing in an unbounded background medium. Permittivity and permeability in $V$ and the background medium are $\varepsilon(r)$ and $\varepsilon_0$ and $\mu_0$, respectively. An incident electric field $E^{\text{inc}}(r, t)$ excites $V$. It is assumed that $E^{\text{inc}}(r, t)$ is vanishingly small for $t \leq 0$, $\forall r \in V$ and essentially band-limited to frequency $f_{\text{max}}$. In response to this excitation, equivalent volumetric current $J(r, t)$ is induced in $V$ and it generates the scattered electric field $E^{\text{sca}}(r, t)$. $E^{\text{sca}}(r, t)$ is represented in terms of retarded-time potentials:

$$E^{\text{sca}}(r, t) = -\frac{\mu_0}{4\pi} \int_{V} \frac{\partial_{t'} J(r', t')|_{t'=t-R/c_0}}{R} dv' + \frac{1}{4\pi \varepsilon_0} \nabla \int_{0}^{t-R/c_0} \int_{V} \nabla' \cdot \frac{J(r', t')}{R} dt' dv'.$$  \hspace{1cm} (2.1)

Here, $\partial_t$ denotes the time derivative, $R = |r - r'|$ is the distance between source and observation points $r'$ and $r$, $c_0 = 1/\sqrt{\varepsilon_0 \mu_0}$ is the speed of the light in the background medium. In $V$, $J(r, t)$ is expressed as

$$J(r, t) = \kappa(r) \partial_t D(r, t)$$  \hspace{1cm} (2.2)

where $\kappa(r) = 1 - \varepsilon_0/\varepsilon(r)$ is the dielectric contrast, and $D(r, t)$ is the electric flux density. Total electric field $E(r, t)$, $E^{\text{inc}}(r, t)$, and $E^{\text{sca}}(r, t)$ satisfy

$$E(r, t) = E^{\text{inc}}(r, t) + E^{\text{sca}}(r, t) = D(r, t)/\varepsilon(r).$$  \hspace{1cm} (2.3)

Inserting (2.2) into (2.1) and the resulting equation into (2.3) and enforcing the final equation for $r \in V$ yield the TD-EFVIE in unknown $D(r, t)$.
\[ E^{\text{inc}}(r, t) = \frac{D(r, t)}{\varepsilon(r)} + \frac{\mu_0}{4\pi} \int_V \frac{\kappa(r') \partial^2 D(r', t')}{R} \left|_{t' = t - R/c_0} \right. \, dv' \]
\[ - \frac{1}{4\pi\varepsilon_0} \nabla \int_V \left\{ \nabla' \cdot \left[ \kappa(r') D(r', t') \right] \right\} \left|_{t' = t - R/c_0} \right. \, dv'. \]

The TD-EFVIE (2.4) is discretized and solved for the samples of \( D(r, t) \) using the MOT scheme as described in the next section.

### 2.2.2 Discretization and Marching On in Time Scheme

To numerically solve the TD-EFVIE (2.4), first, \( V \) is discretized into tetrahedral elements. Then, the unknown electric flux density \( D(r, t) \) is approximated in terms of spatial and temporal basis functions, \( f_{k'}(r) \) and \( T_{l'}(t) \):

\[ D(r, t) \approx \sum_{k'=1}^{N_k} \sum_{l'=0}^{N_t} I_{k',l'} f_{k'}(r) T_{l'}(t) \]  

(2.5)

where \( I_{k',l'} \) are the unknown expansion coefficients associated with \( k' \)th spatial and \( l' \)th temporal basis functions. Here, \( f_{k'}(r) \) are the well-known divergence-conforming Schaubert-Wilton-Glisson (SWG) basis functions, each of which is defined on the triangular face shared by a pair of tetrahedrons \( \{77\} \). The SWG basis function associated with face \( k \) is given as

\[ f_k(r) = \begin{cases} \pm \frac{|A_k|}{3|V_k^\pm|} (r - r_k^\pm), & r \in V_k^\pm \\ 0, & \text{elsewhere} \end{cases} \]

(2.6)

Here, \( A_k = V_k^+ \cap V_k^- \) and \( V_k^\pm \) represent the supports of face \( k \) and the tetrahedrons on its either side, respectively, \( r_k^\pm \) are the free nodes of \( V_k^\pm \) (\( r_k^\pm \in V_k^\pm \) but \( r_k^\pm \notin A_k \)), \( |V_k^\pm| \) are the volumes of \( V_k^\pm \), and \( |A_k| \) is the area of \( A_k \). It should be noted here that
if the face $k$ is on the surface of the scatterer, $f_k(r)$ is defined only on tetrahedron $V_k^+$. Also, it is assumed that the permittivity and contrast are constant inside a given tetrahedron, i.e., $\varepsilon_k(r) = \varepsilon_k^+$ and $\kappa_k(r) = \kappa_k^+$ for $r \in V_k^+$. In (2.5), $T_{l'}(t) = T(t - l'\Delta t)$ are the temporal basis functions constructed by shifting the interpolation function $T(t)$ by $l'\Delta t$. Here, $\Delta t$ is the time step size. Inserting (2.5) into (2.4) and testing the resulting equation with $t_k(r) = \kappa_k(r)f_k(r)$, $k = 1, ..., N$, at times $t = l\Delta t$ yield the MOT system

$$V_l = \sum_{l' = l_{\min}}^{l+N_T-1} Z_{l-l'} I_{l'} , l = 1, ..., N_t. \quad (2.7)$$

Here, $l_{\min} = \max(1, l - N_g)$, $N_g = \floor{(D_{\max}/c_0)/\Delta t + N_T^p}$, $D_{\max}$ is the maximum distance between two points in $V$, and $N_T^p$ and $N_T^f$ are the durations of $T(t)$ (in time steps) in domains $t > 0$ (past) and $t < 0$ (future), respectively. Elements of the tested incident field and unknown coefficient vectors, $V_l$ and $I_{l'}$, and the MOT matrices $Z_{l-l'}$ are

$$\{V_l\}_k = \int_{V_k} t_k(r) \cdot E_{l\Delta t}(r, l\Delta t) dv \quad (2.8)$$

$$\{I_{l'}\}_{k'} = I_{k',l'} \quad (2.9)$$

$$\{Z_{l-l'}\}_{k,k'} = \int_{V_k} t_k(r) \cdot f_{k'}(r) T_{l'}(l\Delta t)\frac{1}{\varepsilon_k(r)} dv \quad (2.10)$$

$$+ \frac{\mu_0}{4\pi} \int_{V_k} t_k(r) \cdot \int_{V_{k'}} \kappa_{k'}(r') f_{k'}(r') \frac{\partial^2 T_{l'}(t)|_{t = l\Delta t - R/c_0}}{R} dv' dv$$

$$+ \frac{1}{4\pi\varepsilon_0} \int_{V_k} \nabla \cdot t_k(r) \int_{V_{k'}} \nabla' \cdot [\kappa_{k'}(r') f_{k'}(r')] T_{l'}(l\Delta t - R/c_0) \frac{1}{R} dv' dv$$
where \( V_k = V_k^+ \cup V_k^- \) is the support of \( f_k(r) \). The divergence operation in the last term of the \( \{ Z_{l-l'} \}_{k,k'} \) is expanded as \( \nabla \cdot [ \kappa_k(r) f_k(r) ] = f_k(r) \cdot \nabla \kappa_k(r) + \kappa_k(r) \nabla \cdot f_k(r) \).

Since \( \kappa_k(r) \) is a discontinuous function across \( A_k \), \( f_k(r) \cdot \nabla \kappa_k(r) \) is evaluated using

\[
f_k(r) \cdot \nabla \kappa_k(r) = \begin{cases} \kappa_k^+ - \kappa_k^-, r \in A_k \\ 0, \text{otherwise.} \end{cases}
\] (2.11)

Consequently, volume integral, which involves the term \( f_k(r) \cdot \nabla \kappa_k(r) \) and is defined over \( V_k \), is reduced to a surface integral defined over \( A_k \).

The MOT scheme casts the system (2.7) into the form

\[
Z_0 I_l = V_l - \sum_{l' = I_{\text{min}}}^{l-1} Z_{l-l'} I_{l'} - \sum_{l' = l+1}^{l + N^T - 1} Z_{l-l'} I_{l'}, \quad l = 1, ..., N_t
\] (2.12)

which is solved for \( I_l \) at the time step \( l \). Here, the matrix \( Z_0 \) represents instantaneous interactions and the second and third terms on the right hand side are the contributions to the electric field at time step \( l \) from “past” and “future” samples of the flux density, respectively. If \( N_t^T = 1 \), there is no contribution from the future samples. Consequently, the MOT system is discretely causal and \( I_l, l = 1, ..., N_t \), are computed via time marching with no further modification to (2.12). On the other hand, if \( N_t^T > 1 \), time marching becomes non-causal and one needs to know \( I_{l'}, l' = l + 1, ..., l + N_t^T - 1 \), to compute \( I_l \). This difficulty is overcome by casting (2.12) into a causal form using an extrapolation scheme.

### 2.2.3 Temporal Basis Function

It is clear from (2.4) that \( E^{\text{sc}}(r,t) \) is expressed in terms of retarded-time integrals of \( D(r,t) \). However, \( D(r,t) \) is sampled at \( t = l \Delta t \), which calls for an interpolation function to evaluate \( D(r,t - R/c_0) \) in the convolution integrals. This is the reason why the expansion in (2.5) uses the temporal basis function \( T(t) \). A common choice
of \( T(t) \) is the piecewise continuous LP interpolator, first proposed in [28]. For this choice of temporal basis function, \( N^T_I = 1 \) and \( N^T_P = p \), [see (2.7) and (2.12)] where \( p \) is the order of the LPs used. This makes the MOT system (2.12) discretely causal as explained in Section 2.2.2. Fig. 2.2 plots \( T(t) \) for \( p = 3 \). Since \( T(t) \) is limited in time, its spectrum might extend beyond the maximum frequency of excitation \( f_{\text{max}} \).

Additionally, derivatives of LP are discontinuous at \( t = l \Delta t \). It has been conjectured before that these two factors reduce the accuracy of the MOT solution and also cause the well-known late time instability problem [59, 60, 61, 62, 63, 64, 65, 66, 41]. To alleviate these problems, use of APSW interpolators as temporal basis functions has been suggested [29, 57]. The APSW interpolator is expressed as [67]

\[
T(t) = \frac{\sin(\omega_0 t)}{\omega_0 t} \frac{\sin \left( \Omega_0 N_{\text{hw}} \Delta t \sqrt{t^2/(N_{\text{hw}} \Delta t)^2 - 1} \right)}{\sinh(\Omega_0 N_{\text{hw}} \Delta t) \sqrt{t^2/(N_{\text{hw}} \Delta t)^2 - 1}} \tag{2.13}
\]

where \( \omega_0 = \pi/\Delta t \) and \( \Omega_0 = \omega_0 - 2\pi f_{\text{max}} \). \( T(t) \) is vanishingly small for \( |t| > N_{\text{hw}} \Delta t \), and therefore \( N^T_P = N^T_I = N_{\text{hw}} \). Fig. 2.2 plots \( T(t) \) with \( N^T_P = N^T_I = N_{\text{hw}} = 5 \) and compares it to \( T(t) \) constructed using third order LPs (\( N^T_I = 1 \) and \( N^T_P = 3 \)). The APSW interpolators have several advantages when used as temporal basis functions in an MOT scheme: (i) They are band-limited therefore they suppress high-frequency numerical errors that deteriorate the stability and accuracy of the solution. (ii) For a given bandwidth, APSW interpolators have the shortest temporal support possible, i.e., \( (N^T_P + N^T_I) \Delta t \) is as small as possible. This reduces the computational cost of evaluating \( Z_{l-l'} \) in (2.10). (iii) APSW interpolators have continuous derivatives. This ensures that the integrands in the elements of \( Z_{l-l'} \) do not have jumps/discontinuities throughout the integration domain, and therefore increases the accuracy of the numerical integration. (iv) Accuracy of interpolation increases exponentially with the number of samples. The band-limitedness, interpolation accuracy and other properties of APSW functions have been demonstrated in [29, 57, 67].
On the other hand, the APSW interpolators are not causal functions \( (N_T^T = N_{hw} > 1) \) and they render the MOT system (2.12) non-causal. As described in Section 2.2.2, the non-causal MOT scheme requires future samples \( I_{l'}, l' = l + 1, ..., l + N_T^T \), to solve (2.12) for \( I_l \). The causality of the MOT system is restored by extrapolating the future samples from the present and past samples \([29, 57]\). Let \( I_{l+j} \) denote the \( j \)th future sample at time step \( l \). The extrapolation scheme approximates \( I_{l+j} \) using

\[
I_{l+j} \approx \sum_{i=1}^{0} \{ p_j \}_{i+N_s} I_{l+i}, j = 1, ..., N_T^T \tag{2.14}
\]

where \( p_j \) are vectors that the extrapolation coefficients and \( N_s \) is the number of the past samples used in the extrapolation. Inserting (2.14) into (2.12) yields a causal MOT system:

\[
\hat{Z}_0 I_l = V_l - \sum_{l'=l_{\min}}^{l-1} \hat{Z}_{l-l'} I_{l'}, l = 1, ..., N_t \tag{2.15}
\]

where the modified MOT matrices \( \hat{Z}_{l-l'} \) are given by

\[
\hat{Z}_n = \begin{cases} 
Z_n + \sum_{j=1}^{N_T^T} \{ p_j \}_{N_s-n} Z_{-j}, & 0 \leq n < N_s \\
Z_n, & n \geq N_s.
\end{cases} \tag{2.16}
\]

It is clear from (2.15) and (2.16) that the extrapolation coefficients inherently modify the MOT matrix system. To maintain the accuracy and stability of its solution, the extrapolation scheme described by (2.15) should be highly accurate within the bandwidth of the excitation up to its maximum frequency \( f_{\text{max}} \).

A wideband-accurate extrapolation scheme, termed as HE in this thesis, has been developed in [29] to restore the causality of the MOT matrix system resulting from the discretization of the time domain electric field surface integral equation (TD-EFSIE) and time domain magnetic field surface integral equation (TD-MFSIE). This
scheme “trains” the extrapolation coefficients using sine and cosine functions. Even though HE-enhanced MOT scheme is stable when solving TD-EFSIE and MFSIE, it introduces instabilities in the solution of the TD-EFVIE enforced on high-contrast dielectric scatterers [68]. In what follows, Section 2.2.4 briefly reviews the HE scheme and Section 2.2.5 proposes an extrapolation method that maintains the stability of the MOT matrix system obtained from the discretization of TD-EFVIE.

2.2.4 Harmonic Function Based Extrapolation

Let $f(t)$ represent a function band-limited to $\omega_{\text{max}} = 2\pi f_{\text{max}}$. Assume that samples of $f(t)$ for $t \leq 0$ are known and its samples for $t > 0$ are to be extrapolated. The HE scheme assumes that $f(t)$ can be approximated accurately by a weighted sum of harmonic functions $\exp(j[n\Delta \omega]t)$:

$$ f(t) = \sum_{n=-N_\omega}^{N_\omega} \gamma_n \exp(j[n\Delta \omega]t). \quad (2.17) $$

Here, $\gamma_n$ are the weighting coefficients (which are never calculated), $n\Delta \omega$, $n = -N_\omega, ..., N_\omega$ represent the frequency samples, $N_\omega$ is the number of harmonics, and
\[ \Delta \omega = \omega_{\text{max}}/(N_\omega - 1). \] Using the extrapolation scheme defined in (2.14), one can approximate \( f(j \Delta t), j = 1, ..., N_f^T \), from \( f(i \Delta t), i = 1 - N_s, ..., 0 \) using:

\[
f(j \Delta t) \approx \sum_{i=1-N_s}^{0} \{p_j\}_{i+N_s} f(i \Delta t).
\] (2.18)

Inserting (2.17) into (2.18) yields a system of equations for every \( j = 1, ..., N_f^T \):

\[
A p_j = b_j
\] (2.19)

Here, elements of \( A \) and \( b_j \) are

\[
\{A\}_{n,i} = \exp \left[ j(n - N_\omega - 1)(i - N_s) \Delta \omega \Delta t \right], n = 1, ..., 2N_\omega + 1, i = 1, ..., N_s
\] (2.20)

\[
\{b_j\}_n = \exp \left[ j(n - N_\omega - 1)j \Delta \omega \Delta t \right], n = 1, ..., 2N_\omega + 1.
\] (2.21)

Choosing \( N_\omega > N_s \) (as recommended in [29]) ensures the accuracy of extrapolation and makes the matrix system in (2.19) over determined. Then, \( p_j \) are obtained through singular value decomposition (SVD) as

\[
p_j = \sum_{n=1}^{r_n(A)} \frac{u_n^\dagger b_j}{\sigma_n} v_n
\] (2.22)

where \( u_n \) and \( v_n \) are the left and right singular vectors and \( \sigma_n \) are the singular values (ordered from largest \( \sigma_1 \) to the smallest \( \sigma_{N_s} \)) obtained from the SVD of \( A \), \( r_n(A) \) is the numerical rank of \( A \), which is the largest \( n \) that satisfies \( \sigma_n < \chi \), and \( \chi \) is determined based on the desired accuracy of the extrapolation. Note that since the system in (2.19) is symmetric in \( n \), \( p_j \) are always real even though the system is complex. The accuracy of the extrapolation in (2.18) is determined by the singular values retained in the SVD, i.e., \( \chi \) and \( r_n(A) \).

The HE scheme described above introduces instabilities in the solution, when used
in the MOT scheme in (2.12) for solving the TD-EFVIE enforced on high-contrast scatterers [68]. This can be explained by the fact that HE coefficients are trained using harmonic functions (only oscillating signals) and can not be used to accurately extrapolate the fields of exponentially decaying and oscillating modes induced inside the dielectric scatterers [69]. When the frequency of excitation or the contrast of the scatterer increase, the number of modes excited inside the scatterer also increases [see Section 2.3.2]. Consequently, HE becomes less and less accurate, making the instability of the MOT solution worse for higher-contrast scatterers.

2.2.5 Complex Exponent Based Extrapolation

The shortcoming of the HE scheme can be overcome by training the extrapolation coefficients using exponential functions with complex exponents (i.e., exponentially decaying and oscillating functions). Such a training scheme has been developed in [70] to compute the predictor-corrector coefficients of a multi-step time integration method. A similar idea is used here to design the CEE scheme as described next. This scheme assumes that $f(t)$ can be approximated accurately by a weighted sum of exponentials:

$$f(t) = \sum_{n=1}^{N_{\lambda}} \alpha_n \exp(\lambda_n t). \quad (2.23)$$

Here, $\alpha_n$ are the weighting coefficients (which are never calculated) and $\lambda_n$ are samples of complex frequency. Unlike the HE, where the frequency samples are chosen on a single axis, choosing $\lambda_n$ is not a straightforward task and is described step by step in what follows:
Support of complex frequency $\lambda$

Assume that $\lambda_n$ represent a set of samples selected in the complex semi-disc $S_D = \{ \lambda \in \mathbb{C} | \text{Re}\{\lambda\} \leq 0 \text{ and } |\lambda| \leq \omega_{\text{max}} \}$ [Fig. 2.3(a)]. Stability of the extrapolation is ensured by selecting $\text{Re}\{\lambda\} \leq 0$, i.e., forcing $S_D$ to be on the left side of the imaginary axis. Also, the condition $|\lambda| \leq \omega_{\text{max}}$, i.e., radius of $S_D$ is $\omega_{\text{max}}$, is enforced to make sure that the approximation in (2.23) is accurate for $|\lambda| \leq \omega_{\text{max}}$. Consequently, the fields of the modes induced inside the scatterer by the incident field can be extrapolated accurately. To simplify sampling/discretization of the complex semi-disc $S_D$, one can make use of the maximum modulus principle [70]. According to maximum modulus principle, the error of the approximation in (2.23) is maximum at the boundary of the semi-disc $S_D$, ($\partial S_D$), i.e., if the error in the approximation constructed using $\exp(\lambda t)$, $\lambda \in \partial S_D$, is ensured to be less than $\delta$, then the error in the approximation constructed using $\exp(\lambda t)$, $\lambda \in S_D$, will also be less than $\delta$. In other words, choosing samples $\lambda_n$ on $\partial S_D$ and using them to compute the extrapolation coefficients ensure that the resulting extrapolation is accurate for all modes with exponents that fall in the semi-disk $S_D$.

Sampling of $\partial S_D$

Let $\lambda_m$, $m = 1, ..., \bar{N}_\lambda$ and $\bar{t}_i = (i - \bar{N}_s)\Delta \bar{t}$, $i = 1, ..., \bar{N}_s$, represent sufficiently dense discretizations of the boundary $\partial S_D$ [Fig. 2.3(b)] and the time interval $[(1 - N_s)\Delta t, 0]$. Note that $[(1 - N_s)\Delta t, 0]$ is the interval where the extrapolation is applied, $\Delta \bar{t} = (N_s\Delta t)/\bar{N}_s$, and $\bar{N}_s \gg N_s$; and it is assumed that $\bar{N}_\lambda \gg N_\lambda$. These selections ensure the accuracy of this dense frequency/time discretization. Using this discretization, one can construct an $\bar{N}_\lambda \times \bar{N}_s$ matrix $S$ with entries

$$\{S\}_{m,i} = \exp(\lambda_m \bar{t}_i), \ m = 1, ..., \bar{N}_\lambda, \ i = 1, ..., \bar{N}_s.$$

(2.24)
Matrix interpolation (skeletonization)

Matrix skeletonization [71] finds the “most important” rows/columns of a matrix that can approximate the matrix itself with a given accuracy. This idea is applied to $\mathbf{S}$ to find its most important rows, i.e., to select $\exp(\lambda_n t_i)$, $\lambda_n$, $n = 1, \ldots, N_\lambda$, which can be used to represent $\exp(\lambda_m t_i)$, $\lambda_m$, $m = 1, \ldots, \tilde{N}_\lambda$ with a given accuracy. For $\mathbf{S}$, there
exists such a selection of \( N_\lambda \) rows such that

\[
S = TS_\lambda + X. \tag{2.25}
\]

Here, \( T \) is an \( \tilde{N}_\lambda \times N_\lambda \) matrix whose elements have magnitudes less than one, \( S_\lambda \) is an \( N_\lambda \times \tilde{N}_s \) matrix that stores the most important \( N_\lambda \) rows of \( S \), \( X \) is an \( \tilde{N}_\lambda \times \tilde{N}_s \) matrix, whose \( L_2 \)-norm is bounded by the \((N_\lambda + 1)\)th singular value of \( S \), \( \sigma_{N_\lambda+1} \):

\[
\|X\| \leq \sigma_{N_\lambda+1}\sqrt{1 + N_\lambda(\min(\tilde{N}_\lambda, \tilde{N}_s) - N_\lambda)}. \tag{2.26}
\]

Since the error of the skeletonization is bounded by \( \|X\| \leq \delta \), the matrix \( S \) can be interpolated using \( T \) from \( S_\lambda \) (most important \( N_\lambda \) rows of \( S \)) with accuracy \( \delta \). Consequently, skeletonization yields \( \lambda_n, n = 1, \ldots, N_\lambda \), corresponding to the most important \( N_\lambda \) rows of \( S \) [Fig. 2.3(c)]. Here, matrix skeletonization is implemented using the rank revealing QR algorithm described in [70].

\section*{Computing/training extrapolation coefficients}

Once \( \lambda_n \) are computed, the extrapolation coefficients can be trained. Inserting (2.23) into (2.18) yields a system of equations for every \( j = 1, \ldots, N_T^T \):

\[
A p_j = b_j. \tag{2.27}
\]

Here, elements of \( A \) and \( b_j \) are

\[
\{A\}_{n,i} = \exp(\lambda_n(i - N_s)\Delta t), n = 1, \ldots, N_\lambda, i = 1, \ldots, N_s \tag{2.28}
\]

\[
\{b_j\}_n = \exp(\lambda_n j \Delta t), n = 1, \ldots, N_\lambda. \tag{2.29}
\]
The matrix equation in (2.27) is an over determined system and the extrapolation coefficients \( p_j \) can be obtained by minimum least squares solution of (2.27). \( A \) and \( b_j \) being complex valued matrices, the least squares solution of (2.27) might yield complex results. There are several ways to enforce the solution to be real. One of them is choosing \( \lambda_n \) and their symmetric values to the real axis, as suggested in [70]. Another way, which is chosen in this thesis, is solving the real and imaginary parts of (2.27) simultaneously. Since \( p_j \) are real, the solution of the matrix equation

\[
\tilde{A}p_j = \tilde{b}_j
\]  

(2.30)

for every \( j = 1, ..., N_s^T \) is real. Here, the elements of \( \tilde{A} \) and \( \tilde{b}_j \) are

\[
\{\tilde{A}\}_{n,i} = \begin{cases} 
\Re\{A\}_{n,i}, & 0 < n \leq N_\lambda \\
\Im\{A\}_{n-N_\lambda,i}, & N_\lambda < n \leq 2N_\lambda 
\end{cases}
\]

(2.31)

\[
\{\tilde{b}_j\}_n = \begin{cases} 
\Re\{b_j\}_n, & 0 < n \leq N_\lambda \\
\Im\{b_j\}_{n-N_\lambda}, & N_\lambda < n \leq 2N_\lambda 
\end{cases}
\]

(2.32)

where \( n = 1, ..., 2N_\lambda \). The values of \( p_j \) can be approximated by the least square solution of (2.30) as described by (2.22), where \( A \) should be replaced by \( \tilde{A} \).

Several observations about the CEE scheme are in order: (i) To ensure that (2.30) is an over determined system, \( N_s \) is always forced to satisfy \( 2N_\lambda > N_s \). (ii) Reducing \( \delta \) down to a certain level increases the accuracy of the matrix skeletonization as well as the extrapolation at the cost of increased \( N_\lambda \) and \( N_s \). On the other hand, if \( \delta \) is very small resulting in a very high \( N_s \) (i.e., a large number of past samples), errors due to the floating point summation of numbers with opposite sign, which has to be carried out many times during extrapolation, are amplified [70]. This eventually reduces the stability of the MOT scheme. (iii) For a fixed set of \( N_\lambda \) and \( N_s \), the accuracy of the extrapolation is controlled by \( \chi \). Reducing \( \chi \) down to a certain level
increases the accuracy of the least squares solution as well as the extrapolation. On the other hand, if $\chi$ is very small, because of the term $1/\sigma_n$ (i.e., due to division by a very small number) in (2.22), floating-point operation errors get amplified decreasing significantly the accuracy of the least squares solution. This results in an unstable MOT scheme. (iv) Numerical results presented in Section 2.3 demonstrate that to obtain an accurate and stable MOT scheme, it is enough to have values of $N_\lambda$ and $N_s$ around 10. Keeping this in mind and realizing that $p_j, j = 1, ..., N^T_f$ are computed only once before time marching is executed, the cost of computing them as described in this section is negligible compared to those of the MOT matrix computation and solution.

2.3 Numerical Results

This section presents numerical examples that demonstrate the accuracy and stability of the proposed MOT-TD-EFVIE solver, especially, when it is used for characterizing transient electromagnetic wave interactions on high-contrast scatterers. For all examples considered here, the excitation is a plane wave with electric field expressed as

$$E^{inc}(r, t) = \hat{p}E_0 G(t - r \cdot \hat{k}/c_0)$$

where $\hat{p}$ and $\hat{k}$ are unit vectors that represent the polarization and the propagation direction of the plane wave, $E_0$ is the electric field amplitude, and $G(t) = \cos[2\pi f_0(t - t_p)] \exp[-(t - t_p)^2/(2\sigma^2)]$ represents a modulated Gaussian pulse with time delay $t_p$, duration $\sigma$, and modulation frequency $f_0$. Excitation parameters are selected as $\hat{p} = \hat{x}$, $\hat{k} = \hat{z}$, $E_0 = 1\text{V/m}$, and $\sigma = 3/(2\pi f_{bw})$. Here, $f_{bw}$ is the effective bandwidth that is selected to ensure that $99.998\%$ of the incident energy is within the frequency band $[f_0 - f_{bw}, f_0 + f_{bw}]$. With this definition of bandwidth, maximum frequency of
excitation $f_{\text{max}} = f_0 + f_{\text{bw}}$. The parameters of $T(t)$ constructed using the APSW and LP interpolators are $N_p^T = N_f^T = N_{\text{hw}} = 7$ and $N_p^T = p = 3$, $N_f^T = 1$, respectively. The coefficients of the HE scheme are obtained by solving the matrix system in (2.19) with $N_s = 5$, $N_\omega = 11$ and $\omega_{\text{max}} = 2\pi f_{\text{max}}$. The accuracy of the least squares solution in (2.22) is $\chi = 10^{-6}$. The CEE scheme is applied to the complex semi-disk $S_D$ with radius $\omega_{\text{max}} = 2\pi f_{\text{max}}$. The matrix skeletonization required by the CEE scheme is carried out using $\tilde{N}_\lambda = 1000$, $\tilde{N}_s = 1000$, and $\delta = 10^{-13}$ [see (2.25) and (2.26)], which results in $N_\lambda = 13$ and $N_s = 7$. Consequently, the coefficients of the CEE scheme are obtained by solving the matrix system in (2.30) with $N_\lambda = 13$ and $N_s = 7$. The accuracy of this least squares solution is $\chi = 2.5 \times 10^{-5}$. The MOT system is constructed using the temporal derivative of the TD-EFIVE (2.3) and is solved iteratively using the transpose-free quasi-minimal residual (TFQMR) method [78]. The TFQMR iterations are terminated when the condition

$$\|I^n_l - I^{n-1}_l\| < \chi_{\text{TFQMR}}$$

(2.34)

is satisfied. Here, $I^n_l$ is the solution at time step $l$ and iteration $n$, and $\chi_{\text{TFQMR}}$ is the convergence threshold and is set to $10^{-16}$ in all simulations.

2.3.1 Accuracy of Harmonic Function and Complex Exponent Based Extrapolation Schemes

The first example compares the accuracy of the HE and CEE schemes in extrapolating the temporal behavior of modes induced in a dielectric unit sphere. Let $f(t) = G(t) * m(t)$, where $m(t) = \exp(\vartheta t) \cos(2\pi \varsigma t)$ represents the temporal behavior of a mode. Consequently, $f(t)$ is equivalent to the temporal behavior of the currents/fields induced in the scatterer. For a unit sphere with relative dielectric permittivity $\varepsilon_r = 12$, parameters of $m(t)$ are found to be $\vartheta = -1.153 \times 10^8 \text{ Np/s}$ and $\varsigma = 41.205 \text{ MHz}$ (see
Appendix). Parameters of \( G(t) \) are selected as \( f_0 = 34 \text{ MHz}, \) \( f_{bw} = 17 \text{ MHz}, \) and \( t_p = 0. \) First, the convolved signal \( f(t) \) is sampled with time step \( \Delta t = 2 \text{ ns}. \) Then, HE and CEE are applied to extrapolate samples as

\[
f^{\text{ext}}([7 + j]\Delta t) = \sum_{i=1-N_s}^{0} \{ p_j \}_{i+N_s} f([7 + i]\Delta t), j = 1, ..., 7. \tag{2.35}
\]

Here, \( p_j \) store the extrapolation coefficients of HE/CEE schemes. Fig. 2.4(a) compares \( f(n\Delta t) \) and \( f^{\text{ext}}(n\Delta t), n = 8, ..., 14 \) computed using HE and CEE schemes. Fig. 2.4(b) plots \( 20\log_{10} \left( \frac{|f(n\Delta t) - f^{\text{ext}}(n\Delta t)|}{|f(n\Delta t)|} \right), n = 8, ..., 14. \) As expected, accuracy of both HE and CEE decreases as \( j \) is increased from 1 to 7. Additionally, figures clearly show that the CEE scheme is three orders of magnitude more accurate than HE scheme for all values of \( j. \)

### 2.3.2 Algebraic Stability

The second example compares the stability characteristics of the MOT-TD-EFVIE solvers with temporal basis functions constructed using the LP and APSW interpolators. For this purpose, eigenvalues of the companion matrices of the MOT systems in (2.12) (constructed using the LP interpolator) and in (2.15) (constructed using the APSW interpolator and HE/CEE schemes) are computed as required by the algebraic stability analysis described in [79]. The MOT systems are generated for unit spheres of dielectric material with relative permittivities \( \varepsilon_r \in \{3, 6, 12\}. \) The flux density induced in the spheres is discretized using \( N = 2114 \) SWG basis functions and time step size is selected as \( \Delta t = 0.5 \text{ ns}. \)

Eigenvalues in the \( z \)-domain are shown in Fig. 2.5(a)-(c) for \( \varepsilon_r \in \{3, 6, 12\}, \) respectively. For \( \varepsilon_r = 3 \), all MOT systems are stable since all the eigenvalues are located inside the unit circle \( |z| = 1 \) as shown in Fig. 2.5(a). For \( \varepsilon_r = 6 \), the MOT system (2.12) constructed using the LP interpolator becomes unstable since some
Figure 2.4: HE and CEE scheme are applied to the samples of $f(t) = G(t) \ast m(t)$, where $G(t)$ and $m(t)$ represent the temporal behaviors of the incident field and one of the modes induced in the unit dielectric sphere with relative permittivity $\varepsilon_r = 12$.

(a) Comparison of $f(n\Delta t)$ and $f^{\text{ext}}(n\Delta t)$ obtained using HE and CEE schemes. The complex frequency of the mode $m(t)$ is marked in the inset. (b) The relative error in $f^{\text{ext}}(n\Delta t)$ computed as $20\log_{10} \left( \frac{|f(n\Delta t) - f^{\text{ext}}(n\Delta t)|}{|f(n\Delta t)|} \right)$.

of the eigenvalues move outside the unit circle, as shown in Fig. 2.5(b). The MOT systems (2.15) constructed using the APSW interpolator and HE/CEE schemes are
stable for $\varepsilon_r = 6$. For $\varepsilon_r = 12$, both the MOT system (2.12) constructed using the LP interpolator and the MOT system (2.15) constructed using the APSW interpolator and HE scheme are unstable as shown in Fig. 2.5(c). The same figure clearly shows that the proposed MOT scheme using the APSW interpolator and CEE scheme maintains its stability when $\varepsilon_r$ is increased to 12.

Next, the eigenvalues of the companion matrices of the MOT system (2.15) constructed using the APSW interpolator and CEE scheme are compared to the (complex) frequencies of the modes induced in the unit dielectric sphere. It should be noted here that for this comparison, the eigenvalues of the companion matrices, which are in $z$-domain, are mapped to $s$-domain (Laplace domain) using $s = 2(z - 1)/\Delta t(z + 1)$. Fig. 2.5(d)-(f) show the mapped eigenvalues and the resonant frequencies of the unit dielectric sphere with $\varepsilon_r \in \{3, 6, 12\}$, respectively. As expected, figures show that eigenvalues of the MOT system’s companion matrix are clustered around the frequencies of the dielectric unit sphere’s modes. The figures also show that as $\varepsilon_r$ is increased more and more mode frequencies shift towards the origin. This means that more and more modes are induced inside the sphere for a given frequency. In other words, there are more mode frequencies in a given semi-disk with fixed radius. To demonstrate this clearly, a semi-disk with a radius of 100 MHz is also plotted on Figs. 2.5(d)-(f). The modes with frequencies within this semi-disk start contributing to the fields induced inside the sphere if the maximum frequency of excitation $f_{\text{max}} = 100$ MHz. Fig. 2.5(d)-(f) clearly explain why the CEE scheme lead to more accurate (and stable) results even for high values of $\varepsilon_r$.

It should also be mentioned here that, in all plots presented in Figs. 2.5(a)-(c) and Figs. 2.5(d)-(f), there are clusters of eigenvalues located around $z = 1$ and $s = 0$, respectively. This is due to the fact that the MOT system is constructed using the temporal derivative of the TD-EFVIE (2.3). Consequently, a DC-component in the solution might be expected due to numerical errors introduced during discretization.
and limited accuracy of matrix inversion carried out at every time step \[80, 81\]. It should be noted here that this DC-instability is not present in the solution of the MOT system constructed using the “regular” TD-EFIVE (2.3). Additionally, if one is interested in obtaining $J(r, t) = \kappa(r)\partial_t D(r, t)$ rather than $D(r, t)$ by solving the temporal derivative of the TD-EFVIE (2.3), the DC-component can be easily eliminated using the scheme described in \[81\].

2.3.3 Dielectric Shell

Next, the accuracy of the proposed MOT-TD-EFVIE solver with APSW interpolator and CEE scheme is demonstrated via the analysis of scattering from a spherical shell with relative dielectric constant $\varepsilon_r$ [inset of Fig. 2.6(a)]. The shell is centered at the origin and its inner and outer radii are 0.75 m and 1 m, respectively. The flux induced inside the shell is discretized using $N = 27546$ SWG basis functions. Two sets of simulations are carried out. For the first set, $\varepsilon_r = 3$, $f_0 = 40 \text{ MHz}$, $f_{bw} = 20 \text{ MHz}$, and $t_p = 14\sigma$. The simulations are carried out using the MOT-TD-EFVIE solvers with the APSW interpolator and HE/CEE schemes for $N_t = 1175$ time steps with step size $\Delta t = 0.6 \text{ ns}$. Fig. 2.6(a) shows the flux density computed at point (0.91 m, -0.08 m, -0.17 m). For this low-contrast problem, both solutions are stable. To demonstrate the accuracy of the solvers, radar cross section (RCS) of the shell is computed for $\phi = 0^\circ$ and $\theta = [0^\circ, 360^\circ]$ at $f = 40 \text{ MHz}$ using the Fourier transformed MOT solutions [denoted by $\text{RCS}^{\text{CEE}}(\theta)$ and $\text{RCS}^{\text{HE}}(\theta)$] and is compared to that computed from the Mie series solution [denoted by $\text{RCS}^{\text{Mie}}(\theta)$]. Fig. 2.6(b) plots $\text{RCS}^{\text{Mie}}(\theta)$, $|\text{RCS}^{\text{CEE}}(\theta) - \text{RCS}^{\text{Mie}}(\theta)|$ and $|\text{RCS}^{\text{HE}}(\theta) - \text{RCS}^{\text{Mie}}(\theta)|$ and shows that both MOT-TD-EFVIE solvers provide accurate results.

For the second set of simulations, $\varepsilon_r = 100$, $f_0 = 18 \text{ MHz}$, $f_{bw} = 9 \text{ MHz}$, $t_p = 14\sigma$, $N_t = 5250$, and $\Delta t = 2 \text{ ns}$. For this high-contrast problem, MOT-TD-EFVIE solver with the APSW interpolator and CEE scheme yields stable results whereas
the one with the HE scheme fails. Fig. 2.7(a) plots the flux density computed at point (0.91 m, -0.08 m, -0.17 m). The RCS of the shell is computed for \( \phi = 0^\circ \) and \( \theta = [0^\circ, 360^\circ] \) at \( f = 15 \text{ MHz} \) and \( f = 23 \text{ MHz} \) using the Fourier transformed MOT solution [denoted by \( \text{RCS}^{\text{CEE}}(\theta) \)] and is compared to that computed from the Mie series solution [denoted by \( \text{RCS}^{\text{Mie}}(\theta) \)]. Fig. 2.7(b) and 2.7(c) plot \( \text{RCS}^{\text{Mie}}(\theta) \) and \( |\text{RCS}^{\text{CEE}}(\theta) - \text{RCS}^{\text{Mie}}(\theta)| \) for \( f = 15 \text{ MHz} \) and \( f = 23 \text{ MHz} \), respectively, and demonstrate the accuracy of the proposed MOT scheme.

### 2.3.4 Layered Dielectric Slab

With this example, the stability of the proposed MOT-TD-EFVIE with the APSW interpolator and CEE scheme is demonstrated via the analysis of scattering from a two-layer dielectric slab (inset of Fig. 2.8). The slab is centered at the origin. Its dimensions are 1.2 m, 1.2 m, and 0.6 m along the \( x, y, \) and \( z \) directions, respectively. The relative dielectric permittivities of the lower and upper halves are \( \varepsilon_r = 100 \) and \( \varepsilon_r = 150 \), respectively. The flux induced inside slab is discretized using \( N = 23880 \) SWG basis functions. For this simulation, \( f_0 = 15 \text{ MHz} \), \( f_{bw} = 15 \text{ MHz} \), and \( t_p = 14\sigma \) and it is carried out using the proposed MOT-TD-EFVIE solver for \( N_t = 4600 \) time steps with step size \( \Delta t = 1 \text{ ns} \). Fig. 2.8 shows the flux density computed at point (0.15 m, -0.51 m, -0.27 m). The solution is clearly stable and exhibits an oscillating behavior because of the physical resonance modes induced inside the dielectric slab. These modes decay very slowly because the reflection coefficients at surfaces of the slab have large values. Consequently, induced fields oscillate around an almost constant value as shown in Fig. 2.8.

### 2.3.5 Luneburg and Eaton-Lippmann Lenses

To demonstrate the applicability of the proposed MOT-TD-EFVIE solver with the APSW interpolator and CEE scheme is used in the analysis of transient field interac-
tions on the Luneburg [82] and Eaton-Lippmann [83, 84] lenses. The lenses are of unit radius and are centered at point $r_c = (19.4 \, \text{m}, 3.0 \, \text{m}, 0 \, \text{m})$. The relative dielectric permittivity of the Luneburg lens varies along the radial direction as $\varepsilon_r(r) = 2 - |r - r_c|^2$ and that of the Eaton-Lippmann lens varies as $\varepsilon_r(r) = \min(20, 2/|r - r_c| - 1)$. Flux induced inside the lenses is discretized using $N = 60250$ SWG basis functions. For both simulations, $f_0 = 450 \, \text{MHz}$, $f_{bw} = 50 \, \text{MHz}$, and $t_p = 6\sigma$ and they are carried out for $N_t = 2500$ time steps with step size $\Delta t = 0.1 \, \text{ns}$. Figs. 2.10 and 2.11 show the distribution of the total electric field on the $xz$-plane of the Luneburg and Eaton Lippmann lenses at different times, respectively. Fig. 2.10 shows that, as expected, the Luneburg lens focuses the fields at the opposite end of the lens. Fig. 2.11 shows that the Eaton-Lippmann lens rotates the incident field around the lens. Fig. 2.9 plots the flux density at point $(19.4 \, \text{m}, 2.8 \, \text{m}, 0 \, \text{m})$ inside the lenses and demonstrates the stability of the solutions.
Figure 2.5: Algebraic stability analysis of the MOT-TD-EFVIE solver. Eigenvalues of the companion matrix (in $z$ domain) associated with the MOT systems constructed using the LP interpolator and the APSW interpolator with the HE and CEE schemes for the unit dielectric sphere with relative permittivity $(a) \varepsilon_r = 3$, $(b) \varepsilon_r = 6$, and $(c) \varepsilon_r = 12$. Corresponding physical resonances of the unit sphere and the eigenvalues of companion matrix (in $s$ domain) associated with the MOT system constructed using the APSW interpolator with the CEE scheme for relative permittivity values $(d) \varepsilon_r = 3$ $(e) \varepsilon_r = 6$, and $(f) \varepsilon_r = 12$. 
Figure 2.6: Scattering from a spherical dielectric shell with inner radius 0.75 m, outer radius 1 m, and relative permittivity $\varepsilon_r = 3$. (a) The flux density computed at point (0.91 m, -0.08 m, -0.17 m) using the MOT-TD-EFVIE solvers with the APSW interpolator and HE/CEE schemes. (b) RCS computed at 40 MHz using the Fourier transformed MOT solutions [denoted by $RCS^{CEE}(\theta)$ and $RCS^{HE}(\theta)$] and the Mie series solution [denoted by $RCS^{Mie}(\theta)$].
Figure 2.7: Scattering from a spherical dielectric shell with inner radius 0.75 m, outer radius 1 m, and relative permittivity $\varepsilon_r = 100$. (a) The flux density computed at point $(0.91 \text{ m}, -0.08 \text{ m}, -0.17 \text{ m})$ using the MOT-TD-EFVIE solver with the APSW interpolator and CEE scheme. RCS computed at (b) 15 MHz and (c) 23 MHz using the Fourier transformed MOT solution [denoted by $\text{RCS}^{\text{CEE}}(\theta)$] and the Mie series solution [denoted by $\text{RCS}^{\text{Mie}}(\theta)$].
Figure 2.8: Scattering from a dielectric slab with two layers with relative permittivites $\varepsilon_r = 150$ and $\varepsilon_r = 100$. The flux density computed at point $(0.15 \text{ m}, -0.51 \text{ m}, -0.27 \text{ m})$ using the MOT-TD-EFVIE solver with the APSW interpolator and CEE scheme.

Figure 2.9: Transient field interactions on the Luneburg and Eaton-Lippman lenses. The flux density computed at point $(19.4 \text{ m}, 2.8 \text{ m}, 0 \text{ m})$ inside the lenses using the MOT-TD-EFVIE solver with the APSW interpolator and CEE scheme.
Figure 2.10: Electric field distribution inside the Luneburg lens at different times.
Figure 2.11: Electric field distribution inside the Eaton-Lippmann at different times.
Chapter 3

An Explicit Marching On in Time Scheme for Solving the Time Domain Magnetic Field Volume Integral Equation

3.1 Introduction

The time domain electric field volume integral equation (TD-EFVIE) solver described in Chapter 2 maintains its stability even when the contrast of the scatterer is high. However, the conditioning of the marching on-in-time (MOT) matrix system becomes worse as the contrast is increased. This significantly increases the computation time, since the solution of the MOT system called for by the implicit scheme at every time step requires higher number of iterations to ensure stability and accuracy. This ill-conditioning effect is a consequence of the fact that the EFVIE starts behaving more like a first kind integral equation as the contrast gets higher [44, 85, 86, 87]. While the research on formulating well-conditioned EFVIEs and developing preconditioning techniques is still in progress [44, 85, 86, 87] in this thesis, this bottleneck is addressed by switching to a time domain magnetic field volume integral equation (TD-MFVIE) formulation and developing a new explicit MOT scheme that calls for solution of an MOT system that is always well-conditioned regardless of the contrast (as well as the time step size).

Even though, unlike their implicit counterparts, the classical explicit MOT schemes do not call for a matrix solution at every time step, they suffer from stability issues [88, 89, 26, 90], which might be remedied using a small time step size at the cost of increased computation time (i.e., they are subject to a Courant-Friedrichs-Lewy (CFL)
constraint). The explicit MOT scheme described in the chapter does not suffer from these shortcomings and is used to efficiently and accurately solve the TD-MFVIE. The TD-MFVIE is a second kind integral equation regardless of the contrast’s value. Using this fact, the TD-MFVIE is cast in the form an ordinary differential equation (ODE), which relates the (unknown) magnetic field to its temporal derivative. The unknown magnetic field is expanded in space using fully linear curl-conforming basis (FLCB) functions [43]. Inserting this expansion into the TD-MFVIE and spatially testing the resulting equation yield a Gram matrix system, which relates time dependent coefficients of the basis expansion to their temporal derivatives. Note that if Galerkin testing is used, the Gram matrix is well-conditioned and sparse. If point testing is used, then it consists of four diagonal blocks. In either case the Gram matrix does not depend on the time step size. This system is integrated in time using a predictor-corrector algorithm, PE(CE)^m, for the coefficients of the unknown expansion. To facilitate the computation of the retarded time integrals, which express the scattered magnetic field in terms of the unknown magnetic field on the scatterer, at discrete time steps as required by the PE(CE)^m, the piece-wise defined Lagrange polynomial [28, 55, 56] or band-limited interpolation functions [20] are used. Since the matrix system that is solved at every evaluation (E) step is either done using an iterative solver if Galerkin testing is used, or by multiplying the right hand side with inverse of the Gram matrix (which also consists of four diagonal blocks) if point testing is used. The resulting MOT schemes are expected to be more efficient than their implicit counterparts, which call for the inversion of a matrix system that gets denser as the time step size gets larger with decreasing frequency. Indeed, the numerical results demonstrate that the proposed MOT schemes use the same time step sizes as the implicit counterparts without sacrificing from stability, and they are more efficient under low frequency excitation. Additionally, the numerical results show that the explicit MOT scheme with Galerkin testing yields the most stable results for scatterers
with high contrast.

The rest of this chapter is organized as follows: Section \textbf{3.2} provides the details of the formulation underlying the proposed MOT scheme, describes its implementations with Galerkin and point testing, and compares its computational complexity to that of its implicit counterpart. Section \textbf{3.3} demonstrates the stability and accuracy of the proposed scheme via numerical experiments.

\section{Formulation}

\subsection{Time Domain Magnetic Field Volume Integral Equation}

Let $V$ represent the volumetric support of a linear, non-dispersive, non-magnetic, isotropic, and possibly inhomogeneous dielectric scatterer with permittivity $\varepsilon(r)$ and permeability $\mu_0$. The scatterer resides in an unbounded and homogenous medium with permittivity $\varepsilon_0$ and permeability $\mu_0$. An incident magnetic field $H^{\text{inc}}(r, t)$, which is essentially band limited to $f_{\text{max}}$ and vanishingly small $\forall r \in V$ and $t \leq 0$, excites the scatterer. Upon excitation, an equivalent current density $J(r, t)$ is induced in $V$, which in return generates a scattered magnetic field $H^{\text{sca}}(r, t)$. $H^{\text{sca}}(r, t)$ is expressed in terms of retarded-time magnetic vector potential $A(r, t)$ as

$$H^{\text{sca}}(r, t) = \frac{1}{\mu_0} \nabla \times A(r, t)$$

$$= \nabla \times \int_V J(r', t - R/c_0) \frac{1}{4\pi R} dv'.$$

(3.1)

Here, $R = |r - r'|$ is the distance between source point $r'$ and observation point $r$, and $c_0 = 1/\sqrt{\varepsilon_0\mu_0}$ is speed of light in the background medium. $J(r, t)$ is expressed in
terms of the total magnetic field $\mathbf{H}(\mathbf{r}, t)$ as

$$\mathbf{J}(\mathbf{r}, t) = \kappa(\mathbf{r}) \nabla \times \mathbf{H}(\mathbf{r}, t)$$  \hspace{1cm} (3.2)$$

where $\kappa(\mathbf{r}) = 1 - \varepsilon_0 / \varepsilon(\mathbf{r})$ is the dielectric contrast. Substituting (3.1) and (3.2) in the derivative form of $\mathbf{H}(\mathbf{r}, t) = \mathbf{H}^{\text{inc}}(\mathbf{r}, t) + \mathbf{H}^{\text{sc}}(\mathbf{r}, t)$ yields the TD-MFVIE:

$$\partial_t \mathbf{H}^{\text{inc}}(\mathbf{r}, t) = \partial_t \mathbf{H}(\mathbf{r}, t) + \frac{1}{4\pi} \int_V \kappa(\mathbf{r}') \hat{\mathbf{R}} \times \left( \frac{\partial^2 \nabla' \times \mathbf{H}(\mathbf{r}', t')}{c_0 R} + \frac{\partial_t \nabla' \times \mathbf{H}(\mathbf{r}', t')}{R^2} \right)_{t'=t-R/c_0} dV'$$  \hspace{1cm} (3.3)$$

where $\hat{\mathbf{R}} = (\mathbf{r} - \mathbf{r}')/R$.

### 3.2.2 Discretization

To numerically solve the TD-MFVIE (3.3), $V$ is divided into a mesh of tetrahedrons. Assume that this mesh has $N$ edges. $\mathbf{H}(\mathbf{r}, t)$ is approximated in terms of the FLCB functions [43], each of which is defined along one of these edges as

$$\mathbf{H}(\mathbf{r}, t) = \sum_{n=1}^{N} \{\mathbf{I}^1(t)\}_n \mathbf{f}^1_n(\mathbf{r}) + \sum_{n=1}^{N} \{\mathbf{I}^2(t)\}_n \mathbf{f}^2_n(\mathbf{r}).$$  \hspace{1cm} (3.4)$$

Note that this expansion follows the interpretation/description in [45], where the FLCB functions are separated to solenoidal and irrotational edge basis functions. In (3.4), $\mathbf{f}^1_n(\mathbf{r})$ and $\mathbf{f}^2_n(\mathbf{r})$ are the first order irrotational edge basis functions [45] and the lowest mixed order solenoidal edge basis functions [91], $\{\mathbf{I}^1(t)\}_n$ and $\{\mathbf{I}^2(t)\}_n$ are their unknown time dependent coefficients. $\mathbf{f}^s_n(\mathbf{r})$, $s \in \{1, 2\}$ are expressed as

$$\mathbf{f}^s_n(\mathbf{r}) = \begin{cases} 
\lambda_n^{d_1}(\mathbf{r}) \nabla \lambda_n^{d_2}(\mathbf{r}) \pm \lambda_n^{d_2}(\mathbf{r}) \nabla \lambda_n^{d_1}(\mathbf{r}), & \mathbf{r} \in S_n \\
0, & \mathbf{r} \notin S_n 
\end{cases}$$  \hspace{1cm} (3.5)$$
where “+” and “-” signs should be selected for $s = 1$ and $s = 2$, respectively, $S_n = \cup_{q=1}^{Q_n} S_n^q$ is the combined support of all $Q_n$ tetrahedrons sharing edge $n$, $d^1_n$ and $d^2_n$ represent the two nodes of this edge, and $\lambda_n^d(r)$, $d \in \{d^1_n, d^2_n\}$, are the barycentric coordinate functions that change linearly from 1 at $d$ to 0 at the face opposite to $d$. Note that from the definitions above, one can easily show that $\nabla \times f^1_n(r) = 0$ and $\nabla \times f^2_n(r) \neq 0$.

Inserting (3.5) in (3.3) and testing the resulting equation with functions $t^1_m(r)$ and $t^2_m(r)$ yield a semi-discrete time dependent system of equations:

$$
\begin{bmatrix}
G^{11} & G^{12} \\
G^{21} & G^{22}
\end{bmatrix}
\begin{bmatrix}
\dot{I}^1(t) \\
\dot{I}^2(t)
\end{bmatrix}
= \begin{bmatrix}
V^{\text{inc},1}(t) \\
V^{\text{inc},2}(t)
\end{bmatrix}
+ \begin{bmatrix}
V^{\text{sca},1}(t) \\
V^{\text{sca},2}(t)
\end{bmatrix}.
$$

(3.6)

Here, $G^{ps}, p, s \in \{1, 2\}$ of dimension $N \times N$ are blocks of the Gram matrix $G$. Their elements given by

$$
\{G^{ps}\}_{m,n} = \int_{P^p_m} t^p_m(r) \cdot f^s_n(r) dv.
$$

(3.7)

Here, $P^p_m$ is the support of $t^p_m(r)$, $p \in \{1, 2\}$. Two sets of choices are considered for $t^1_m(r)$ and $t^2_m(r)$, which result in Galerkin and point testing, respectively. The specific choice of testing procedure changes the sparseness structure of $G$ and consequently affects the efficiency and accuracy of the time marching scheme described in Sec. 3.2.3.

In (3.6), $\dot{\mathbf{I}^s}(t)$, $s \in \{1, 2\}$ are vectors of dimension $N$ with entries $\{\partial_t \mathbf{I}^s(t)\}_n$. $V^{\text{inc},p}(t)$ and $V^{\text{sca},p}(t)$, $p \in \{1, 2\}$ are vectors of dimension $N$ and hold the spatially tested incident and scattered magnetic fields, respectively. Their entries are given by

$$
\{V^{\text{inc},p}(t)\}_m = \int_{P^p_m} t^p_m(r) \cdot \partial_t \mathbf{H}^{\text{inc}}(r, t) dv.
$$

(3.8)
\[
\{V^\text{sca,}p(t)\}_{m} = \frac{1}{4\pi} \sum_{n=1}^{N} \int_{P^p_m} t^p_m(r) \cdot \sum_{q=1}^{Q_n} \kappa^q_n \int_{S^q_n} \hat{R} \times \nabla' \times f^2_n(r') \left( \frac{\partial_{r^q_n}^2 \{I^2(t')\}_n}{c_0 R} + \frac{\partial_{t'} \{I^2(t')\}_n}{R^2} \right)_{t'=t-R/c_0} \int_{S^q_n} \hat{R} \times dv'b'dv.
\]

In (3.9), \( \kappa(r) \) is assumed to be a constant in \( S^q_n \), i.e., \( \kappa^q_n = \kappa(r^q_n) \), where \( r^q_n \) is the center of the tetrahedron \( S^q_n \). Also note that since \( \nabla \times f^1_n(r) = 0 \), only contribution to \( V^\text{sca,}p(t) \) comes from \( \nabla \times f^2_n(r) \).

Temporal discretization of (3.6) is described next. A PE(CE)^m algorithm is used to integrate the system of ODEs (3.6) in time to yield the samples of the unknown vectors \( I^s(t), s \in \{1, 2\} \). This means that (3.6) has to be sampled in time, i.e. it is evaluated at times \( j\Delta t \):

\[
\begin{bmatrix}
G^{11} & G^{21} \\
G^{12} & G^{22}
\end{bmatrix}
\begin{bmatrix}
\dot{I}^1_j \\
\dot{I}^2_j
\end{bmatrix}
= \begin{bmatrix}
V^{\text{inc,}1}_j \\
V^{\text{inc,}2}_j
\end{bmatrix}
+ \begin{bmatrix}
V^{\text{sca,}1}_j \\
V^{\text{sca,}2}_j
\end{bmatrix}
\]

(3.10)

where \( j = 1, \ldots, N_t \), \( \Delta t \) is the time step size, \( N_t \) is the number of time steps, \( \dot{I}^s_j = I^s(j\Delta t), s \in \{1, 2\} \) and \( V^{\text{inc,}}_j = V^{\text{inc,}}(j\Delta t), V^{\text{sca,}}_j = V^{\text{sca,}}(j\Delta t), p \in \{1, 2\} \). \( V^{\text{inc,}}_j \) are computed using (3.8) (\( H^{\text{inc}}(r, t) \) and \( \partial_t H^{\text{inc}}(r, t) \) are known) and \( V^{\text{sca,}}_j \) are computed using (3.9), where the time-retardation should be carefully accounted for. This is achieved by using interpolation on samples of \( I^2(t) \):

\[
\{I^2(t)\}_n = \sum_i \{I^2_i\}_n T(t-i\Delta t)
\]

(3.11)

where \( T(t) \) is a piecewise polynomial Lagrange interpolation function \([28, 55, 56]\). Note that \( T(t) \) is discretely causal: \( T(t) = 0 \) for \( t \leq -\Delta t \). This means that during the computation of \( V^{\text{sca,}}_j \), “future” samples of \( I^2(t) \), i.e., \( I^2_i, i \leq j \) are not required. Additionally, \( T(t) \) is of finite duration: \( T(t) = 0 \) for \( t > t_{\text{max}}\Delta t \), where \( t_{\text{max}} \) is the order of the polynomial interpolation. Substituting (3.11) in (3.9) and evaluating the
resulting expression at \(j\Delta t\) yield:

\[
V_{j}^{sca,p} = \sum_{i=0}^{j} Z_{j-i}^{p} I_{i}^{2}, \quad p \in \{1, 2\} \tag{3.12}
\]

where the elements of the MOT matrices \(Z_{j-i}^{p}\), are given by

\[
\{Z_{j-i}^{p}\}_{m,n} = \frac{1}{4\pi} \int_{\mathcal{P}_{m}} \mathbf{t}_{m}^{p}(r) \cdot \sum_{q=1}^{Q_{n}} k_{n}^{q} \int_{\mathcal{S}_{n}} \hat{\mathbf{R}} \times \nabla' \times f_{n}^{2}(r') \left( \frac{\partial^{2}\{T(t')\}^{m}_{n}}{c_{0}R} + \frac{\partial_{t}\{T(t')\}^{m}_{n}}{R^{2}} \right)_{t'=\Delta t} dv' dv. \tag{3.13}
\]

Note that \(Z_{j-i}^{p} = 0\) for \(j - i > D_{\text{max}}/(c_{0}\Delta t) + t_{\text{max}}\). Consequently, as \(\Delta t\) increases (i.e., for low-frequency excitations), the number of non-zero \(Z_{j-i}^{p}\) decreases. However, these non-zero matrices become fuller. For example, for \(Z_{j-i}^{p}\) to be completely full, \(t_{\text{max}} > j - i > D_{\text{max}}/(c_{0}\Delta t) - 1\), which can only be satisfied when \(D_{\text{max}} < c_{0}\Delta t\) since \(j \geq i\). Here, \(D_{\text{max}}\) is the maximum distance between any two points in \(V\).

Substituting (3.12) into (3.10) yields the final form of the system of ODEs that relates the samples of the derivative of the unknown coefficients \(\dot{I}_{j}^{s}\), \(s \in \{1, 2\}\) to the samples of the unknown coefficients, \(I_{j}^{s}\), \(s \in \{1, 2\}\):

\[
\begin{bmatrix}
G^{11} & G^{12} \\
G^{21} & G^{22}
\end{bmatrix}
\begin{bmatrix}
\dot{I}_{j}^{1} \\
\dot{I}_{j}^{2}
\end{bmatrix} =
\begin{bmatrix}
V_{j}^{\text{inc,1}} \\
V_{j}^{\text{inc,2}}
\end{bmatrix} + \sum_{i=0}^{j} \begin{bmatrix}
Z_{j-i}^{1} \mathbf{0} \\
Z_{j-i}^{2} \mathbf{0}
\end{bmatrix}
\begin{bmatrix}
I_{j}^{1} \\
I_{i}^{2}
\end{bmatrix}. \tag{3.14}
\]

The MOT system (3.14) is integrated in time to yield the unknown coefficients \(I_{j}^{s}\), \(s \in \{1, 2\}\) using a PE(CE)\(m\) scheme as described in Sec. 3.2.3. Note that to have a more compact notation, (3.14) is rewritten as:

\[
G \dot{I}_{j} = V_{j}^{\text{inc}} + \sum_{i=0}^{j} Z_{j-i} I_{i}. \tag{3.15}
\]
It should also be noted here that $T(t)$ can be a non-causal interpolation function: For example one can use the approximate prolate spheroidal wave functions (AP-SWFs) \[67, 57\] since they can interpolate bandlimited functions with exponentially increasing accuracy and they have continuous derivatives everywhere along their support. A non-causal $T(t)$ means that $Z_{p-i} \neq 0$, $i > j$ and consequently the time marching requires “future” values of the unknown coefficients to determine their values at the current time step. The causality of the time marching can be restored using various extrapolation schemes which express future values of the coefficients in terms of their past values \[57, 92, 93\].

### 3.2.3 Explicit Time Marching Scheme

The MOT system (3.15) is a system of ODEs that relates samples of the temporal derivative of the unknown coefficients $\dot{I}_j$ to the samples of the unknown coefficients $I_j$. This means that $I_j$ can be determined by integrating (3.15) using a PE(CE)$^m$ type linear multi-step method, similar to the one used in [47] to solve the time domain magnetic field surface integral equation. The PE(CE)$^m$ scheme used here is a $k$-step method: it requires the values of $I_i$ and $\dot{I}_i$, $i = j-k, \ldots, j-1$ to compute $I_j$. Assuming $I_i$ and $\dot{I}_i$, $i = 0, \ldots, k-1$ are known, the steps of the time marching algorithm, which makes use of the $k$-step PE(CE)$^m$, are detailed below.

At each time step $j = k, \ldots, N_t$:

- **Step 1**: The components of the right-hand side of (3.15), which are not updated within the time step $j$, are computed:

\[
V_{j}^{\text{fixed}} = V_{j}^{\text{inc}} + \tilde{V}_{sca}^{j} \tag{3.16}
\]

\[
V_{j}^{\text{fixed}} = V_{j}^{\text{inc}} + \sum_{i=0}^{j-1} Z_{j-i}I_i.
\]

Here, $V_{j}^{\text{fixed}}$ and $\tilde{V}_{sca}^{j}$ are vectors of dimension $2N$. Note that $\tilde{V}_{sca}^{j}$ does not
include the contributions from \( I_j \), i.e., the matrix-vector product \( Z_0 I_j \).

- **Step 2:** Predictor (P) step. \( I_j \) is predicted using \( k \) past (known) values of \( I_i \) and \( \dot{I}_i \), \( i = j - k, \ldots, j - 1 \), respectively:

\[
I_j = \sum_{l=1}^{k} \left[ \{p\}_l I_{j-l-k} + \{p\}_k \dot{I}_{j-l-k} \right].
\]  

(3.17)

Here, \( p \) is a vector of dimension \( 2k \), which stores the predictor coefficients.

- **Step 3:** Evaluation (E) step. First compute the right hand side using the predicted \( I_j \):

\[
V_j = Z_0 I_j + V_j^{\text{fixed}}.
\]  

(3.18)

Here, \( V_j \) is a vector of dimension \( 2N \). Then, compute \( \dot{I}_j \) by solving

\[
G \dot{I}_j = V_j.
\]  

(3.19)

- **Step 4:** Set \( \dot{I}_j^{(0)} = \dot{I}_j \). Repeat step 4.1 and 4.2 until convergence \( (m = 1, \ldots, m_{\text{max}}) \):

  - **Step 4.1:** Corrector (C) step. \( I_j^{(m)} \) corrected/updated using \( k \) past values of \( I_i \) and \( \dot{I}_i \), \( i = j - k, \ldots, j - 1 \), and the \( \dot{I}_j^{(m-1)} \):

\[
I_j^{(m)} = \sum_{l=1}^{k} \left[ \{c\}_l I_{j-l-k} + \{c\}_k \dot{I}_{j-l-k} \right] + \{c\}_{2k+1} \dot{I}_j^{(m-1)}.
\]  

(3.20)

Here, \( c \) is a vector of dimension \( 2k + 1 \), which stores the corrector coefficients.

  - **Step 4.2:** Evaluation (E) step. First compute the right hand side using the
Figure 3.1: The steps involved in the explicit time marching scheme.

corrected \( I_j^{(m)} \):

\[
V_j^{(m)} = Z_0 I_j^{(m)} + V_j^{\text{fixed}}. \tag{3.21}
\]

Then, compute \( \dot{I}_j^{(m)} \) by solving

\[
G \dot{I}_j^{(m)} = V_j^{(m)}. \tag{3.22}
\]

- **Step 5:** Once convergence is reached, i.e., \( \|I_j^{(m)} - I_j^{(m-1)}\| < \chi_{\text{PECE}} \), the solutions are stored to be used at the next time step: \( I_j = I_j^{(m)} \) and \( \dot{I}_j = \dot{I}_j^{(m)} \).

The steps involved in the explicit time marching scheme are schematically represented using the flow chart shown in Fig. 3.1(a).

The predictor and corrector coefficients, \( p \) and \( c \) used in the above scheme can be those obtained by polynomial interpolation between time samples resulting in well-known schemes such as Adam-Moulton, Adam-Bashfort, or backward difference methods [94] or those obtained numerically under the assumption that the solution can be represented in terms of decaying and oscillating exponentials [70]. In this work,
p and c obtained through polynomial interpolation are preferred since k associated with these coefficients is much smaller resulting in a more time- and memory-efficient scheme.

At the beginning of time marching, it is assumed that $I_i = 0$ and $\dot{I}_i = 0$, $i = 0, \ldots, k - 1$. This assumption does not introduce any significant error since $H_{\text{inc}}(r, t)$ is vanishingly small $\forall r \in V$ and $t \leq 0$. For other types of excitations, the Euler method or spectral-deferred correction type methods can be used to initialize $I_i$ and $\dot{I}_i$, $i = 0, \ldots, k - 1$.

The method used for solving the MOT system of equations in (3.19) and (3.22) is selected based on the sparsity structure of $G$, which depends on type of spatial testing used as detailed in Sec. 3.2.4.

3.2.4 Choice of Spatial Testing Function

Two different approaches have been developed to spatially test the MFVIE: Point testing [45] and Galerkin testing [42]. The choice of testing functions $t_{p m}^p(r)$, $p \in \{1, 2\}$, affects the sparsity structure of the Gram matrix $G$ resulting in changes in the implementation of the time marching algorithm described in Sec. 3.2.3 and in its efficiency and accuracy.

Point testing

For point testing, $t_{p m}^p(r) = \hat{q}_m \delta(r - r_{p m}^m)$, $p \in \{1, 2\}$, where $\hat{q}_m$ is a unit vector that points from node $d_{1 m}^1$ to $d_{2 m}^2$ (along edge $m$) and $r_{p m}^p$ are selected from Gaussian quadrature points defined on edge $m$. Inserting the expression for $t_{p m}^p(r)$ into (3.7) and using the facts that, one edge, the tangential component of $f_{n m}^i(r)$ linearly increases from
−1 to 1 and the tangential component of $f^2_n(r)$ stays constant at 1 yield

$$G^{12} = G^{22} = I$$

$$G^{11} = -G^{21} = -\frac{1}{\sqrt{3}}I$$

The inverse of $G^{-1}$ can be expressed as:

$$G^{-1} = \frac{1}{2} \begin{bmatrix} I & I \\ \sqrt{3}I & -\sqrt{3}I \end{bmatrix}.$$  \hfill (3.24)

$G^{-1}$ is stored using $O(N)$ memory before the time marching starts. Using the pre-computed $G^{-1}$, the solution of the MOT system of equations in (3.19) and (3.22) is obtained only in $O(N)$ operations. This makes the proposed MOT algorithm with point testing significantly faster than its implicit counterpart as shown by the computational complexity analysis carried out in Sec. 3.2.5 (as also demonstrated by the numerical results presented in Sec. 3.3).

**Galerkin testing**

For Galerkin testing, $t^1_m(r) = f^1_m(r)$ and $t^2_m(r) = f^2_m(r)$. Inserting the expressions for $t^p_m(r)$ into (3.7), the resulting equation yields a summation of integrals, each of which has a second-order polynomial integrand defined over a tetrahedron. These integrals are evaluated exactly using a Gaussian quadrature rule specifically designed for tetrahedrons [95]. Analytical expressions can be derived for these integrals but evaluating those would be computationally more expensive than using a quadrature rule.

When Galerkin testing is used, $G$ is sparse and well-conditioned regardless of $\Delta t$. Therefore the solution of the MOT system of equations in (3.19) and (3.22) is obtained very efficiently using an iterative scheme. The resulting MOT algorithm with Galerkin
testing is faster than its implicit counterpart at low frequencies (i.e., for large \( \Delta t \)). This is because the matrix system of equations that the implicit scheme has to solve at every time step becomes fuller (less sparse) as \( \Delta t \) increases. Implicit and explicit schemes have similar computational costs at high frequencies (i.e., smaller \( \Delta t \)). These are shown by the computational complexity analysis carried out in Sec. 3.2.5 (also by the numerical results presented in Sec. 3.3).

### 3.2.5 Computational Complexity

In this section, computational complexity of the explicit time marching algorithm presented in Sec. 3.2.3 is analyzed in detail and compared to that of its implicit counterpart. Let the computational costs of explicit schemes with point and Galerkin testing and the implicit scheme be represented by \( C_{\text{exp}}^{\text{PT}} N_t + C \), \( C_{\text{exp}}^{\text{GT}} N_t + C \), and \( C_{\text{imp}} N_t + C \), respectively. Note that the implicit time marching algorithm can also be implemented using Galerkin or point testing, but the expression for these implementations’ computational complexity would be the same. That is why \( C_{\text{imp}} \) does not distinguish between these two implementations.

Here, \( C \) represents the total cost of computing \( V_j^{\text{fixed}} \) for all time steps \( j = 1, \ldots, N_t \) and is dominated by the cost of computing \( \tilde{V}_j^{\text{sca}} \). Since \( \tilde{V}_j^{\text{sca}} \) is computed by the implicit and the explicit schemes in the same way, \( C \) is same for all schemes. Note that this computation could be accelerated significantly using the time-domain adaptive integral method [36] or (multilevel) plane wave time-domain algorithm [55] (for both explicit and implicit schemes).

The differences between the explicit scheme and its implicit counterpart are the other operations executed at a given time step. The computational costs of these operations are represented by \( C_{\text{PT}}^{\text{exp}} \), \( C_{\text{GT}}^{\text{exp}} \), and \( C_{\text{imp}} \) for explicit schemes with point and Galerkin testing and the implicit scheme, respectively. The estimates for \( C_{\text{PT}}^{\text{exp}} \) and \( C_{\text{GT}}^{\text{exp}} \) are obtained by following (3.17)-(3.22) step by step.
The $k$-step predictor update in (3.17) and the $k$-step corrector update in (3.20) require $O(2k[2N])$ and $O(m_{\text{max}}[2k + 1][2N])$ operations, respectively. Updating the right hand sides of (3.18) and (3.21) requires the computation of $\mathbf{Z}_0 \mathbf{I}_j$ once and $\mathbf{Z}_0 \mathbf{I}_j^{(m)}$ $m_{\text{max}}$ times. Assuming $\gamma$ represents the sparseness factor of $\mathbf{Z}_0^1$ and $\mathbf{Z}_0^2$, these updates require $O([m_{\text{max}} + 1] \gamma[2N])$ operations in total for predictor and corrector steps. Solution of the MOT matrix systems in (3.19) and (3.22) has two different complexities depending on the testing procedure used. For point testing, computing the solution requires multiplying the right hand side with pre-computed sparse $\mathbf{G}^{-1}$ (Sec. 3.2.4) resulting in $O((m_{\text{max}} + 1)[4N])$ operations in total for predictor and corrector steps. For Galerkin testing $\mathbf{G}$ is sparse without a specific structure (Sec. 3.2.4) and the solution is obtained using an iterative solver. This results in $O((m_{\text{max}} + 1)N_{\text{iter}}^G F_{\text{iter}}^2[\delta N])$ operations in total for predictor and corrector steps. Here, $N_{\text{iter}}^G$ is the number of iterations required, $F_{\text{iter}}$ is the number of matrix-vector multiplications required at each iteration, and $\delta$ is the sparseness factor of $\mathbf{G}$.

The implicit scheme solves the MOT matrix system using an iterative solver, which results in $C^{\text{imp}} \sim O(N_{\text{iter}}^\text{imp} F_{\text{iter}}^2[\gamma N])$. Note that the MOT matrix system solved by the implicit scheme at a given step is not same as the system in (3.15). However, the implicit MOT system’s sparseness level is same as that of $\mathbf{Z}_0^1$ and $\mathbf{Z}_0^2$ and is also represented with $\gamma$. Here, $N_{\text{iter}}^\text{imp}$ is the number of iterations and $F_{\text{iter}}$ is the number of matrix-vector multiplications required at a given iteration (explicit and implicit schemes use the same iterative solver).

In the complexity estimates above, $k$ depends on the order of the PE(CE)$^m$ therefore it is considered as a user defined input for a given level accuracy. Also, $N_{\text{iter}}^G$ is always small since $\mathbf{G}$ is well-conditioned and sparse regardless of $\Delta t$. Assuming $m_{\text{max}}$ is the same for explicit schemes with point and Galerkin testing, the former scheme is faster since $N_{\text{iter}}^G F_{\text{iter}}^2 \delta \gg 4$. Numerical results in Sec. 3.3 show that for scatterers with smaller permittivity ($\varepsilon(r) < 6$), $m_{\text{max}}$ is indeed the same for both of the schemes.
Under high frequency excitation, i.e., when $c_0 \Delta t$ is comparable to the spatial discretization length, $\gamma \leq N$ and a direct analytical comparison of $C^{\text{imp}}$ to $C^{\text{exp}}_{PT}$ or $C^{\text{exp}}_{GT}$ becomes challenging since it is difficult to accurately estimate which contributions discussed above are dominant.

Under low frequency excitation, i.e., when $c_0 \Delta t$ is comparable to or larger than the size of the scatterers, i.e., $c_0 \Delta t \sim D_{\text{max}}$, $\gamma \sim N$, which means that $Z_0$ and the implicit MOT matrix become fuller. Consequently, $C^{\text{imp}} \sim O(N_{\text{iter}}^{\text{imp}} F_{\text{iter}} N^2)$, $C^{\text{exp}}_{PT} \sim O(m_{\text{max}} N^2)$ (assuming $\gamma \sim N \gg k$) and $C^{\text{exp}}_{GT} \sim O(m_{\text{max}} N^2)$ (assuming $\gamma \sim N \gg k$ and $\gamma \sim N \gg N_{\text{iter}}^{\text{imp}} F_{\text{iter}} 2 \delta$). This means that explicit schemes are faster than the implicit scheme as long as $m_{\text{max}} < N_{\text{iter}}^{\text{imp}} F_{\text{iter}}$. Numerical results presented in Sec. 3.3 show that this condition is indeed satisfied and the explicit solvers are faster.

Note that one can use the low-frequency extension of the time-domain adaptive integral method \[96\] to accelerate the matrix-vector multiplications required by the iterative method in solving the implicit MOT system. However, the same extension can also be used to accelerate the computation of the matrix product $Z_0 I_j$ required by the explicit scheme during the predictor updates. Therefore, the conclusions drawn above remains unchanged even when acceleration methods are used.

### 3.3 Numerical Results

This section presents numerical examples to demonstrate the advantages of the proposed explicit schemes. In all examples, the scatterer is illuminated by a Gaussian modulated plane wave travelling in the $\hat{z}$ direction with a $\hat{y}$-polarized magnetic field:

$$H^{\text{inc}}(\mathbf{r}, t) = \sqrt{\mu_0/\varepsilon_0} \mathbf{\hat{y}} H_0 G(t - \mathbf{r} \cdot \mathbf{\hat{z}}/c_0)$$  \hspace{1cm} (3.25)

where $H_0 = 1 \text{A/m}$ is the amplitude and $G(t) = \cos[2\pi f_0(t - t_p)]e^{-(t-t_p)^2/(2\sigma^2)}$ is the modulated Gaussian pulse. Here, $\sigma = 3/(2\pi f_{bw})$ is the duration, $f_{bw}$ is the effective
bandwidth, $f_0$ is the center frequency, and $f_{\text{max}} = f_0 + f_{\text{bw}}$ is the maximum frequency of the pulse. It is assumed that the scatterer resides in free space (vacuum). Accuracy and efficiency of four time marching schemes are compared: The explicit scheme with Galerkin testing, the explicit scheme with point testing, the implicit scheme with Galerkin testing, and the implicit scheme with point testing. For sake of briefness, in the rest of this section, these schemes are referred to as $[\text{MOT}]^{\text{exp}}_{\text{GT}}$, $[\text{MOT}]^{\text{exp}}_{\text{PT}}$, $[\text{MOT}]^{\text{imp}}_{\text{GT}}$, and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$, respectively.

The $[\text{MOT}]^{\text{exp}}_{\text{GT}}$, $[\text{MOT}]^{\text{imp}}_{\text{GT}}$, and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$ use the transpose-free quasi-minimal residual (TFQMR) method [78] to iteratively solve the relevant MOT systems. The iterations of the TFQMR solver and the correction updates of the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$ and $[\text{MOT}]^{\text{exp}}_{\text{PT}}$ are terminated when the following stopping criteria is satisfied:

$$
\|I^u_l - I^{u-1}_l\| < \chi
$$

(3.26)

Here, $I^u_l$ represents the solution vector at the $l$th time step and the $u$th TFQMR iteration or at the $l$th time step and the $u$th correction update and $\chi = 10^{-15}$ is the convergence threshold. The PE(CE)$^m$ scheme uses the 4th order Adam-Bashworth and backward difference coefficients at the prediction and correction steps, respectively [94].

After the time domain simulations are completed, the solutions are Fourier transformed and divided by the Fourier transform of $G(t)$ to yield the time harmonic magnetic field, $\tilde{H}(r,f)$. Time harmonic electric field $\tilde{E}(r,f)$ and the time harmonic current density $\tilde{J}(r,f)$ are computed using the curl of (3.4). The radar cross section (RCS) and the scattering cross section (SCS) are computed using $\tilde{J}(r,f)$. 
3.3.1 Accuracy of Basis Functions

The scatterer is a unit sphere with $\varepsilon(\mathbf{r}) = \varepsilon_0$. Since $\kappa(\mathbf{r}) = 0$, $\mathbf{H}^{ca}(\mathbf{r}, t) = 0$ and $\mathbf{H}(\mathbf{r}, t) = \mathbf{H}^{inc}(\mathbf{r}, t)$, i.e. the solution should match the incident field. The excitation parameters $f_0 = 5$ MHz and $f_{bw} = 2$ MHz. Four different meshes are used. The average edge length of the meshes changes from 63.28 cm to 24.84 cm. These correspond to $\lambda/94.81$ and $\lambda/241.5$ at $f_0$. Two sets of simulations are carried out using
the [MOT]^{\text{exp}}_{\text{GT}} for N_t = 4000 with $\Delta t = 1 \text{ ns}$. In the first set, $\mathbf{H}(\mathbf{r}, t)$ is expanded using both $\mathbf{f}_n^1(\mathbf{r})$ and $\mathbf{f}_n^2(\mathbf{r})$ in (3.4) while in the second test only $\mathbf{f}_n^2(\mathbf{r})$ is used. Two error measures are defined:

$$
err^H = \sqrt{\frac{\sum_{k=1}^{N_v} \left| \tilde{\mathbf{H}}(\mathbf{r}_k, f_0) - \tilde{\mathbf{H}}^{\text{inc}}(\mathbf{r}_k, f_0) \right|^2}{\sum_{k=1}^{N_v} \left| \tilde{\mathbf{H}}^{\text{inc}}(\mathbf{r}_k, f_0) \right|^2}}
$$

(3.27)

$$
err^E = \sqrt{\frac{\sum_{k=1}^{N_v} \left| \tilde{\mathbf{E}}(\mathbf{r}_k, f_0) - \tilde{\mathbf{E}}^{\text{inc}}(\mathbf{r}_k, f_0) \right|^2}{\sum_{k=1}^{N_v} \left| \tilde{\mathbf{E}}^{\text{inc}}(\mathbf{r}_k, f_0) \right|^2}}
$$

(3.28)

Here, $\mathbf{r}_k$ represent the centers of the tetrahedrons and $N_v$ is their number, $\{\tilde{\mathbf{E}}^{\text{inc}}(\mathbf{r}, f), \tilde{\mathbf{H}}^{\text{inc}}(\mathbf{r}, f)\}$ and $\{\tilde{\mathbf{E}}(\mathbf{r}, f), \tilde{\mathbf{H}}(\mathbf{r}, f)\}$ are the time harmonic incident and total electric and magnetic fields, respectively. Fig. 3.2(a) plots $err^H$ versus average edge length for the two sets of simulations. The figure shows that both $\mathbf{f}_n^1(\mathbf{r}) \cup \mathbf{f}_n^2(\mathbf{r})$ (the FLCB basis functions) and $\mathbf{f}_n^2(\mathbf{r})$ (the Nedelec basis functions) are reasonably accurate in representing $\mathbf{H}(\mathbf{r}, t)$ and the error decreases as the mesh gets finer. Fig. 3.2(b) plots $err^E$ versus average edge length for the same sets of simulations. The figure shows that using only $\mathbf{f}_n^2(\mathbf{r})$ (the Nedelec basis functions) results in an inaccurate electric field $\mathbf{E}(\mathbf{r}, t)$ while using $\mathbf{f}_n^1(\mathbf{r}) \cup \mathbf{f}_n^2(\mathbf{r})$ (the FLCB basis functions) renders $\mathbf{E}(\mathbf{r}, t)$ as accurate as $\mathbf{H}(\mathbf{r}, t)$. In other words, the Nedelec functions accurately represent the solution, but the curl of the resulting solution is not accurate. When $\kappa(\mathbf{r}) \neq 0$, the curl of the solution is needed to compute $\nabla_{j}^{\text{ind}}$, $p \in \{1, 2\}$ [see for example (3.3), (3.9), or (3.12)]. This means that using only the Nedelec functions makes the MOT solution inaccurate (and consequently unstable). The results and the discussion presented here justify why the FLCB basis functions are used by the explicit schemes developed in
this work.

3.3.2 Unit Sphere

For this example, scattering from a unit sphere is analyzed. The sphere is discretized using 1924 tetrahedrons resulting in $N = 6324$ unknowns. The excitation parameters $f_0 = 5 \text{ MHz}$ and $f_{bw} = 0.5 \text{ MHz}$.

First, the permittivity of the sphere is set to $10\varepsilon_0$. A total of four simulations are carried out for $N_t = 2500$ with $\Delta t = 6 \text{ ns}$ using the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$, $[\text{MOT}]^{\text{exp}}_{\text{PT}}$, $[\text{MOT}]^{\text{imp}}_{\text{GT}}$, and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$. Fig. 3.3(a) plots $H(r, t)$ computed by these schemes at the point $r = (0.51, -0.64, 0.12)$. The figure shows that all four schemes provide practically the same result. Fig. 3.3(b) provides the number of correction updates ($m_{\text{max}}$) required by the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$ and $[\text{MOT}]^{\text{exp}}_{\text{PT}}$ as well as the number of TFQMR iterations ($N_{\text{iter}}^{\text{imp}}$) required by the $[\text{MOT}]^{\text{imp}}_{\text{GT}}$ and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$ to achieve the convergence criteria in (3.26) at every time step. For the the $[\text{MOT}]^{\text{imp}}_{\text{GT}}$ and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$, $N_{\text{iter}}^{\text{imp}}$ reaches roughly 100 and 2500, respectively. For the implicit MOT systems, the sparseness factor ($\gamma$) is 1.000 and 0.9983, respectively. For $[\text{MOT}]^{\text{exp}}_{\text{GT}}$ and $[\text{MOT}]^{\text{exp}}_{\text{PT}}$, $m_{\text{max}}$ reaches roughly 30. For the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$, the sparseness factor of $Z_0^1$ and $Z_0^2$ ($\gamma$) is 0.9984, the sparseness factor of $G$ ($\delta$) is 0.0037, the number of iterations required to solve the MOT systems in (3.19) and (3.22) ($N_{\text{iter}}^G$) is 26. Inserting these values in the computational complexity estimates described in Sec. 3.2.5 shows that the $[\text{MOT}]^{\text{exp}}_{\text{PT}}$ is faster than the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$, which is faster than both the $[\text{MOT}]^{\text{imp}}_{\text{GT}}$ and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$. Indeed, measured computation times, which are presented in Table 3.1, verify this result. Note that in Table 3.1, the first column is the time required to compute all relevant MOT matrices, the second column refers to $C_{\text{PT}}^{\text{exp}} N_t + C$, $C_{\text{GT}}^{\text{exp}} N_t + C$, or $C_{\text{imp}}^{\text{imp}} N_t + C$ (see Sec. 3.2.5) depending the scheme used, and the last column is the total of the first two.

The RCS of the sphere is computed for $0^\circ < \theta < 180^\circ$ and $\phi = 0^\circ$ at $f = 5 \text{ MHz}$. Let $\sigma_{\text{GT}}^{\text{imp}}$, $\sigma_{\text{PT}}^{\text{imp}}$, $\sigma_{\text{GT}}^{\text{exp}}$, and $\sigma_{\text{PT}}^{\text{exp}}$ represent the RCS computed from the solu-
Figure 3.3: Scattering analyzed for unit sphere with $\varepsilon_r = 10$. (a) shows the magnetic field density computed using the solvers against time, (b) shows the iterations required for obtaining the result in each time step, and (c) shows the accuracy of the RCS computed using the solvers, compared with analytical solution obtained using Mie series solution.
Figure 3.4: Scattering analyzed for unit sphere with $\varepsilon_r = 50$. (a) shows the magnetic field density computed using the solvers against time, (b) shows the iterations required for obtaining the result in each time step, and (c) shows the accuracy of the RCS computed using the solvers, compared with analytical solution obtained using Mie series solution.
Matrix fill time [s] | MOT time [s] | Total time [s]
----------------|--------------|-------------
$[\text{MOT}]^{\text{imp}}_{\text{GT}}$ | 1977 | 2654 | 4631
$[\text{MOT}]^{\text{exp}}_{\text{GT}}$ | 1974 | 1350 | 3324
$[\text{MOT}]^{\text{imp}}_{\text{PT}}$ | 43 | 64891 | 64934
$[\text{MOT}]^{\text{exp}}_{\text{PT}}$ | 45 | 476 | 521

Table 3.1: Times required for the 4 different marching schemes for scattering analysis of unit sphere with $\varepsilon_r = 10$.

Fig. 3.3(c) plots the RCS computed using Mie series (denoted by $\sigma_{\text{Mie}}$), $|\sigma_{\text{GT}}^{\text{imp}} - \sigma_{\text{Mie}}|$ , $|\sigma_{\text{GT}}^{\text{exp}} - \sigma_{\text{Mie}}|$ , $|\sigma_{\text{PT}}^{\text{imp}} - \sigma_{\text{Mie}}|$, and $|\sigma_{\text{PT}}^{\text{exp}} - \sigma_{\text{Mie}}|$ in dB scale. The figure shows that all solvers practically have the same accuracy, as the largest error is 30dB below $\sigma_{\text{Mie}}$.

For the next simulation, the permittivity of the sphere is set to 50$\varepsilon_0$. The simulation is carried out for $N_t = 1000$ with $\Delta t = 5$ ns using the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$. Fig. 3.4(a) plots $H(\mathbf{r}, t)$ computed during the simulation at the point $\mathbf{r} = (0.51, -0.64, 0.12)$. Fig. 3.4(b) provides the number of correction updates ($m_{\text{max}}$) required by the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$ to achieve the convergence criteria in (3.26) at every time step. Note that for this problem, other three schemes do not produce stable results. The RCS (denoted by $\sigma_{\text{GT}}^{\text{exp}}$) is computed for $0^0 < \theta < 180^0$ and $\phi = 0^0$ at $f = 5$ MHz from the solution obtained by the $[\text{MOT}]^{\text{exp}}_{\text{PT}}$. Fig. 3.4(c) plots the RCS computed using Mie series (denoted by $\sigma_{\text{Mie}}$) and $|\sigma_{\text{GT}}^{\text{exp}} - \sigma_{\text{Mie}}|$ in dB scale. The error is less than 40dB.

3.3.3 Piece-wise Slab

For this example, scattering from piece-wise dielectric slab is analyzed. The slab consists of two equal volumes with permittivities $3\varepsilon_0$ and $9\varepsilon_0$ [as shown in the inset of Fig. 3.5(a)]. The slab is discretized using 2106 tetrahedrons resulting in $N = 6088$ unknowns. The excitation parameters $f_0 = 5$ MHz and $f_{\text{bw}} = 0.5$ MHz. A total of four simulations are carried out for $N_t = 2500$ with $\Delta t = 6$ ns using the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$, $[\text{MOT}]^{\text{exp}}_{\text{PT}}$, $[\text{MOT}]^{\text{imp}}_{\text{GT}}$, and $[\text{MOT}]^{\text{imp}}_{\text{PT}}$. 
Figure 3.5: Scattering analyzed for inhomogeneous slab (a) shows the magnetic field density computed using the solvers, (b) shows the iterations required in each time step, and (c) shows the accuracy of the RCS computed using the 4 different solvers, compared with frequency domain EFVIE solver.
Fig. 3.5(a) plots $\mathbf{H}(r, t)$ computed by these schemes at the point $r = (0.23, 0.14, 0.57)$. The results agree very well. Fig. 3.5(b) provides the number of correction updates ($m_{\text{max}}$) required by the $[\text{MOT}]_{\text{exp}}^{\text{GT}}$ and $[\text{MOT}]_{\text{PT}}^{\text{exp}}$ as well as the number of TFQMR iterations ($N_{\text{iter}}^{\text{imp}}$) required by the $[\text{MOT}]_{\text{imp}}^{\text{GT}}$ and $[\text{MOT}]_{\text{PT}}^{\text{imp}}$ to achieve the convergence criteria in (3.26) at every time step. Sparseness factor for the implicit MOT systems is $\gamma = 1.000$. For the $[\text{MOT}]_{\text{exp}}^{\text{GT}}$, the sparseness factor of $\mathbf{Z}_0^1$ and $\mathbf{Z}_0^2$ is $\gamma = 1.000$, the sparseness factor of $\mathbf{G}$ is 0.0047, the number of iterations required to solve the MOT systems in (3.19) and (3.22) $N_{\text{iter}}^{\text{G}} = 24$. Inserting these values and the ones provided in Fig. 3.5(b) in the computational complexity estimates described in Sec. 3.2.5 shows that the $[\text{MOT}]_{\text{PT}}^{\text{exp}}$ is faster than the $[\text{MOT}]_{\text{GT}}^{\text{exp}}$, which is faster than both the $[\text{MOT}]_{\text{GT}}^{\text{imp}}$ and $[\text{MOT}]_{\text{PT}}^{\text{imp}}$. This result is verified by the computation times provided in Table 3.2.

<table>
<thead>
<tr>
<th>Matrix fill time [s]</th>
<th>MOT time [s]</th>
<th>Total time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[\text{MOT}]_{\text{GT}}^{\text{imp}}$</td>
<td>1199</td>
<td>1240</td>
</tr>
<tr>
<td>$[\text{MOT}]_{\text{GT}}^{\text{exp}}$</td>
<td>1201</td>
<td>940</td>
</tr>
<tr>
<td>$[\text{MOT}]_{\text{PT}}^{\text{imp}}$</td>
<td>28</td>
<td>7198</td>
</tr>
<tr>
<td>$[\text{MOT}]_{\text{PT}}^{\text{exp}}$</td>
<td>29</td>
<td>203</td>
</tr>
</tbody>
</table>

Table 3.2: Times required for different marching schemes for scattering analysis of piece-wise slab.

The solutions obtained by the $[\text{MOT}]_{\text{GT}}^{\text{imp}}$, $[\text{MOT}]_{\text{PT}}^{\text{imp}}$, $[\text{MOT}]_{\text{GT}}^{\text{exp}}$, and $[\text{MOT}]_{\text{PT}}^{\text{exp}}$ are used to compute $\sigma_{\text{GT}}^{\text{imp}}$, $\sigma_{\text{PT}}^{\text{imp}}$, $\sigma_{\text{GT}}^{\text{exp}}$, and $\sigma_{\text{PT}}^{\text{exp}}$ for $0^0 < \theta < 180^0$ and $\phi = 0^0$ at $f = 5$ MHz, respectively. Fig. 3.5(c) plots the RCS computed using the solution obtained by a frequency domain electric field volume integral equation solver (denoted by $\sigma_{\text{FD}}$), $|\sigma_{\text{GT}}^{\text{imp}} - \sigma_{\text{FD}}|$, $|\sigma_{\text{PT}}^{\text{imp}} - \sigma_{\text{FD}}|$, $|\sigma_{\text{GT}}^{\text{exp}} - \sigma_{\text{FD}}|$, and $|\sigma_{\text{PT}}^{\text{exp}} - \sigma_{\text{FD}}|$ in dB scale. Results agree very well.
3.3.4 Thin Film Detection

In this example, a thin film detection scheme, which makes use of a photonic nanojet (PNJ), is studied using the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$. The PNJ is a narrow high intensity light beam generated using a microspherical dielectric lens. High intensity electromagnetic field focused in the proximity of the thin film results in a detectable change in the scattering efficiency of the whole system (in comparison to the same system without the thin film) [26, 97].

For the system studied here, the PNJ is generated using a six layered microsphere [Fig. 3.6]. The radius of the core and the thickness of the layers are set to 0.416 $\mu$m. Their permittivities (in the order from the core to the outermost layer) are 1.02$\varepsilon_0$, 1.04$\varepsilon_0$, 1.06$\varepsilon_0$, 1.08$\varepsilon_0$, 1.10$\varepsilon_0$, and 1.12$\varepsilon_0$, respectively. The thickness of the thin film is 100 nm and its permittivity is 1.96$\varepsilon_0$. It is located on the plane that divides the substrate vertically into two equal volumes. The substrate is a cube of dimension 2 $\mu$m and its permittivity is 1.69$\varepsilon_0$. The scatterer (microsphere + cube + thin film) is discretized using 19856 tetrahedrons resulting in 49460 unknown. The excitation parameters are $f_0 = 300$ THz and $f_{bw} = 15$ THz. Two simulations are carried out for $N_t = 6000$ with $\Delta t = 0.1$ fs using the $[\text{MOT}]^{\text{exp}}_{\text{GT}}$: (i) The scatterer consists of the microsphere, cube, and thin film. (ii) The scatterer consists of the micropshere...
Figure 3.7: (a) shows the magnetic field density observed at the point \( \mathbf{r} = (4.0, 0.0, 0.0) \mu\text{m} \) and (b) shows the change in the scattering efficiency after inserting the thin film.

and cube with the thin film removed. Fig. 3.7(a) plots \( \mathbf{H}(\mathbf{r}, t) \) computed at the point \( \mathbf{r} = (4.0, 0.0, 0.0) \mu\text{m} \) in the first and second simulations. Fig. 3.7(b) plots the scattering efficiency computed using the solutions obtained using the time domain simulations. The difference between the two results is clear, demonstrating that this system can indeed be used to detect a thin film.
Chapter 4

Time Domain Volume Integral Equation Solver for Analyzing Nonlinear Scatterers

4.1 Introduction

The chapter introduces an extension of the marching on-in-time (MOT) schemes described in the previous chapters, which enables their application to nonlinear scatterers, i.e., scatterers where the permittivity is a (nonlinear) function of the electric field intensity. More specifically, scatterers with Kerr nonlinearity are considered.

Kerr nonlinear materials find applications in the fields of electromagnetics and photonics for harmonic generation, self-wave modulation, self-focusing, and wave mixing [98]. Therefore, simulation tools capable of accounting for nonlinear permittivity models are needed. Since the linearity assumption that forms the basis of frequency domain solvers breaks, time domain solvers lead the way in characterizing the electromagnetic wave interactions on nonlinear scatterers. From the several classes of time domain solvers, finite different time domain (FDTD) schemes are often preferred for this purpose [99] because their explicit nature allows for straightforward incorporation of nonlinear permittivity models. This is typically done using the nonlinear constitutive relation between the electric field intensity and the flux density as an auxiliary equation [99] complementing the Maxwell equations. On the other hand, use of time domain volume integral equation (TD-VIE) solvers in characterizing nonlinear scatterers is limited to two-dimensional scatterers [100]. Extension of the (three-dimensional) implicit MOT developed to solve the time domain electric field
volume integral equation (TD-EFVIE) (Chapter 2) to the analysis of the Kerr nonlinear scatterer is not straightforward since this extension would call for a Newton like nonlinear solver at every time step. Whereas the traditional explicit MOT solvers, which can be extended for characterizing nonlinear effects in a more straightforward way, suffer from poor stability [88, 89, 26, 90].

The explicit MOT solver described in Chapter 3 offers improved stability and accuracy compared to these traditional explicit MOT solvers. In this chapter, an extension of this new explicit MOT scheme to solve the TD-EFVIE enforced on Kerr nonlinear scatterers is developed. The stability of the solution is ensured using the temporal interpolation scheme discussed in the Chapter 2, and the PE(CE)\textsuperscript{m} based marching scheme discussed in Chapter 3. To account for the nonlinearity, the TD-EFVIE is formulated in terms of both electric field intensity and flux density, and their spatial discretization is carried out by half and full Schaubert-Wilton-Glisson (SWG) functions [72, 73, 77], respectively. Similar to the FDTD schemes, the nonlinear constitutive relation is used as the auxiliary equation to complement the TD-EFVIE. The explicit nature of the proposed scheme allows for the incorporation of the nonlinearities as function evaluations on the right-hand side of the MOT system. Therefore the resulting scheme does not call for Newton-like nonlinear equation solvers.

The rest of this chapter is organized as follows. Section 4.2 describes the proposed explicit MOT-TD-EFVIE solver. Sections 4.2.1 and 4.2.2 present the TD-EFVIE and the constitutive equation, respectively. Section 4.2.3 and 4.2.4 discusses some observation about the proposed scheme and illustrates the steps involved in the explicit MOT scheme, respectively. Section 4.3 demonstrates the stability and accuracy of the proposed explicit MOT solver in characterizing transient electromagnetic wave interactions on the nonlinear Kerr media via numerical experiments.
4.2 Formulation

4.2.1 Time Domain Electric Field Volume Integral Equation

The equivalent current $\mathbf{J}(\mathbf{r}, t)$ in (2.1), is related to the total electric field intensity $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{D}(\mathbf{r}, t)$ as

$$\mathbf{J}(\mathbf{r}, t) = \partial_t \mathbf{D}(\mathbf{r}, t) - \varepsilon_0 \partial_t \mathbf{E}(\mathbf{r}, t)$$  (4.1)

where, the total electric field $\mathbf{E}(\mathbf{r}, t)$ is

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}^{\text{inc}}(\mathbf{r}, t) + \mathbf{E}^{\text{sca}}(\mathbf{r}, t)$$  (4.2)

Inserting (4.1) into (2.1) and the resulting equation into (4.2) and enforcing the temporal derivative of the final equation for $\mathbf{r} \in V$ yield the temporal derivative of TD-EFVIE in unknowns $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{D}(\mathbf{r}, t)$:

$$\partial_t \mathbf{E}^{\text{inc}}(\mathbf{r}, t) = \partial_t \mathbf{E}(\mathbf{r}, t) + \mathcal{L}\{\mathbf{E}(\mathbf{r}, t)\} - \varepsilon_0^{-1} \mathcal{L}\{\mathbf{D}(\mathbf{r}, t)\}$$  (4.3)

where the volume integral operator $\mathcal{L}\{\cdot\}$ is defined as

$$\mathcal{L}\{\mathbf{X}(\mathbf{r}, t)\} = -\frac{\varepsilon_0 \mu_0}{4\pi} \int_V \frac{1}{R} \partial_{t'}^3 \mathbf{X}(\mathbf{r}', t')|_{t' = t - R/c_0} d\mathbf{r}'$$

$$+ \frac{1}{4\pi} \nabla \int_V \frac{1}{R} \left[ \nabla' \cdot \partial_{t'} \mathbf{X}(\mathbf{r}', t') \right]|_{t' = t - R/c_0} d\mathbf{r}'$$  (4.4)

To numerically solve (4.3) scatterer $V$ is discretized with tetrahedral elements. $\mathbf{D}(\mathbf{r}, t)$ is spatially approximated using the full Schaubert-Wilton-Glisson (SWG) basis functions $f^D_n(\mathbf{r})$ (2.6) as
\[ D(r, t) \approx \sum_{n=1}^{N_D} \{I^D(t)\}_n f^D_n(r) \quad (4.5) \]

where \( \{I^D(t)\}_n = I^D_n(t) \) are the time dependent coefficients associated with the \( n \)th spatial basis function. To model the discontinuous behavior of the electric field intensity half SWG functions \( f^E_n(r) \) defined as

\[
f^E_n(r) = \begin{cases} 
\frac{a_n}{3n_f^+} (r - r^+_n), r \in V^+_n \\
0, \text{ elsewhere}
\end{cases} \quad (4.6)
\]

are used. Subsequently, \( E(r, t) \) is approximated as [72, 73]:

\[ E(r, t) \approx \sum_{n=1}^{N_E} \{I^E(t)\}_n f^E_n(r) \quad (4.7) \]

where \( \{I^E(t)\}_n = I^E_n(t) \) is the time dependent coefficients associated with the \( n \)th spatial half SWG function. Substituting (4.5) and (4.7) in (4.3) and testing the resulting equation with \( f^E_m(r) \) yield the spatially discretized time dependent TD-EFVIE:

\[
G \partial_t I^E(t) = V^{inc}(t) + V^{sca}_E(t, I^E(t)) + V^{sca}_D(t, I^D(t)) \quad (4.8)
\]

Here the elements of Gram matrix \( G \), tested incident field \( V^{inc}(t) \), \( V^{sca}_E(t, I^E(t)) \)
and $V_{sca}^D(t, I^E(t))$ are

\[
\{G\}_{m,n} = \int_{V_m} f_m^E(r) \cdot f_n^E(r) dr \\
\{V^{inc}(t)\}_m = \int_{V_m} f_m^E(r) \cdot \partial_t E^{inc}(r, t) dr \\
\{V_{sca}^E(t, I^E(t))\}_m = \sum_{n=1}^{N_E} \int_{V_m} f_m^E(r) \cdot L\{\{I^E(t)\}_n f_n^E(r)\} dr \\
\{V_{sca}^D(t, I^D(t))\}_m = -\sum_{n=1}^{N_D} \int_{V_m} f_m^E(r) \cdot L\{\varepsilon^{-1}\{I^D(t)\}_n f_n^E(r)\} dr
\]

To obtain a fully discretized system, (4.8) should be sampled in time with step size $\Delta t$. However once (4.8) is temporally discretized, the time retardation in the operator $L\{\cdot\}$ required for computing the contribution from $V_{sca}^E(t, I^E(t))$ and $V_{sca}^D(t, I^D(t))$ may not fit into the sampled time steps. To overcome this $I^E(t)$ and $I^D(t)$ are interpolated from its samples using approximate spheroidal wave functions augmented with complex exponential extrapolation (Section 2.2.3), denoted as $T_i(t) = T(t - i\Delta t)$. This results in the expansion of $I^E(t)$ and $I^D(t)$ as

\[
I^E(t) = \sum_{i=1}^{N_t} I^E_i T_i(t) \\
I^D(t) = \sum_{i=1}^{N_t} I^D_i T_i(t)
\]

Here $I^E_i = I^E(t)|_{t=i\Delta t}$, $I^D_i = I^D(t)|_{t=i\Delta t}$ and $N_t$ is number of time steps. As a result, fully discretized MOT system at $j$th time step is given as

\[
G \dot{I}^E_j = Z_0^{EE} I^E_j - \varepsilon^{-1}_0 Z_0^{ED} I^D_j + V^{inc}_j + \sum_{i=1}^{j-1} Z_{j-i}^{EE} I^E_i - \varepsilon^{-1}_0 \sum_{i=1}^{j-1} Z_{j-i}^{ED} I^D_i
\]

where $\dot{I}^E_j = \partial_t I^E(t)|_{t=j\Delta t}$, $V^{inc}_j = V^{inc}(t)|_{t=j\Delta t}$ and the elements of MOT matrices
\( Z_{j-i}^{EE} \) and \( Z_{j-i}^{ED} \) are given as

\[
\{Z_{j-i}^{EU}\}_{m,n} = \int_{V_m} f_m^E(r) \cdot \mathcal{L}\{f_m^U(r)T_i(t)\}|_{t=j\Delta t} dr; \quad U \in \{E, D\} \quad (4.16)
\]

It should be noted here that the range of both the matrices \( Z_{j-i}^{EE} \) and \( Z_{j-i}^{ED} \) is half SWG function space. Since the half SWG functions are defined as positive half of SWG, \( f_n^D(r) \) can be constructed by combining two associated \( f_n^E(r) \) functions with appropriate sign. Subsequently, a sparse mapping operator \( P \) from the half SWG function space to full SWG function space can be defined. Using \( P \), the MOT matrices \( Z_{j-i}^{ED} \) can be constructed as \( Z_{j-i}^{ED} = Z_{j-i}^{EE}P^\dagger \), where \( \dagger \) is the transpose operator. Using this, the need for storing MOT matrices \( Z_{j-i}^{ED} \) can be completely avoided.

This completes the discretization of the TD-EFVIE.

### 4.2.2 Constitutive Relation

Constitutive equation that relates the total electric field intensity \( E(r, t) \) to flux density \( D(r, t) \) is used as an auxiliary equation in the explicit MOT scheme:

\[
D(r, t) = \varepsilon(r, t, E)E(r, t) \quad (4.17)
\]

The constitutive equation has been incorporated to MOT solvers to model the dispersive and lossy media \[72, 73\]. But in this thesis incorporation of nonlinearity in an instantaneous Kerr medium is presented. For an instantaneous Kerr nonlinear scatterer the time and field dependent permittivity is given as \[19\]

\[
\varepsilon(r, t, E) = \varepsilon_0 \left[ \chi^{(1)} + \chi^{(3)} |E(r, t)|^2 \right] \quad (4.18)
\]

Here, \( \chi^{(1)} \) and \( \chi^{(3)} \) and are the relative linear and third order nonlinear terms. Even though, the explicit MOT scheme is equally valid in the presence of second order
nonlinear terms \( \chi^{(2)} \), only \( \chi^{(3)} \) nonlinearity is considered here, assuming the presence of centro-symmetry in the scatterer [98].

In MOT based VIE solvers, permittivity is assumed to be constant throughout the tetrahedron. Using this fact (4.18) is discretized at the center of the tetrahedrons and the value is assumed to be constant throughout the tetrahedron. Using the expansion (4.7), (4.18) can be discretized as

\[
\varepsilon(r^c_k, t, E) = \varepsilon_k^c(t) = \varepsilon_0 \left[ \chi^{(1)} + \chi^{(3)} \sum_{n=1}^{N_e} \left| \left\{ I^E_n(t) \right\}_n f^E_n(r^c_k) \right| \right]^2 \tag{4.19}
\]

where \( r^c_k \) is the center of the \( k \)th tetrahedron. Since there is no retardation in (4.17) and (4.18), (4.17) can be discretized temporally at the discrete time steps \( t = j \Delta t \), without a need for temporal interpolation functions. Using the expansions (4.5), (4.7), and (4.19) in (4.17) and testing the resulting equations with \( f^D_n(r) \), we obtain the discretized constitutive equation as

\[
\text{PGP}^\dagger I^D_j = \text{PG} \varepsilon_j I^E_j \tag{4.20}
\]

where, the elements of \( \{ \varepsilon_j \}_k_n = \varepsilon^c_{k_n}(j \Delta t) \) are the samples of time and field dependent permittivity at the center of the tetrahedron \( k_n \), that is the part of the \( n \)th half SWG function consists.

After evaluating \( I^D_j \), \( I^E_j \) is updated using Pade approximation [101] as:

\[
I^E_j = \left( \left[ \chi^{(1)} \right]^3 + 2 \chi^{(3)} |D|^2 \right) \frac{\text{PG}^\dagger I^D_j}{\varepsilon_0 \chi^{(1)}} \left[ \chi^{(1)} \right]^3 + 3 \chi^{(3)} |D|^2 \tag{4.21}
\]

This completes the discretization of the constitutive relation.
4.2.3 Observations and Discussions

Several observations about the MOT system in (4.15) with the auxiliary equation (4.20) are listed as follows:

1. The MOT system in (4.15) connects the samples of the unknowns $I_E^j$ and $I_D^j$ to the temporal derivative of $I_E^j$. As a result (4.15) is a form of an ordinary differential equation and can be integrated in time using a predictor-corrector scheme as described in citeulku2013. The constitutive equation (4.20) is used as auxiliary equation to update $I_D^j$ in the predictor corrector scheme.

2. In (4.15) the temporal interpolation functions can be Lagrange interpolation function as well as the band limited interpolation functions. Lagrange interpolation functions provide a causal MOT system (4.15), whereas the band limited interpolation functions result in a non-causal system. In such cases, causality can be retrieved using an extrapolation scheme specially tailored for TD-EFVIE as described in [93].

3. EFVIE is a second kind Volterra integral equation. However its second kind behavior strictly depends on the permittivity of the scatterer. If the permittivity of the scatterer is high, or when the electric field intensity is high, the contribution from the electric flux density dominates the matrix elements and resulting equation system resembles a first kind integral equation [44, 85]. This results in unstable MOT systems and slow convergence in time marching since the proposed explicit MOT scheme in this thesis benefits from the second kind behavior of integral equations.

4. The MOT matrices $Z_{j-i}^{EE}$ are determined as in the implicit MOT scheme without the self-term contribution [44, 93]. Therefore implementation of the given explicit scheme in this thesis can be obtained with small changes in time marching. As in the implicit case, the gradient operation in the retarded-time scalar
potential part in $\mathcal{L}\{\cdot\}$ operator in (4.16) is moved to testing function in the MOT matrix elements as explained in [47, 77, 93]. Since $f^E_m(r)$ is a discontinuous function on the common face $A_m$, the divergence operation is determined as

$$\nabla \cdot f^E_m(r) = \begin{cases} 
\frac{a_m}{u^+_m}, & r \in V^+_m \\
-1, & r \in A_m \\
0, & \text{elsewhere}
\end{cases} \quad (4.22)$$

for both testing and basis functions. Here $A_m$ denotes the support of the face where $f^E_m(r)$ is defined. As a result a surface integral over $A_m$ should be calculated to determine the MOT matrix elements.

### 4.2.4 Explicit Marching On in Time Scheme

Similar to Section 3.2.3, an explicit time marching method based on the predictor-corrector scheme developed in [47] can be used to integrate the MOT system in (4.15) with the auxiliary equation (4.20). $I^E_j$ can be determined by solving (4.15) if the values of $I^E_i$ and $I^D_i$, $i = 0, \ldots, j$, are known. The values of $I^E_i$ are extrapolated, and $I^P_i$ and $I^E_j$ evaluated from (4.20) and (4.15), respectively. This leads to the PE(CE)$^m$ scheme. At every time step the PE(CE)$^m$ scheme is employed to obtain the solution. However direct implementation of PE(CE)$^m$ scheme as developed in [47] to TD-EFVIE results in high number of corrector steps and slow converging solution. Therefore the algorithm is modified to provide faster convergence rate and stable solution using successive over relaxation (SOR) ([74]. The algorithm for the solution of (4.15) with the auxiliary equation (4.20) at $j$th time step using the predictor-corrector based time marching is describe below.

At each time step $j = k, \ldots, N_t$:
• **Step 1**: The components of the right-hand side of (3.15), which are not updated within the time step \(j\), are computed:

\[
V_{j}^{\text{fixed}} = V_{j}^{\text{inc}} + \sum_{i=1}^{j-1} Z_{j-i}^{EE} I_{i}^{E} - \varepsilon_{0}^{-1} \sum_{i=1}^{j-1} Z_{j-i}^{ED} I_{i}^{D}
\]

• **Step 2**: Predictor (P) step. \(I_{j}^{E,(0)}\) is predicted using \(k\) past (known) values of \(I_{j}^{E,(0)}, \dot{I}_{j}^{E,(0)}\), \(i = j - k, \ldots, j - 1\), respectively:

\[
I_{j}^{E,(0)} = \sum_{i=1}^{k} \left[ \{p\}_{i} I_{j-1+i-k}^{E} + \{p\}_{k+i} \dot{I}_{j-1+i-k}^{E} \right]
\]

Here, \(p\) is a vector of dimension \(2k\), which stores the predictor coefficients.

• **Step 3**: Compute \(\varepsilon_{j}^{(0)}\):

\[
\{\varepsilon_{j}^{(0)}\}_{n} = \varepsilon_{0} \left[ \chi^{(1)} + \chi^{(3)} \left| \{I_{j}^{E,(0)}\}_{n} f_{n}^{E}(r_{k}) \right|^{2} \right]
\]

• **Step 4**: Compute \(I_{j}^{D,(0)}\) as

\[
\text{PGP}^{\dagger} I_{j}^{D,(0)} = \text{PG} \varepsilon_{j}^{(0)} I_{j}^{E,(0)}
\]

• **Step 5**: Update \(I_{j}^{E,(0)}\):

\[
I_{j}^{E,(0)} = \left( \frac{[\chi^{(1)}]^{3} + 2\chi^{(3)}|D|^{2}}{[\chi^{(1)}]^{3} + 3\chi^{(3)}|D|^{2}} \right) \frac{\text{PG}^{\dagger} I_{j}^{D,(0)}}{\varepsilon_{0} \chi^{(1)}}
\]

• **Step 6**: Evaluate \(\dot{I}_{j}^{E,(0)}\) by solving:

\[
G I_{j}^{E,(0)} = V_{j}^{\text{fixed}} + Z_{j}^{EE} I_{j}^{E,(0)} - \varepsilon_{0}^{-1} Z_{j}^{ED} I_{j}^{D,(0)}
\]
• Step 7 Repeat step 7.1 and 7.2 until convergence ($m = 1, ..., m_{\text{max}}$):

- Step 7.1: Corrector (C) step. $I_{j}^{E,(m)}$ corrected/updated using $k$ past values of $I_{j}^{E}$ and $\dot{I}_{j}^{E}$, $i = j - k, ..., j - 1$, and the $I_{j}^{E,(m-1)}$:

$$I_{j}^{E,(m)} = \sum_{l=1}^{k} \left[ \{\mathbf{c}\}_l I_{j-1+l-k}^{E} + \{\mathbf{c}\}_{k+l} \dot{I}_{j-1+l-k}^{E} + \{\mathbf{c}\}_{2k+l} I_{j}^{E,(m-1)} \right]$$

Here, $\mathbf{c}$ is a vector of dimension $2k + 1$, which stores the corrector coefficients.

- Step 7.2: Compute $\varepsilon_{j}^{(m)}$:

$$\{\varepsilon_{j}^{(m)}\}_n = \varepsilon_0 \left[ \chi^{(1)} + \chi^{(3)} \left| \{I_{j}^{E,(m)}\}_n \dot{r}_{n}(\mathbf{r}_k) \right|^{2} \right]$$

- Step 7.3: Compute $I_{j}^{D,(m)}$ as

$$\text{PGP} I_{j}^{D,(m)} = \text{PG} \varepsilon_{j}^{(m)} I_{j}^{E,(m)}$$

- Step 7.4: Update $I_{j}^{E,(m)}$:

$$I_{j}^{E,(m)} = \left( \frac{\left[ \chi^{(1)} \right]^{3} + 2\chi^{(3)}|D|^{2}}{\left[ \chi^{(1)} \right]^{3} + 3\chi^{(3)}|D|^{2}} \right) \frac{\text{PG} I_{j}^{D,(m)}}{\varepsilon_0 \chi^{(1)}}$$

- Step 7.5: Evaluate $\dot{I}_{j}^{E,(m)}$ by solving:

$$\mathbf{G} I_{j}^{E,(m)} = \mathbf{V}_{j}^{\text{fixed}} + \mathbf{Z}_{0}^{E} I_{j}^{E,(m)} - \varepsilon_0^{-1} \mathbf{Z}_{0}^{E} \dot{I}_{j}^{D,(m)}$$

• Step 8: Once convergence is reached, i.e., $\|I_{j}^{E,(m)} - I_{j}^{E,(m-1)}\| < \chi^{\text{PECE}}$, the solutions are stored to be used at the next time step: $I_{j}^{E} = I_{j}^{E,(m)}$ and $\dot{I}_{j}^{E} = \dot{I}_{j}^{E,(m)}$.

The steps involved in the explicit time marching scheme are schematically represented using the flow chart shown in Fig. 4.1(a).
4.3 Numerical Results

This section presents numerical examples that demonstrate the stability and accuracy of the proposed explicit MOT-TD-EFVIE solver in characterizing electromagnetic wave interactions on nonlinear Kerr media with same excitation as used in (2.33). The PE(CE)\textsuperscript{m} scheme uses the sixth order Adam-Bashworth and backward difference formulas at the predictor and corrector stages, respectively. Unless specified otherwise, SOR parameter \( \beta = 0.3 \) is used. The matrix systems (4.15) and (4.20) are solved iteratively using the transpose-free quasi-minimal residual (TFQMR) method [78]. The TFQMR iterations are terminated when the condition

\[ \| \mathbf{I}_l^n - \mathbf{I}_l^{n-1} \| < \| \mathbf{b} \| \delta_{\text{TFQMR}} \]  \hspace{1cm} (4.23) \]

is satisfied. Here, \( \mathbf{I}_l^n \) is the solution at time step \( l \) and iteration \( n \), \( \mathbf{b} \) is the RHS, and
\( \delta_{\text{TFQMR}} = 10^{-12} \) is the convergence threshold. Similarly, step 7 is terminated when

\[
\| \mathbf{I}_t^n - \mathbf{I}_t^{n-1} \| < \| \mathbf{I}_t^n \| \delta_{\text{EXP}}, \quad \delta_{\text{EXP}} = 10^{-13}
\]  

(4.24)

### 4.3.1 Accuracy for Linear Sphere

In the first example, the accuracy of the proposed MOT-TD-EFVIE solver is demonstrated via comparing the radar cross section (RCS) with analytical solutions. Since, the analytical RCS solutions are available only for linear problems, the proposed solver is used for scattering analysis from a unit sphere with \( \chi^{(1)} = 2 \) and \( \chi^{(3)} = 0 \). The fields inside the sphere are discretized using \( N_E = 12820 \) and \( N_D = 6642 \). The incident field has \( f_0 = 10 \) MHz, \( f_{bw} = 5 \) MHz, and \( t_p = 8\sigma \). The simulations are carried out for \( N_t = 500 \) with \( \Delta t = 3 \) ns. Fig. 4.2(a) shows the field intensity computed at the origin, demonstrating that the solver provided stable results for the entire simulation duration. In 4.2(b), the RCS computed for \( \phi = 0^0 \) and \( \theta = [0^0, 180^0] \) at \( f = 10 \) MHz using the Fourier transformed MOT solution is compared to that computed from the analytical Mie series solution. The difference between the two solutions is less than 30 dB demonstrating that the proposed solver is providing accurate solutions.

### 4.3.2 Accuracy for Nonlinear Cube

In the second example, accuracy of the nonlinear solution obtained from the proposed solver is compared with that of an open source finite difference time domain (FDTD) solver. Here, the proposed solver and the FDTD solver MEEP [18] are used to study the scattering from a cube of edge length 0.1 m. The optical parameters of the cube are \( \chi^{(1)} = 2 \) and \( \chi^{(3)} = 8.854 \times 10^{-14} \). The fields are discretized using \( N_E = 7596 \) and \( N_D = 4002 \). The incident field has \( f_0 = 1498.962 \) MHz, \( f_{bw} = 149.896 \) MHz, and \( t_p = 10\sigma \). The simulations are carried out for \( N_t = 6000 \) time steps with step size \( \Delta t = 13.343 \) ps. In the MEEP, the simulations are carried out with \( \Delta x = 5 \) mm.
Figure 4.2: Scattering analysis from a unit sphere with \( \chi^{(1)} = 2 \) and \( \chi^{(3)} = 0 \). (a) Electric field intensity at the center of the sphere, (b) RCS for \( \phi = 0^\circ \) and \( \theta = [0^\circ, 180^\circ] \) at \( f = 10 \) MHz compared with the analytical Mie series solution.

and \( \Delta t = 8.33 \) ps. The whole computational domain is \( 1m \times 1m \times 2m \) with PML thickness of 0.3 m.

Fig. 4.3(a) compares the flux density computed at the center of the cube from the proposed solver to that of MEEP, showing good agreement between the two results.
Note that the MOT solution is saturated at a better accuracy compared to the MEEP solution. The Fourier spectrum of these two results is compared in Fig. 4.3(b). The results reveal several harmonics generated due to the nonlinearity of the medium. Both the solutions match well unto the fourth harmonic, demonstrating the accuracy of the proposed solver. The mismatch from the fifth harmonic is in the order of difference in the saturation levels of the two solutions shown in Fig. 4.3(a).
Figure 4.4: Comparison of flux density computed from TD-EFVIE and FDTD at the center of a unit sphere with $\chi^{(1)} = 1.5$ for $\chi^{(3)} = 0$ and $\chi^{(3)} = 6.64 \times 10^{-13}$ (a) in time domain and (b) spectrum showing additional harmonics generated due to the Kerr nonlinearity.

4.3.3 Four-wave Mixing

In the next example, frequency conversion using four-wave mixing phenomena in a nonlinear sphere is studied [102]. Here, the electric field of the incident wave is modulated using

$$G(t) = [0.25 \times \cos[2\pi f_1(t - t_p)] + 0.5 \times \cos[2\pi f_2(t - t_p)]] \exp[-(t - t_p)^2/(2\sigma^2)]$$
where, \( f_1 = 10.5 \text{ MHz} \), \( f_2 = 15 \text{ MHz} \), \( f_{bw} = 1 \text{ MHz} \), and \( t_p = 14\sigma \). The fields inside the sphere are discretized using \( N_E = 4444 \) and \( N_D = 2686 \). The optical parameters of the sphere are \( \chi^{(1)} = 1.5 \) and \( \chi^{(3)} = 6.6405 \times 10^{-13} \). The simulations are carried out for \( N_t = 15000 \) time steps with step size \( \Delta t = 1 \text{ ns} \). For comparison, scattering from a linear sphere with \( \chi^{(3)} = 0.0 \) is also studied for the same input.

Fig. 4.4(a) shows that flux density computed at the center of the sphere for both linear and nonlinear cases. The result shows that proposed solver provides stable results for both cases. The spectrum of these two solutions is shown in Fig. 4.4(b). The linear solution shows two harmonics at \( f_1 \) and \( f_2 \) matching with the input frequencies. However, the nonlinear solution shows two extra harmonics at frequencies \( 2f_1 - f_2 \) and \( 2f_2 - f_1 \), demonstrating the frequency conversion due to the Kerr nonlinearity.

### 4.3.4 Nonlinear Bragg Grating

In the last example, scattering from a nonlinear Bragg grating (shown in Fig. 4.5) is studied using the proposed solver. The Bragg grating considered here is composed of 20 unit cells of size \( 0.5\mu m \times 0.5\mu m \times 0.25\mu m \), where each unit cell has a linear and a nonlinear slab of thicknesses \( 0.125 \mu m \) with \( \{ \chi^{(1)}_1 = 2.25, \chi^{(3)}_1 = 0.0 \} \) and
Figure 4.6: Comparison of field transmission through a linear and nonlinear Bragg grating (a) decay in the field in a linear Bragg grating and (b) increase in the transmission due to Kerr nonlinearity.

\[ \chi_2^{(1)} = 4.5, \chi_2^{(3)} = -5.3126 \times 10^{-13} \] respectively. It is shown that, an equivalent linear structure \( \left( \chi_2^{(3)} = 0.0 \right) \) has a stop band ranging from 300 THz to 370 THz \[103\]. By introducing a negative Kerr nonlinearity, this stop band can be partially closed \[103\]. To demonstrate this, the proposed solver is used to study the scattering from a linear and a nonlinear structure from a plane wave that has
\begin{equation}
G(r, t) = \begin{cases} 
\cos(2\pi f_0(t - t_1)) e^{-(t-t_1)^2/2\sigma^2}, & t < t_1 \\
\cos(2\pi f_0(t - t_1)), & t_1 \leq t < t_2 \\
\cos(2\pi f_0(t - t_2)) e^{-(t-t_2)^2/2\sigma^2}, & t_2 \leq t 
\end{cases}
\end{equation}

where, $f_0 = 353$ THz, $\sigma = 2.3873$ fs, $t_1 = 6\sigma$ and $t_2 = 17.87\sigma$. The simulation is carried out with $N_t = 1000$, $\Delta t = 0.13$ fs and $\beta = 0.4$. The fields recorded at the feeding end $(0, 0, -2.6\mu m)$ and at the trailing end $(0, 0, 2.6\mu m)$ are shown for the linear case in Fig. 4.6(a). It is clear that the field has decayed significantly, as the signal frequency is within the stop band for the structure. The fields at $(0, 0, 2.6\mu m)$ for the linear and nonlinear cases are compared in the Fig. 4.6(b). This result shows that due to the introduction of the nonlinearity, there is a significant improvement in the field values at the trailing end.
Chapter 5

A Time Domain Volume Integral Equation Solver for Analyzing Ferrite Scatterers

5.1 Introduction

This chapter introduces a marching on-in-time (MOT) scheme for solving the time domain magnetic field volume integral equation (TD-MFVIE) enforced on anisotropic scatterers. This solver is built upon the explicit MOT scheme described in Chapter 3. In this chapter, scatterers made of ferrite material are considered as an example of anisotropic scatterers.

The electrical properties of a ferrite can be controlled using an external DC bias. This property makes ferrite substrates good candidates in designing reconfigurable and/or nonreciprocal microwave and millimeter devices. Several microwave devices like circulators, isolators, phase shifters, and patch antennas are indeed fabricated using ferrite substrates [48, 49, 50]. Accurate modeling and fabrication of these microwave devices in computer-aided design has to be supported with simulation tools that can accurately model the field dynamics on a ferrite substrate.

The nonlinear dynamics of magnetization inside ferrite materials are modeled using Landau-Lifshitz-Gilbert (LLG) equation. Henceforth simulation tools for analyzing electromagnetic wave interactions on magnetized ferrites requires the solution of the coupled system of LLG and Maxwell equations. Frequency domain solvers [2] linearize the LLG equation using a small signal approximation to obtain a (frequency dependent) permeability tensor, which is then inserted into the Maxwell equations.
On the other hand, time domain finite difference (FDTD) solvers use the LLG equation as an auxiliary relation to complement the Maxwell equations [3]. This type of time domain modeling can take into account the nonlinear terms in the LLG equation, which are linearized/simplified/approximated by frequency domain solvers. It is well known that time domain volume integral equation (TD-VIE) solvers offer several advantages over FDTD schemes (see Chapter 1 for example). To fully benefit from these advantages in the simulation of electromagnetic wave interactions on ferrite substrates, this chapter develops an approach based on the solving a TD-VIE.

More specifically, the explicit MOT scheme described in Chapter 3, is extended to solve the coupled system of the LLG and the TD-MFVIE enforced on a ferrite scatterer. The unknown magnetic field intensity and flux density in this coupled system are expanded using half and full Schaubert-Wilton-Glisson (SWG) basis functions [72, 73, 77], respectively. The equations are converted to an ordinary differential equation (ODE) and spatially tested to yield a matrix system that relates the time dependent coefficients of the unknown expansion to their temporal derivatives. This system is integrated in time using a PE(CE)m scheme [47] to obtain the samples of the unknown coefficients.

The rest of this chapter is organized as follows. Section 5.2 provides the formulation underlying the explicit MOT scheme for solving TD-MFVIE and details of its implementation. Sections 5.2.1 and 5.2.2 present the formulation of the TD-MFVIE and the LLG equation, respectively. Section 5.2.3 illustrates the steps involved in implementation of the MOT scheme. Section 5.3 demonstrates the stability and accuracy of the scheme in characterizing transient electromagnetic wave interactions magnetized ferrites via numerical experiments.
5.2 Formulation

5.2.1 Time Domain Magnetic Field Volume Integral Equation

Let $V$ denote the support of magnetized ferrite residing in an unbounded background medium with permittivity $\varepsilon_0$ and permeability $\mu_0$. An incident wave with magnetic field intensity $H^\text{inc}(r, t)$ that is vanishingly small $\forall r \in V, t \leq 0$ and essentially band-limited to frequency $f_{\text{max}}$, excites the scatterer. In response to this excitation, equivalent volumetric magnetic current $J_m(r, t)$ is induced in $V$. The scattered magnetic field $H^\text{sca}(r, t)$ is related to $J_m(r, t)$ through $\mathcal{L}\{ \cdot \}$ as

$$H^\text{sca}(r, t) = \frac{1}{\mu_0} \mathcal{L} \left( \int_{-\infty}^{t-R/c_0} J_m(r, t')dt' \right)$$

(5.1)

In $V$, $J_m(r, t)$ is related to the total magnetic field intensity $H(r, t)$ and the flux density $B(r, t)$ as

$$J_m(r, t) = \partial_t B(r, t) - \mu_0 \partial_t H(r, t)$$

(5.2)

where, the total magnetic field $H(r, t)$ is

$$H(r, t) = H^\text{inc}(r, t) + H^\text{sca}(r, t)$$

(5.3)

Inserting (5.2) into (5.1) and the resulting equation into (5.3) and enforcing the temporal derivative of the final equation for $r \in V$ yield the temporal derivative of TD-MFVIE in unknowns $H(r, t)$ and $B(r, t)$:

$$\partial_t H^\text{inc}(r, t) = \partial_t H(r, t) + \mathcal{L}(H(r, t)) - \mu_0^{-1} \mathcal{L}(B(r, t))$$

(5.4)
To numerically solve (5.4) scatterer $V$ is discretized with tetrahedral elements. $B(r, t)$ is spatially approximated using the full Schaubert-Wilton-Glisson (SWG) basis functions $f_n^B(r)$ (2.6) as

$$B(r, t) \approx \sum_{n=1}^{N_B} \{I^B(t)\}_n f_n^B(r) \tag{5.5}$$

where $\{I^B(t)\}_n = I_n^B(t)$ are the time dependent coefficients associated with the $n$th spatial basis function.

$H(r, t)$ is approximated using as half SWG function $f_n^H(r)$ (4.8) as

$$H(r, t) \approx \sum_{n=1}^{N_H} \{I^H(t)\}_n f_n^H(r) \tag{5.6}$$

where $\{I^H(t)\}_n = I_n^H(t)$ is the time dependent coefficients associated with the $n$th spatial half SWG function. Substituting (5.5) and (5.6) in (5.4) and testing the resulting equation with $f_m^H(r)$ yield the spatially discretized time dependent TD-EFVIE:

$$G \partial_t I^H(t) = V^{inc}(t) + V^{sca}_H(t, I^H(t)) + V^{sca}_B(t, I^B(t)) \tag{5.7}$$

Here the elements of Gram matrix $G$, tested incident field $V^{inc}(t)$, $V^{sca}_H(t, I^H(t))$ and
\( \mathbf{V}_{\text{B}}^{\text{sca}}(t, \mathbf{I}^B(t)) \) are

\[
\{ \mathbf{G} \}_{m,n} = \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \mathbf{f}_n^H(\mathbf{r}) d\mathbf{r} \tag{5.8}
\]

\[
\{ \mathbf{V}^{\text{inc}}(t) \}_m = \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \partial_t \mathbf{H}^{\text{inc}}(\mathbf{r}, t) d\mathbf{r} \tag{5.9}
\]

\[
\{ \mathbf{V}_{\text{H}}^{\text{sca}}(t, \mathbf{I}^H(t))) \}_m = \sum_{n=1}^{N_H} \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \mathcal{L}\{ \mathbf{I}_n^H(t) \} \mathbf{f}_n^H(\mathbf{r}) d\mathbf{r} \tag{5.10}
\]

\[
\{ \mathbf{V}_{\text{B}}^{\text{sca}}(t, \mathbf{I}^B(t)) \}_m = -\sum_{n=1}^{N_B} \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \mathcal{L}\{ \varepsilon_0^{-1} \mathbf{I}_n^B(t) \} \mathbf{f}_n^H(\mathbf{r}) d\mathbf{r} \tag{5.11}
\]

Following the temporal sampling the interpolation same as in (4.15) and (4.16), we obtain

\[
\mathbf{G}_j^H = \mathbf{Z}_0^H \mathbf{I}_j^H - \varepsilon_0^{-1} \mathbf{Z}_0^H \mathbf{I}_j^B + \mathbf{V}_j^{\text{inc}} + \sum_{i=1}^{j-1} \mathbf{Z}_{j-i}^H \mathbf{I}_i^H - \varepsilon_0^{-1} \sum_{i=1}^{j-1} \mathbf{Z}_{j-i}^H \mathbf{I}_i^B \tag{5.12}
\]

where \( \mathbf{I}_j^H = \partial_t \mathbf{I}^H(t)|_{t=j\Delta t} \), \( \mathbf{V}_j^{\text{inc}} = \mathbf{V}^{\text{inc}}(t)|_{t=j\Delta t} \) and the elements of MOT matrices \( \mathbf{Z}_{j-i}^H \) and \( \mathbf{Z}_{j-i}^B \) are given as

\[
\{ \mathbf{Z}_{j-i}^{\text{HU}} \}_{m,n} = \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \mathcal{L}\{ \mathbf{f}_m^U(\mathbf{r}) T_i(t) \} |_{t=j\Delta t} d\mathbf{r}; \ U \in \{ \text{H,B} \} \tag{5.13}
\]

The observations regarding the matrices \( \mathbf{Z}_{j-i}^{\text{EE}} \) and \( \mathbf{Z}_{j-i}^{\text{ED}} \) is also valid for the matrices \( \mathbf{Z}_{j-i}^H \) and \( \mathbf{Z}_{j-i}^B \).

### 5.2.2 Discretization of Landau-Lifshitz-Gilbert Equation

Landau-Lifshitz-Gilbert equation is

\[
\partial_t \mathbf{M}(\mathbf{r}, t) = -\gamma \mathbf{M}(\mathbf{r}, t) \times \mathbf{H}_{\text{eff}}(\mathbf{r}, t) + \frac{\alpha}{M_s} \mathbf{M}(\mathbf{r}, t) \times \partial_t \mathbf{M}(\mathbf{r}, t) \tag{5.14}
\]
where, the magnetization $M(r, t)$ is given as

$$M(r, t) = \mu_0^{-1} B(r, t) - H(r, t) \quad (5.15)$$

Without loss of generality, we can assume that a DC Field $H_{dc}(r) = \hat{z} H_{dc}$, and in response a static magnetization $M_s(r) = \hat{z} M_s$ are developed inside the ferrite. Under small signal approximation, we have $H_{eff}(r, t) = H_{dc}(r)$, and the total magnetic field $H_t(r, t)$ and the total magnetization $M_t(r, t)$ are

$$H_t(r, t) = \hat{z} H_{dc} + H(r, t) \quad (5.16)$$
$$M_t(r, t) = \hat{z} M_s + M(r, t)$$

Substituting (5.16) in (5.14), we have

$$\partial_t M_t(r, t) = -\gamma [\hat{z} M_s + M(r, t)] \times [\hat{z} H_{dc} + H(r, t)] + \alpha \hat{z} \times \partial_t M(r, t) \quad (5.17)$$

Under small signal approximation, and using (5.15) in (5.17), we get

$$\mu_0^{-1} \partial_t B(r, t) - \partial_t H(r, t) = -\gamma [M_s \hat{z} \times H(r, t) - H_{dc} \hat{z} \times \mu_0^{-1} B(r, t) + H_{dc} \hat{z} \times H(r, t)]$$
$$+ \alpha \hat{z} \times \{ \mu_0^{-1} \partial_t B(r, t) - \partial_t H(r, t) \} \quad (5.18)$$

Using the resonance frequency $\omega_0 = \gamma H_{dc}$ and the magnetization frequency $\omega_m = \gamma M_s$, (5.18) can be written as

$$\mu_0^{-1} \partial_t B(r, t) - \partial_t H(r, t) = \mu_0^{-1} \omega_0 (\hat{z} \times B(r, t)) - [\omega_0 + \omega_m] (\hat{z} \times H(r, t))$$
$$+ \alpha \hat{z} \times \{ \mu_0^{-1} \partial_t B(r, t) - \partial_t H(r, t) \} \quad (5.19)$$
Testing (5.19) using \( f_m^B(r) \) and subsequently sampling in time results in the matrix equation

\[
\mu_0^{-1} G^{BB} \partial_t I_j^B - G^{BH} \partial_t I_j^H = \mu_0^{-1} H^{BB} I_j^B - M^{BB} I_j^H + \mu_0^{-1} L^{BB} \partial_t I_j^B - L^{BH} \partial_t I_j^H \quad (5.20)
\]

where,

\[
\{G^{BB}\}_{m,n} = \int_{V_m} f_m^B(r) \cdot f_n^B(r) dr
\]

\[
\{G^{BH}\}_{m,n} = \int_{V_m} f_m^B(r) \cdot f_n^H(r) dr
\]

\[
\{H^{BB}\}_{m,n} = \omega_0 \int_{V_m} f_m^B(r) \cdot \hat{z} \times f_n^B(r) dr
\]

\[
\{H^{BH}\}_{m,n} = \left[ \omega_0 + \omega_m \right] \int_{V_m} f_m^B(r) \cdot \hat{z} \times f_n^H(r) dr
\]

\[
\{L^{BB}\}_{m,n} = \alpha \int_{V_m} f_m^B(r) \cdot \hat{z} \times f_n^B(r) dr
\]

\[
\{L^{BH}\}_{m,n} = \alpha \int_{V_m} f_m^B(r) \cdot \hat{z} \times f_n^H(r) dr
\]

Combining (5.12) and (5.22), we have the coupled system

\[
\begin{bmatrix}
G^{HH} & 0 \\
L^{BH} - G^{BH} & G^{BB} - L^{BB}
\end{bmatrix} \frac{\partial}{\partial t} U_j =
\begin{bmatrix}
Z_0^{HH} & -Z_0^{HB} \\
-M^{BB} & H^{BB}
\end{bmatrix} U_j +
\begin{bmatrix}
V_j^{\text{fixed}} \\
0
\end{bmatrix}; \quad (5.22)
\]

\[
U_j =
\begin{bmatrix}
I_j^B \\
\mu^{-1} I_j^H
\end{bmatrix}
\]

### 5.2.3 Explicit Marching On in Time Scheme

To solve (5.22), we modify the explicit time marching method based on the predictor-corrector scheme described in Section 3.2.3. The steps involved are describe below:
At each time step $j = k, \ldots, N_t$:

- **Step 1**: The components of the right-hand side of (3.15), which are not updated within the time step $j$, are computed:

$$V_j^{\text{fixed}} = V_j^{\text{inc}} + \sum_{i=1}^{j-1} Z_{j-i}^{HH} I_i^{H} - \mu_0^{-1} \sum_{i=1}^{j-1} Z_{j-i}^{HB} I_i^{B}$$

- **Step 2**: Predictor (P) step. Predict $U_j^{(0)}$ is predicted using $k$ past (known) values of $U_j^{(0)}, \dot{U}_j^{(0)}$, $i = j - k, \ldots, j - 1$, respectively:

$$U_j^{(0)} = \sum_{l=1}^{k} [\{p\}_l U_{j-1+l-k} + \{p\}_{k+l} \partial_t U_{j-1+l-k}]$$

Here, $p$ is a vector of dimension $2k$, which stores the predictor coefficients.

- **Step 3**: Evaluate $\partial_t U_j^{(0)}$ solving:

$$\begin{bmatrix} G^{HH} & 0 \\ L^{BH} - G^{BH} & G^{BB} - L^{BB} \end{bmatrix} \partial_t U_j^{(0)} = \begin{bmatrix} Z_0^{HH} & -Z_0^{HB} \\ -M^{BB} & H^{BB} \end{bmatrix} U_j^{(0)} + \begin{bmatrix} V_j^{\text{fixed}} \\ 0 \end{bmatrix}$$

- **Step 4** Repeat step 4.1 and 4.2 until convergence ($m = 1, \ldots, m_{\text{max}}$):

  - **Step 4.1**: Corrector (C) step. $U_j^{(m)}$ corrected/updated using $k$ past values of $U_j$ and $\dot{U}_j$, $i = j - k, \ldots, j - 1$, and the $U_j^{(m-1)}$:

$$U_j^{(m)} = \sum_{l=1}^{k} [\{c\}_l U_{j-1+l-k} + \{c\}_{k+l} \partial_t U_{j-1+l-k}] + \{c\}_{2k+1} \partial_t U_j^{(m-1)}$$

Here, $c$ is a vector of dimension $2k + 1$, which stores the corrector coefficients.
Step 4.2: Apply SOR on $U_j^{(m)}$:

$$U_j^{(m)} = \beta U_j^{(m)} + (1 - \beta) U_j^{(m-1)}$$

Step 4.2: Evaluate $\partial_t U_j^{(m)}$ by solving:

$$\begin{bmatrix}
G^{HH} & 0 \\
L^{BH} - G^{BH} & G^{BB} - L^{BB}
\end{bmatrix}
\begin{bmatrix}
\partial_t U_j^{(m)}
\end{bmatrix}
= 
\begin{bmatrix}
Z_0^{HH} & -Z_0^{HB} \\
-M^{BB} & H^{BB}
\end{bmatrix}
\begin{bmatrix}
U_j^{(m)}
\end{bmatrix}
+ 
\begin{bmatrix}
V_j^{fixed} \\
0
\end{bmatrix}$$

• Step 8: Once convergence is reached, i.e., $\|U_j^{(m)} - U_j^{(m-1)}\| < \chi_{PECE}$, the solutions are stored to be used at the next time step: $U_j = U_j^{(m)}$ and $\partial_t U_j = \partial_t U_j^{(m)}$.

5.3 Numerical Results

This section presents numerical examples that demonstrate the stability and accuracy of the proposed explicit MOT-TD-MFVIE solver in characterizing electromagnetic wave interactions on magnetized ferrites. Similar to Section 3.3, all the examples considered here, a plane wave excitation with magnetic field $H^{inc}(r, t) = \hat{y} G(t - r \cdot \hat{z}/c_0)$ is used.

The temporal interpolators developed in Chapter 2 are used the temporal basis functions. The PE(CE)$^m$ scheme uses the fourth order Adam-Bashworth and backward difference formulas at the predictor and corrector stages, respectively with $\beta = 0.6$. The coupled matrix systems (5.22) is solved iteratively using the generalized minimal residual method (GMRES) method [15]. The GMRES iterations are terminated when the condition

$$\|I^l_n - I^{n-1}_l\| < \|b\| \delta_{GMRES}$$

is satisfied. Here, $I^l_n$ is the solution at time step $l$ and iteration $n$, $b$ is the RHS, and
\( \delta_{\text{GMRES}} = 10^{-12} \) is the convergence threshold. Similarly, step 3 is terminated when

\[
\| I^n - I^{n-1} \| < \| I^n \| \delta_{\text{EXP}}, \quad \delta_{\text{EXP}} = 10^{-13}
\]  

(5.24)

5.3.1 Accuracy

In the first example, the accuracy of the proposed MOT-TD-MFVIE solver is demonstrated via comparing the radar cross section (RCS) with analytical solutions [104]. The proposed solver is used for scattering analysis from a unit sphere ferrite that has a set of loss factor \( \alpha = [0.0, 0.1, 0.2, 0.4] \). The ferrite with \( \gamma = 2.8 \text{ MHz/Oe} \) is biased using \( H_{\text{DC}} = 67.32 \text{ Oe} \) and a resulting magnetization of \( M_S = 20.2 \text{ Oe} \). This corresponds to \( \omega_0 = 1.885 \times 10^8 \text{ rad/s} \) and \( \omega_m = 5.655 \times 10^7 \text{ rad/s} \). Fields inside the sphere are discretized using \( N_H = 17600 \) and \( N_B = 9108 \). The incident field has \( f_0 = 24 \text{ MHz}, \quad f_{\text{bw}} = 5 \text{ MHz}, \) and \( t_p = 8\sigma \). The simulations are carried out for \( N_t = 5000 \) with \( \Delta t = 0.5 \text{ ns} \). Fig. 5.1(a) shows the field intensity recorded at the origin for different loss factors, demonstrating that the solver provided stable results for all the examples. The result also shows that when there is no loss factor, the decay is very slow. In Fig. 5.1(b), the RCS computed for \( \phi = 0^\circ \) and \( \theta = [0^\circ, 180^\circ] \) at \( f = 24 \text{ MHz} \) in the loss-less case (\( \alpha = 0.0 \)) using the Fourier transformed MOT solutions are compared to the analytical Mie series solution. In Fig. 5.1(c), same comparison is performed for \( \alpha = 0.4 \). Both results demonstrate that the solver provides accurate results.

To study the effect of loss factor and the resonance frequency on the accuracy of the proposed solver, the previous test case is also performed for a set of center frequencies, i.e., for \( f_0 = [24, 25, 28, 30] \text{ MHz} \). Please note that, among this set, \( f_0 = 30 \text{ MHz} \) matches with the resonance frequency \( \omega_0 = 1.885 \times 10^8 \text{ rad/s} \) of the ferrite material. The RCS computed from the solver for \( \phi = 0^\circ \) and \( \theta = [0^\circ, 180^\circ] \) is then compared with the analytical Mie series solution as shown in Fig 5.2. It is clear
Figure 5.1: Scattering analysis from a magnetized ferrite sphere with $\omega_0 = 1.885 \times 10^8$ rad/s and $\omega_m = 5.655 \times 10^7$ rad/s. (a) Magnetic field intensity at the center of the sphere, (b) RCS for $\phi = 0^\circ$ and $\theta = [0^\circ, 180^\circ]$ at $f = 24$ MHz for $\alpha = 0.0$ solution, and (c) RCS for $\phi = 0^\circ$ and $\theta = [0^\circ, 180^\circ]$ at $f = 24$ MHz for $\alpha = 0.4$ compared with the analytical Mie series solution.
Figure 5.2: Scattering analysis from a magnetized ferrite sphere with $\omega_0 = 1.885 \times 10^8$ rad/s and $\omega_m = 5.655 \times 10^7$ rad/s. Comparison of error in RCS calculation (a) for different frequencies and (b) for different loss factor values.

From the Fig 5.2(a) that the solution accuracy increases as we move away from the resonance frequency. Also Fig 5.2(b) shows that increase in loss factor also makes the solution more accurate. Please note that the Mie Series solution could not be used for the case of $f_0 = 30$ MHz with $\alpha = 0.0$. 

5.3.2 Polarizer

In the last example, scattering from a Polarizer is studied using the proposed solver. The polarizer considered is a thin ferrite sheet with dimensions of $4 \times 4 \times 0.2$ m$^3$. The ferrite with $\gamma = 2.8$ MHz/Oe is biased using $H_{DC} = 67.32$ Oe and a resulting magnetization of $M_S = 20.2$ Oe. This corresponds to $\omega_0 = 1.885 \times 10^8$ rad/s and $\omega_m = 5.655 \times 10^7$ rad/s and the ferrite has the loss factor $\alpha = 0.1$. Fields inside the sphere are discretized using $N_H = 14036$ and $N_B = 7802$. The polarized is excited with a plane wave with

$$G(r, t) = \begin{cases} 
\cos[2\pi f_0(t - t_1)]e^{-(t-t_1)^2/2\sigma^2}, & t < t_1 \\
\cos[2\pi f_0(t - t_1)], & t_1 \leq t < t_2 \\
\cos[2\pi f_0(t - t_2)]e^{-(t-t_2)^2/2\sigma^2}, & t_2 \leq t 
\end{cases} 
$$

(5.25)

where, $f_0 = 304.8$ MHz, $\sigma = 2.3873$ ns, $t_1 = 8\sigma$ and $t_2 = 35.48\sigma$. The simulation is carried out with $N_t = 2000$, $\Delta t = 0.05$ ns and $\beta = 0.6$. The reflected field at $(0,0,-0.25m)$ and at the transmitted field at $(0,0,0.25m)$ are shown Fig. 5.3(a) and in Fig. 5.3(b), respectively. It is clear that the polarizer converts the linearly polarized incident field to elliptically polarized reflected and transmitted fields.
Figure 5.3: Reflected field at (0, 0, −0.25m) and (b) transmitted field at (0, 0, 0.25m).
Chapter 6

Concluding Remarks

6.1 Summary

Simulation tools that can model the electromagnetic wave interactions on complex scatterers are indispensable for the design of microwave, millimeter wave, photonic, and plasmonic devices [1, 2, 3, 4, 5, 6, 7]. The material complexities present in these devices can be heterogeneity, high permittivity, nonlinearity, dispersion and anisotropy. The wave interactions on these complex geometries can be studied using either frequency domain or time domain solvers. When the problem is over a narrow band of frequencies with only linear field interactions, frequency domain solvers, which assume time-harmonic excitation, are often preferred. However, when the analysis needs to be carried out over a wide band, and/or when there is nonlinearity in the field dynamics, time domain solvers are preferred over their frequency domain counterparts [13, 14, 15]. Time domain solvers can be classified as either differential equation solvers such as finite difference time domain (FDTD) schemes or time domain finite element method (TD-FEM) schemes or time domain volume integral equation (TD-VIE) solvers [22, 23, 24]. Oftentimes, the FDTD schemes are the method of choice because their formulation and implementation are straightforward. On the other hand, time domain volume integral equation (TD-VIE) solvers work with fewer unknowns (only the volume of the scatterer is discretized) and produce better accuracy (radiation condition is implicitly enforced without the need for (approximate) absorbing boundary conditions). Moreover, the time step size is chosen to resolve the maximum frequency
of the excitation and is independent of the spatial discretization size.

Even though TD-VIE solvers have several advantages over differential equation solvers, they have not been widely preferred by practitioners of computational electromagnetics because of their high computational cost and difficulty in extending them for the simulation of electromagnetic wave interactions on complex scatterers. Two different classes of accelerators have been developed to reduce the computational cost. Plane wave time domain (PWTD) solvers [33, 34, 35] use plane wave decompositions and diagonal translation operators, whereas time domain adaptive integral equation method (TD-AIM) [36, 37, 38] employs blocked fast Fourier transforms to accelerate the matrix-vector multiplications. These accelerators have enabled TD-VIE solvers to work on large-scale problems with affordable computational resources.

This thesis aims at addressing the second drawback, i.e. limited applicability of the TD-VIE solvers to complex scatterers. It describes several solvers that are developed for transient analysis of electromagnetic wave interactions on heterogeneous, high-contrast, nonlinear, dispersive and anisotropic scatterers, by addressing each level of complexity step by step. The solver’s accuracy is verified by numerical experiments where solutions are compared to analytical Mie series solutions or to those obtained by well-established methods. Additionally, their applicability is demonstrated by using them to simulate practical real-life problems.

### 6.2 Contribution of the Thesis

The thesis first focuses on addressing the instability of the marching on in time (MOT) solution of the time domain electric field volume integral equation (TD-EFVIE) enforced on scatterer with high dielectric permittivity. Studying the resonant modes of homogeneous spheres with increasing permittivity has revealed that existing temporal basis functions and extrapolation schemes (used for ensuring the causality of the time marching) do not accurately model the oscillating and decaying fields, and this re-
results in instabilities when the simulation is run for a long time. A novel implicit MOT solver, which maintains its stability (and accuracy) when applied to the analysis of electromagnetic wave interactions on high-contrast scatterers, is developed. The stability is achieved by using a specially designed highly accurate extrapolation scheme. This new scheme trains the extrapolation coefficients using exponential functions with exponents sampled on the complex frequency plane. Consequently, this increases the stability of the resulting MOT scheme since oscillating and decaying modes (with complex wave numbers) induced inside the scatterers are now accounted for more accurately. Numerical results, which demonstrate the stability of the MOT-TD-EFVIE solver, are presented.

Even though the proposed MOT-TD-EFVIE solver is stable, the conditioning of the MOT matrix becomes worse with the increasing contrast of the scatterer. This results in a large number of iterations (required to solve the MOT matrix system) at every time step and consequently increases the computation time significantly. To alleviate this problem, an explicit MOT scheme to solve the time domain magnetic volume integral equation (TD-MFVIE) enforced on dielectric scatterers, is developed. For this approach, TD-MFVIE is preferred, because, upon discretization, the MFVIE operator produces a well-conditioned matrix even when the scatterer has high contrast [44]. The TD-MFVIE is first cast in the form of an ordinary differential equation (ODE) and it is integrated in time using a PE(CE)\(m\) scheme for the (unknown) coefficients of the expansion discretizing the magnetic field. The resulting MOT algorithm calls for the solution of a Gram matrix system at the evaluation (E) steps of every time step. However, the Gram matrix is well conditioned and sparse (for Galerkin testing) or consists of four diagonal blocks. Either way, this Gram matrix system can be solved very efficiently. Numerical results, which demonstrate that this explicit MOT scheme is significantly faster than its implicit MOT counterpart for low-frequency problems and has comparable performance for high-frequency problems, are presented. Ad-
ditionally, numerical experiments show that it maintains its stability for scatterers with high contrast. In addition to developing two novel MOT schemes, this thesis has focused on enabling the use of these schemes in characterization of electromagnetic wave interactions on nonlinear and anisotropic scatterers. First, nonlinear scatterers, more specifically, scatterers with Kerr nonlinearity are considered. This solver builds upon the $\text{PE(CE)}^m$ based explicit MOT scheme applied to solving the TD-EFVIE complemented with the nonlinear constitutive relation. The coupled system of the TD-EFVIE and the constitutive relation are cast in the form of an ODE system, where the electric field intensity and flux density are separately discretized. Then $\text{PE(CE)}^m$ scheme is used to integrate this ODE system in time for the (unknown) coefficients of the expansion discretizing the field and flux. This explicit scheme avoids the need for a Newton-like nonlinear solver by casting the nonlinear constitutive relation as a function evaluation on the right-hand side. Numerical results demonstrating the applicability of the solver are presented.

Next, anisotropic scatterers, more specifically scatterers made of ferrite, are considered. The predictor-corrector based explicit MOT scheme applied to the solution of the coupled ODE system of the TD-MFVIE and the Landau-Lifshitz-Gilbert (LLG) equation (which describes the behavior magnetization vector). Numerical results demonstrate that the proposed solver provides an accurate solution to the wave interactions on (magnetized) ferrite substrates.

### 6.3 Future Research Work

Development of preconditioning techniques to accelerate the iterative solution of the implicit MOT-TD-EFVIE solver at every time step is underway. These techniques are needed since the conditioning of the MOT matrix gets worse as the contrast and the inhomogeneity of the scatterer increases. Work is also in progress to apply the proposed solver to the analysis of electromagnetic wave interactions on (dispersive)
plasmonic nanostructures. The dispersive permittivity is modeled using a pole-zero representation in the frequency domain that is converted to a convolution in the time domain.

For nonlinear scatterers, increasing strength of nonlinearity naturally results in faster varying transient fields. This means that the MOT scheme has to use a smaller time step size to resolve the fast variations while maintaining the accuracy and stability of the solution. Decreasing the time step size for the whole simulation duration might unnecessarily increase the computation time. This can be avoided using multi-time step integration schemes as well as methods to track (localized) windows of fast variations.

Unlike the EFVIE, Galerkin testing does not result in conformal testing of the MFVIE. In return, the solution of the resulting matrix system deteriorates. To alleviate this problem, conformal testing schemes, which use mixed basis functions (between curl- and divergence conforming spaces) need to be formulated and developed.

The MOT scheme developed to solve the TD-MFVIE on ferrite scatterers operates under the assumptions of small signal, which linearizes the LLG equation, and saturated hysteresis loop. This is valid in many practical problems, where a high external DC field is used to saturate the ferrite. However, novel applications might potentially need LLG equation to be solved for without using a small signal approximation (i.e., internal and external fields are on the same level) and for ferrite substrates that are only partially saturated. This requires the LLG equation to be treated in the original form without any approximation. Additionally, the explicit MOT scheme can be extended to the analysis of scattering from objects that are dielectric and magnetic and can also have bi-anisotropy.
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APPENDICES
A Appendix

A.1 Cavity Mode of Dielectric Sphere

Cavity modes of a homogenous non-magnetic dielectric sphere residing in free space are studied in [69]. Characteristic equations of the transverse electric and magnetic field (TE and TM) modes are obtained by enforcing the continuity conditions of the modes’ electric and magnetic fields represented in the spherical coordinate system on the sphere surface:

\[
\psi_{\text{TE}}(\beta a) = \frac{J_{n-1/2}(\beta a)}{J_{n+1/2}(\beta a)} - \frac{H^{(2)}_{n-1/2}(\beta a/\sqrt{\varepsilon_r})}{H^{(2)}_{n+1/2}(\beta a/\sqrt{\varepsilon_r})} = 0 \quad (A.1)
\]

\[
\psi_{\text{TM}}(\beta a) = \frac{n}{\beta a} - \frac{J_{n-1/2}(\beta a)}{J_{n+1/2}(\beta a)} - \frac{n\varepsilon_r}{\beta a} + \sqrt{\varepsilon_r} \frac{H^{(2)}_{n-1/2}(\beta a/\sqrt{\varepsilon_r})}{H^{(2)}_{n+1/2}(\beta a/\sqrt{\varepsilon_r})} = 0 \quad (A.2)
\]

Here, \(J_{n+1/2}(\cdot)\) and \(H^{(2)}_{n+1/2}(\cdot)\) are the first kind Bessel and second kind Hankel functions of order \(n + 1/2\), \(a\) is the radius of the sphere, and the \(\beta = \omega\sqrt{\varepsilon_r\varepsilon_0\mu_0}\) is the mode wave number, \(\varepsilon_r\) is the relative permittivity of the sphere, and \(\omega = \omega' + j\omega''\) is the complex frequency which determines the oscillation frequency (\(\omega'\)) and decay constant (\(\omega''\)) of the modes. Note that while deriving (A.1) and (A.2), it is assumed that the modes vary with \(e^{j\omega t} = e^{j\omega' t - \omega'' t}\). To find the unknown \(\omega = \omega' + j\omega''\) for a given mode index \(n\), the roots of (A.1) and (A.2) are computed using Newton-Raphson iterations:

\[
\beta_{p+1} = \beta_p - \frac{\psi_{\text{type}}(\beta_p a)}{\partial \psi_{\text{type}}(\beta_p a) / \partial \beta}|_{\beta_p}
\]  

(A.3)
where \( type \in \{ \text{TE}, \text{TM} \} \) and \( \beta_p \) is the root at the \( p^{\text{th}} \) iteration. The iterations are terminated when \( |\beta_{p+1} - \beta_p| < 10^{-13} \) and \( \omega \) is computed as \( \omega = \beta_{p+1}/\sqrt{\varepsilon_\varepsilon_0\mu_0} \).
B List of papers

B.1 Journal papers


5. R. Chen, S. B. Sayed, and H. Bagci, ”A Nyström-based explicit time marching scheme for solving the time domain magnetic field integral equation”, IEEE

### B.2 Conference papers


10. S. B. Sayed, H. A. Ulku, and H. Bagci, ”Transient Analysis of Electromagnetic Wave Interactions on Nonlinear Dispersive Scatterers using Volume Integral


