Stabilizing 3D Volterra Time Domain Integral Equation Algorithms

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1. Introduction

An accurate and stable 3D Volterra Time Domain Integral Equation TDIE algorithm capable of running on both structured rectangular grids and unstructured tetrahedral meshes is presented here for the first time. This development is in response to recent demands for numerical methods to solve volume integral equations in the time domain. The derivation of a flexible, stable, accurate and effective numerical tool is presented and moreover it is demonstrated that it is capable of accurately approximating the solution of problems accommodating arbitrarily shaped dielectric structures with complex features and time varying material properties. Canonical structures are considered here to demonstrate stability and accuracy of the algorithm.

Substantial progress has been reported in order to make TDIE algorithms computationally efficient in comparison to established numerical methods that are based on the differential form of the Maxwell equations such as the FDTD [1] and TLM [2]. As in the case of FDTD [3], it has also been observed that almost all numerical approximation of higher dimensional TDIE solutions suffer from late time instabilities [4]. In the case of MoM [5] and FE [6] approaches, compensatory numerical treatment has focused on a combination of careful design and the choice of spatial and temporal bases functions. Nevertheless, complete removal of these late time oscillations has met with limited success in the general case. Consequently, it is still often required that special attention must be given to the geometry of the structure, its physical parameters and the mesh used.

The problems of instabilities are often attributed to an accumulation on numerical errors due to the discretisation on the integrals involved. Consideration of the stability of computer algorithms based upon the Volterra TDIE formulation in 1D has previously been reported and their solution was significantly improved from the earlier implementations by means of both a semi-implicit formulation and a central difference Crank-Nicholson technique [7]. Also their solution has been demonstrated on a modified rectangular space-time meshes [7], and on unstructured triangular space-time meshes [8]. These simple modifications were found to radically increase the flexibility of the computer implementations of the algorithm, allowing numerical solutions that are both stable and accurate for various media without any reservation on the structure, its mesh or permittivity contrast between the discontinuity region and background [7, 8].

However, in the 3D case, a more general treatment of such numerical instabilities is needed, and this can be achieved by employing low pass filtering. A digital filter approach is used to successfully remove the components of the solution which are prone to instability [9]. Here we find that the use of the simple low pass filtering technique, also known as an averaging scheme, is adequate to stabilise the computations. This only requires the use of three field values at any given moment in time, and therefore saves on the overall computational overhead required to obtain the solution. Higher order, finite impulse response FIR filtering, [9] can also be considered; a future step towards complete characterisation of this approach which is promising to yield an unconditionally stable and accurate algorithm.

2. Theory

In general, the electric field in a 3D structure satisfies a Volterra integral equation [10],

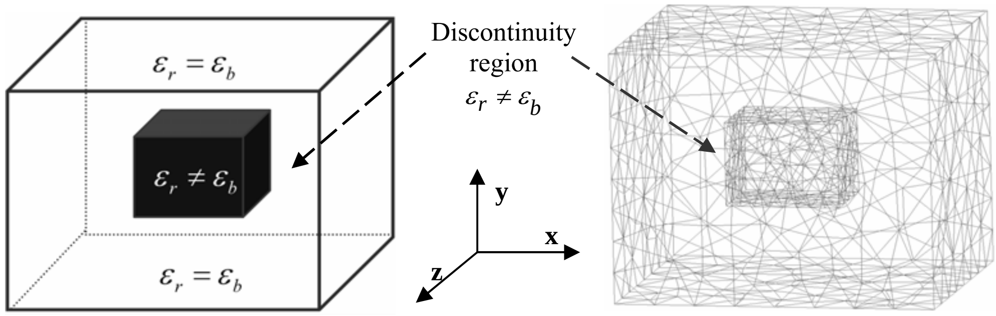
$$\mathbf{E}(t,r) = \mathbf{E}_o(t,r) - \left(\nabla\nabla\cdot - \frac{\partial^2}{v_b^2 \partial t^2} \right) \times \int_V dr' \frac{1}{4\pi} \frac{1}{|r-r'|} \left[\mathbf{P}(t - \frac{1}{v_b}|r-r'|, r') - (\varepsilon_b - 1)\varepsilon_o \mathbf{E}(t - \frac{1}{v_b}|r-r'|, r') \right] \quad (1)$$

where ε_b and v_b are the relative permittivity and speed of light in the background medium, **P** is the polarisation of the media, $\mathbf{E}_o$ is the excitation field and *t* and $r=(x,y,z)$ denotes the time and space coordinates. The equations are based upon generalized functions and are convenient for investigating electromagnetic transients, especially those with moving wave fronts and an arbitrary time-spatial dependence of the medium parameters, such as plasmas, semiconductors, non-linear dielectrics and dissipative media with losses. In principle these modifications can be implemented by merely redefining the functions describing the incident field or the medium polarization [7, 10]. At each instant of time, the present electric field in (1) is determined via a 4D integral over the space-time history of the field. However, this is immediately reduced to a 3D integral due to the properties of the delta function, yielding a process which is visualized as integrating over the surface of spheres of the time-retarded field values.

When evaluating the spatial integrals, special consideration must be given to the weak singularity that exists when the observation point coincides with a source, i.e. |r-r'|=0. At this point a small spherical exclusion region is introduced and its contribution to the total integral evaluated analytically. Furthermore, simple interpolation is performed to obtain field values in between the surfaces of the spheres of integration from the values on the uniform time mesh. It is also noted that at each instant in time and space the integrand in (1) is evaluated first as a pre-processing step before applying the Green's tensor $\nabla\nabla. - \partial^2 / v_b^2 \partial t^2$. The time and space derivative operators are then discretised in a straightforward manner using a combination of second order spatial and temporal finite differencing schemes respectively. Using basic central difference formulae to evaluate the spatial differential operator has been found to be robust in practice. However when this is also used for the time derivatives; it has proven less reliable as overall it leads to an explicit scheme. This is consistent with experience gained from the 1D case, [7]. To overcome this problem, an implicit difference formula for the time derivatives has been adopted [7] and this has proven successful in improving stability and therefore accuracy, however, only for a limited range of practical material parameters [11]. Thus, a more robust stability analysis is needed to underpin this phenomenon as considered thereafter.

For accurate modelling in the 3D formulation, it is also necessary to incorporate a stabilisation procedure besides satisfying both the causality and the Courant stability conditions. This phenomenon is common to most of the time-marching methods [4, 9], where a number of different causes have been attributed such as insufficient sampling of the very high frequencies, existence of internal numerical resonances, and/or errors caused while evaluating the intermediate quantities. Known stabilising procedures operate through averaging in time [4] and rarely in space. For averaging in space or time, the underlying concept is simply a de-correlation of accumulated computational noise and therefore, modest supplementary computer resources are required as a result. In this work we propose the use of a simple three term averaging scheme [4], which is found to be sufficient enough to accurately model the solution.

In this work, the generality of the algorithm is demonstrated by evaluating the discretised field values on both Cartesian structured meshes [11] and unstructured tetrahedral meshes [12] with equal validity, if not ease for the former case. The choice of spatial mesh size is dictated by the need to sufficiently and accurately sample the field behaviour in the structure. The choice of the time step is more flexible than that in the FDTD and TLM methods, and dictated by the Courant condition of the underlying Mesh. In the development of TDIE approach, structures are subdivided into an adequate number of small elements *e*, as shown in Fig 1 below, where the sampling 3D field points are specified to fall on the center of mass of each element. These elemental values then evolve in time with a fixed time step size allowing for signal propagation in time.



1(a) 1(b)

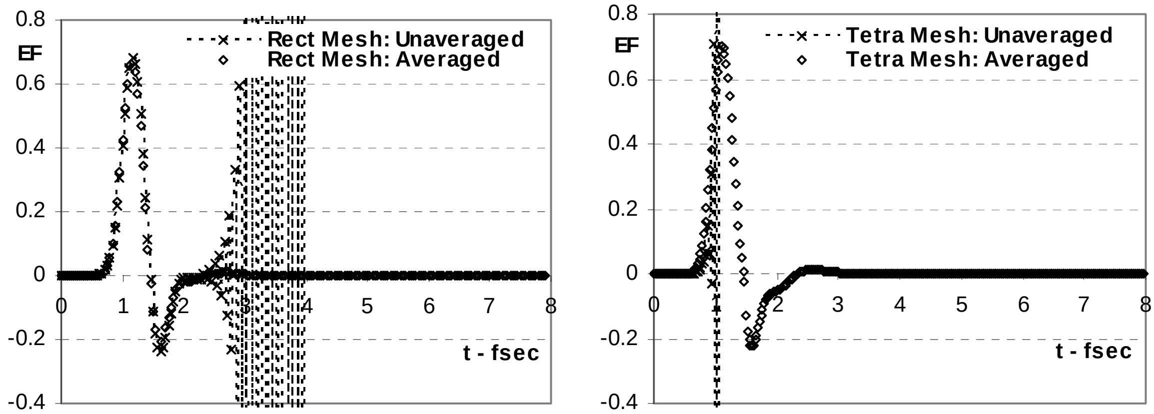
Figure1: Structured rectangular mesh in 1(a) and its equivalent unstructured tetrahedral mesh in 1(b) (Open space ε_b =1 containing a dielectric $\varepsilon_r \neq \varepsilon_b$)

3. Results

The general scheme is now investigated for validation on both structured rectangular and unstructured tetrahedral meshes. For clarity of the algorithmic development, the discontinuity region is characterised here by a simple homogeneous, linear, isotropic and nondissipative material of relative permittivity ε_1 whose polarisation function is defined by

$$\mathbf{P}(t', z') = (\varepsilon_1 - 1)\varepsilon_o \mathbf{E}(t', z') \qquad (2)$$

To assess the stability and convergence of the numerical results we choose a simple cubic structure where the discontinuity region is situated at 0.1μm≤x,y,z≤0.225μm in an otherwise homogeneous background, as illustrated in Fig. 1. In this case, the initial field is launched outside the discontinuity region, whose permittivity switches from ε_b=1.0 to ε_1=4.0 at t = 0 whilst the pulse is inside it. It is noted that an instant reflection takes place at zero moment in time and this travels in the opposite direction to that of the forward propagation with amplitude proportional to ε_1 and reversed in polarity. The transmitted and reflected signals then undergo multiple reflections in time.



2(a) 2(b)

Figure 2: A Gaussian pulse launched inside the discontinuity region with ε_1 =4.0 for (0.1μm≤x,y,z≤0.225μm), ε_b=1.0 otherwise and r=(0.157μm,0.173μm,0.168μm). (Pulse width=0.065μm centred at 0.0μm) 2(a) simulation from structured mesh and 2(b) is the corresponding equivalent unstructured mesh.

The field distribution at fixed point in space r = (0.157μm, 0.173μm, 0.168μm) is observed and the corresponding temporal of the signal are plotted as shown in Fig. 2. A total number of 1000 and 1027 nodal sample values, denoted as *e*, are used to obtain the solution with a time step size of 0.0416fsec and 0.0245fsec for the rectangular structured and tetrahedral unstructured meshes respectively. The set of results plotted is presented to demonstrate both stability and convergence of the algorithm, where it is observed that the instabilities are completely eliminated upon the application of a third order averaging filter technique [4, 9].

A detailed analysis of the solution accuracy is to be demonstrated. In addition, the significant reduction in computer resources that can be exploited via the tetrahedral meshing, and the generality of the algorithm, promises to be advantageous when implementing the TDIE to the more complex systems. Furthermore, the specific tetrahedral pattern being defined as opposed to a uniform rectangular mesh, which takes into account discontinuity and field distribution, promises to offer significant scope for adaptive schemes and structures containing a diverse range of feature sizes or boundaries that are curved or non-tangential to the coordinate axes.

4. Conclusion

For the first time, a stable 3D, fully vectorial numerical algorithm is investigated for validation of the Volterra TDIE method on structured rectangular and unstructured tetrahedral meshes. Initial simulations have demonstrated the algorithm both stable and convergent. Notwithstanding that there is substantial scope for further assessment of this approach as well as for rigorous analysis of its theoretical properties. Also higher order, finite impulse response FIR filtering, can also be considered; a future step towards complete characterisation of this approach which is promising to yield an unconditionally stable and accurate algorithm.

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