Time-Domain Analysis of Temporally and Spatially Dispersive Metasurfaces in GSTC-FDTD Frameworks

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Abstract—In this paper, we propose two different methods for time-domain finite-difference analysis of uniform temporally and spatially dispersive metasurfaces using their zero thickness sheet representations using the Generalized Sheet Transition Conditions (GSTCs). Metasurfaces are described here using their effective surface susceptibilities which are assumed to exhibit Lorentzian temporal dispersion characteristics. For both methods, the spatial dispersion of the, the surface susceptibilities (i.e., their dependence on angle of incidence) are represented using the extended GSTCs presented in [1]–[3]. However, the first method takes advantage of a polynomial expansion of the angle-dependent surface susceptibilities in terms of the transverse wavevector to implement spatial derivatives of the electric and magnetic polarization as well as the average field on the surface, leading to a coupled set of field equations encompassing the entire surface. Limitations for this method are presented in terms of poor conditioning for a coupled system of equations and an inconvenient extension to the higher-order expansion of the susceptibility terms. The second method lifts these limitations by solving the spatial dispersion problem in the spatial frequency domain at every time step. Both methods are validated for custom Lorentzian models and two canonical physical cells while comparing their transmission and reflection coefficients with analytical results.

Index Terms—Electromagnetic Metasurfaces, Spatial Dispersion, Electromagnetic Propagation, Generalized Sheet Transition Conditions (GSTCs), Surface Susceptibility Tensors, Lorentz Oscillator Model, Finite-Difference Time-Domain, Spatial Frequency Domain.

I. INTRODUCTION

More recently, metasurfaces, which are arrays of subwavelength arrays of resonating structures, have received a lot of attention since they are capable of presenting electromagnetic characteristics not available from simple material interfaces and surfaces [4]. Therefore enabling the design of exotic functionalities like electromagnetic cloaking and holography [5], [6], besides being used for beam shaping and improving the performance of antenna designs [7], among others. The broadband scattered field computation and analysis of resonant metasurfaces is a multi-scale problem as the resonant structures themselves are sub-wavelength, while the overall metasurface is typically orders of wavelength in size. To reduce the computational complexity of brute-force simulations of metasurfaces, a compact zero thickness sheet model based on Generalized Sheet Transition Conditions (GSTCs) has recently become popular, where the metasurface is instead described in term of their constitutive parameters using their homogenized effective surface susceptibilities, $\tilde{\chi}$. By sacrificing the microscopic field characteristics, the zero thickness sheet model greatly simplifies the computation of macroscopic scattered fields.

Due to resonant characteristics of the underlying resonators forming the surface, typical metasurfaces are intrinsically temporally dispersive, i.e., $\tilde{\chi}(\omega)$. Moreover, for a general metasurface, these effective surface susceptibilities may also be spatially dispersive (or non-local), where their constitutive parameters are also functions of angle of plane-wave incidences (related to the transverse wave-vector $k_\parallel$), i.e. $\tilde{\chi}(\omega, k_\parallel)$. Therefore, due to the interaction of broadband incident signals with dispersive metasurfaces, the scattered time-domain waveforms are distorted in both time and space, and these interactions are thus naturally captured using time-domain analysis, typically implemented using Finite-Difference Time-Domain (FDTD) technique.

Finite-Difference Time-Domain (FDTD) is a widely used numerical technique for simulating electromagnetic wave propagation and interactions in various media [8]. FDTD discretizes both the spatial and temporal domains of the electromagnetic field equations into finite differences, allowing for the efficient and accurate simulation of complex wave phenomena. By discretizing space and time with the Yee cell, the FDTD method becomes a versatile tool for solving Maxwell’s equations without the need for complex meshes or grid structures. Despite its advantages, the Yee cell does have limitations, particularly in dealing with structures that involve small geometric features compared to the wavelength, where the Yee cell resolution may become impractically large. Nevertheless, over the years, various extensions and adaptations of the original FDTD method, such as the introduction of higher-order Yee cells or hybrid approaches with other numerical techniques, have been developed to address these challenges and further expand the method’s applicability to a wide array of electromagnetic problems [9]–[11].

Several works have been reported in the literature on FDTD analysis of metasurfaces, particularly using their zero-thickness sheet representation via the GSTCs. In [13], the GSTCs were introduced to the FDTD scheme via electric current densities source terms in the curl equations for non-dispersive real-valued electric susceptibilities. Other non-dispersive implementations are presented in [14]–[16]. In [17], Smy and Gupta...
introduced an explicit time-dispersive model where the electric and magnetic surface susceptibilities were described using the Lorentz model to take into account the temporal dispersion characteristics of the metasurface unit cell. In [18], authors used a rational polynomial in the temporal frequency domain to represent temporal dispersion of the surface susceptibilities and then incorporated that representation in a piecewise linear convolution method. They evaluate the surface polarizations inside an explicit method to solve the GSTCs within a regular Yee-cell-based FDTD solver. More recently, an explicit Drude dispersive model was presented in [19] and an implicit Lorentz model in [12] that was later extended for time-modulated metasurfaces in [20]. Authors in [21] presented a vector fitting procedure to represent a multi-Lorentz susceptibility form in an explicit GSTC-FDTD solver.

However, all these recent works only modeled the temporally dispersive nature of the resonating structures composing the metasurfaces, while assuming a local response, point by point, along the surface, i.e. non-spatially dispersive metasurface. In such a description, the surface susceptibilities terms are functions of the temporal frequency but represent a delta function in terms of the spatial frequency domain and are implicitly independent of the angle of incidence of the exciting fields. These approaches may be sufficient only if the resonator unit cells of the metasurfaces are deeply sub-wavelength and can be represented by angle-independent effective surface susceptibilities.

More recently, the works presented in [1]–[3] showed that the constitutive parameters of the resonating cells can also change with respect to the transverse wavevector, \( k_{||} \), i.e., the angle of incidence of the interacting fields at the surface, especially in cases where the periodicity of the cell is not deep sub-wavelength (\( > \lambda/5 \), as a current rule of thumb) and close to the diffraction limit of \( \lambda/2 \). Thus, the surface susceptibilities ended up being dependent on the spatial frequency, which corresponds to a general non-local response of the cell. As part of those works, a Boundary Element method (BEM) was developed for frequency domain analysis of uniform and non-uniform, periodic and finite, flat and curved spatially dispersive metasurfaces. However, to the best of our knowledge, no GSTC-FDTD method in the literature models spatially dispersive metasurfaces.

Therefore, in this work, we present, for the first time, a GSTC-FDTD-SD framework that can simultaneously incorporate both time- and space-dispersive (i.e., TD and SD) susceptibilities. We start describing the GSTC-FDTD-TDSD method for a uniform mono-anisotropic metasurface with electric and magnetic tangential susceptibilities under TE incidence, for simplicity and base the framework on the time-dispersive tight-asymmetric cell of [12] and the extended GSTCs of [1]. We validate the methodology by comparing the reflection and transmission phases and magnitudes with their analytical solution for a custom temporally and spatially dispersive electric and magnetic Lorenzian response. Then, we present a few limitations of this method and proceed with an improved mixed Finite-Difference Time-Domain/Spatial-Frequency-Domain (Mixed GSTC-FDTD-TDSD) method that solves the GSTC implicit problem in the spatial frequency domain at each time step. This version of the method shows improved accuracy and a more straightforward form to incorporate higher-order terms in the polynomial expansion of the Lorentz parameters with respect to the transverse wavevector. Finally, the methodology is further validated using data extracted from two practical unit cell structures: the wire dipole cell and the dielectric puck Huygens’ unit cell presented in [1].

II. STANDARD 2D-FDTD METHOD

Initially, we define the system setup of a standard Yee cell 2D-FDTD region and a coordinate system. Propagation will happen in the \( x-z \) plane with the angle of incidence, \( \theta \) defined with respect to the \( z \)-axis. At the edges of the \( z \)-axis, we have...
convolutional perfectly matched layers (CPML) as absorbing boundary conditions, and at the edges of the x-axis, we have periodic boundary conditions (PBC). The overall simulation setup can be seen in Fig. 1(a).

The 2D-FDTD method is developed in Matlab using the standard FDTD equations and boundary conditions provided in [22] and [23]. For a solution in 2D with TEexcitation, we are going to consider \( H_x, E_y, \) and \( H_z \) field components with no variation along the y direction, for simplicity. Hence, Maxwell’s curl equations in free space with no impressed current sources are

\[
\begin{align*}
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon_0} \left( \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) \quad (1a) \\
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu_0} \frac{\partial E_y}{\partial z} \quad (1b) \\
\frac{\partial H_z}{\partial t} &= - \frac{1}{\mu_0} \frac{\partial E_y}{\partial x} \quad (1c)
\end{align*}
\]

This set of equations can be discretized using regular Yee-cells shown in Fig. 1(b) whose finite difference form using Forward Euler for time derivatives and space derivatives in E and Backward Euler for space derivatives in H, as

\[
\begin{align*}
E_{yi,k}^{n+1} &= E_{yi,k}^n + \frac{\Delta t}{\epsilon_0 \Delta z} \left( H_{xi,k}^{n+\frac{1}{2}} - H_{xi,k-1}^{n+\frac{1}{2}} \right) \quad (2a) \\
H_{xi,k}^{n+\frac{1}{2}} &= H_{xi,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_0 \Delta z} \left( E_{yi,k+1}^n - E_{yi,k}^n \right) \\
H_{zi,k}^{n+\frac{1}{2}} &= H_{zi,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_0 \Delta z} \left( E_{yi,k+1}^n - E_{yi,k}^n \right)
\end{align*}
\]

where \( \epsilon_0 \) is the free space permittivity, \( \mu_0 \) is the free space permeability, \( \Delta t \) is the time step, and \( \Delta x \) and \( \Delta z \) are the space steps along the x and z directions, respectively, while the space indices \( i \) and \( k \) are used to index the respective Yee-cells while keeping the physical half step different between E and H field. Using the leap-frog approach, the fields can be updated by first computing \( H \) values at half-time steps with past values of \( E \) and then proceeding with \( E \) field calculations at integer time steps using past values of \( H \).

III. TIME-DOMAIN GENERALIZED SHEET TRANSITION CONDITIONS

The generalized sheet transition conditions (GSTC) rely on the zero thickness model presented by Idemen in [24]. Assuming the surface normal to be \( \mathbf{n} = \hat{\mathbf{z}} \), parallel directions \( \hat{x} \) and \( \hat{y} \) and the transverse gradient operator as \( \nabla \parallel = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, 0 \right] \), we can then write the GSTC’s as follows:

\[
\begin{align*}
\hat{z} \times \Delta H &= \frac{\partial P}{\partial t} - \hat{z} \times \nabla \| M_z \quad (3a) \\
\hat{z} \times \Delta E &= -\mu_0 \frac{\partial M}{\partial t} - \hat{z} \times \nabla \| \left( \frac{P_r}{\epsilon_0} \right) \quad (3b)
\end{align*}
\]

where \( \mathbf{E} = [E_x, E_y, E_z]^T \) and \( \mathbf{H} = [H_x, H_y, H_z]^T \) are the fields interacting with the surface, \( \mathbf{P} = [P_x, P_y, P_z]^T \) and \( \mathbf{M} = [M_x, M_y, M_z]^T \) are the surface electric and magnetic polarizations, and \( \Delta \psi = \psi_i - \psi_s \) is the difference operator with \( \psi \in \{E, H\} \) and \( \{i, t, r\} \) corresponding to the incident, reflect and transmitted field at the surface, respectively. Evaluation of (3), leads to

\[
\begin{align*}
\begin{bmatrix} -\Delta H_y \\ \Delta H_x \end{bmatrix} &= \begin{bmatrix} \frac{\partial P_r}{\partial t} + \frac{\partial M_x}{\partial y} \\ -\frac{\partial M_y}{\partial x} \end{bmatrix} \quad (4a) \\
\begin{bmatrix} -\Delta E_y \\ \Delta E_x \end{bmatrix} &= \begin{bmatrix} -\mu_0 \frac{\partial M_x}{\partial t} + \frac{\partial P_y}{\epsilon_0} \\ -\mu_0 \frac{\partial M_y}{\partial t} - \frac{\partial P_x}{\epsilon_0} \end{bmatrix} \quad (4b)
\end{align*}
\]

which represents the GSTC’s in the time domain, relating the difference in the transverse fields with time-derivatives of the tangential surface polarization and transverse spatial derivatives of the normal components of the surface polarizations. Moreover, the surface polarization terms at the surface for a non-local, temporally and spatially dispersive response can be related to the average fields on the surface using the following constitutive relations [11],

\[
\begin{align*}
\mathbf{P} &= \epsilon_0 \overline{\mathbf{E}}_{av} + \frac{1}{\epsilon_0} \overline{\mathbf{M}}_{em} \times \mathbf{H}_{av} \\
\mathbf{M} &= \overline{\mathbf{H}}_{mm} \times \mathbf{H}_{av} + \frac{1}{\mu_0} \overline{\mathbf{H}}_{me} \times \mathbf{E}_{av},
\end{align*}
\]

where \( \psi_{av} = (\psi_i + \psi_r + \psi_s)/2 \) is the average fields on the surface and \( \overline{\mathbf{E}}_{av}, \overline{\mathbf{H}}_{av} \) with \( \{a, b\} \in \{e, m\} \) correspond to the surface susceptibility tensors,

\[
\overline{\mathbf{E}}_{ee} = \begin{bmatrix} \chi_{ee} & \chi_{ex} & \chi_{ey} \\ \chi_{xe} & \chi_{ee} & \chi_{xy} \\ \chi_{ye} & \chi_{yx} & \chi_{ee} \end{bmatrix}, \quad \overline{\mathbf{E}}_{em} = \begin{bmatrix} \chi_{em} & \chi_{et} & \chi_{ey} \\ \chi_{me} & \chi_{em} & \chi_{xy} \\ \chi_{ye} & \chi_{ym} & \chi_{em} \end{bmatrix}
\]

\[
\overline{\mathbf{H}}_{mm} = \begin{bmatrix} \chi_{mm} & \chi_{mx} & \chi_{my} \\ \chi_{xm} & \chi_{mm} & \chi_{xy} \\ \chi_{ym} & \chi_{yx} & \chi_{mm} \end{bmatrix}, \quad \overline{\mathbf{H}}_{me} = \begin{bmatrix} \chi_{me} & \chi_{et} & \chi_{ym} \\ \chi_{me} & \chi_{em} & \chi_{xy} \\ \chi_{me} & \chi_{ym} & \chi_{em} \end{bmatrix}
\]

For simplicity and without loss of generality in the upcoming derivations and methods, we are going to consider the case of a monoanisotropic surface with no normal components under TE excitation. Therefore, simplifying the GSTC’s and constitutive relations to the following

\[
\begin{align*}
\Delta E_y &= \mu_0 \frac{\partial M_x}{\partial t}, \quad M_x = \chi_{xx} \times H_{x,av} \\
\Delta H_z &= \frac{\partial P_y}{\partial t}, \quad P_y = \epsilon_0 \chi_{ye} \times E_{y,av}
\end{align*}
\]

Consider now that this zero-thickness surface is placed between nodes \( k_x \) and \( k_x + 1 \) in the Yee-cell, as shown in Fig. 1(c). Following the tight-asymmetric (TA) cell scheme in [12], virtual surface nodes, \( E_{y|i+s-} \), \( H_{x|i+s+} \) and \( H_{z|i,s-} \) are inserted right before and after the surface so that Maxwell’s curl equations can be evaluated for bulk field nodes interacting with the surface field nodes. Following this discretization scheme, difference and average fields are defined as

\[
\begin{align*}
\Delta E_y &\to E_y|i,k_x+1 - E_y|i,k_x \\
\Delta H_z &\to H_z|i,s+ - E_y|i,k_x \\
E_{y,av} &\to \frac{E_y|i,k_x+1 + E_y|i,k_x}{2}, \\
H_{x,av} &\to \frac{H_z|i,s+ + E_y|i,k_x}{2}
\end{align*}
\]
For the case of a monoanisotropic metasurface, under TE oblique incidence, the tangential electric and magnetic susceptibilities can be obtained from full-wave simulation according to [25],

\[
\chi_{ee}(k_z = k_0 \sin \theta) = \frac{2j \cos \theta}{k_0} \left( \frac{R + T - 1}{T + R + 1} \right) \quad \text{(5a)}
\]

\[
\chi_{mm}(k_z = k_0 \sin \theta) = \frac{2j \sin \theta}{k_0 \cos \theta} \left( \frac{R - T + 1}{T - R + 1} \right). \quad \text{(5b)}
\]

where \(k_0\) is the free space wavenumber and \(R\) and \(T\) are the reflection and transmission coefficients for a given frequency and angle of incidence. From (5), we can obtain the reflection and transmission as a function of the susceptibilities according to,

\[
R = \frac{2j k_0 \{ \cos^2 \chi_{ee} - \chi_{yy} \}}{\{ k_0 \chi_{ee} - 2 \cos \theta \} \{ k_0 \cos \theta \chi_{mm} + 2 \}} \quad \text{(6a)}
\]

\[
T = \frac{2j k_0 \{ \cos \theta \chi_{mm} \chi_{ee} \}}{\{ k_0 \chi_{ee} - 2 \cos \theta \} \{ k_0 \cos \theta \chi_{mm} + 2 \}} \quad \text{(6b)}
\]

Completing the set of equations that form the background required for constructing temporal and spatial dispersion in the GSTC-FDTD methods in the subsequent sections.

IV. LORENTZIAN TEMPORAL AND SPATIAL DISPERSION METHOD (GSTC-FDTD-TDS)

A. Method Formulation

Let us start with the implicit method in the time and space domain, referred to in this work as GSTC-FDTD-TDS. The polarization at the metasurface can be described as a summation of polarization components based on the susceptibilities excited. For instance, the tangential \(P_y\) and \(M_x\) components can be described as

\[
P_y = P_{y,ee} + P_{y,yy} + P_{y,em} + P_{y,me} + P_{y,mm}
\]

\[
M_x = M_{x,mm} + M_{x,mm} + M_{x,me} + M_{x,me} + M_{x,me}.
\]

Time and spatial dispersion can be incorporated for each one of these terms using the extended Lorentz model [1],

\[
\frac{\partial^2 P_{yy}}{\partial t^2} + \gamma(k_x) \frac{\partial P_{yy}}{\partial t} + \omega_p^2(k_x) P_{yy} = \epsilon_0 \omega_p^2(k_x) E_y, \quad \text{(7)}
\]

where \(k_x\) is the transverse wavenumber and

\[
\gamma = \alpha_0 + \alpha_1 k_x + \alpha_2 k_x^2 + O(k_x^3)
\]

\[
\omega_p^2 = \beta_0^2 + \beta_1 k_x + \beta_2 k_x^2 + O(k_x^3)
\]

\[
\omega_0^2 = \xi_0^2 + \xi_1 k_x + \xi_2 k_x^2 + O(k_x^3),
\]

is the polynomial expansion of the Lorentz parameters in the spatial frequency domain, referred to as the extended Lorentz parameters.

Let us now consider the uniform monoanisotropic TE case with only tangential electric and magnetic polarization terms \(P_{yy}\) and \(M_{x,mm}\) described by tangential electric and magnetic susceptibilities \(\chi_{yy}\) and \(\chi_{mm}\) respectively. For a compact notation, let us write \(P_{yy} \rightarrow P_y\) and \(M_{x,mm} \rightarrow M_x\).

Assuming without loss of generality, a symmetric spatial response in (8) (even powers of \(k_x\) for terms up to second-order. We obtain for the description of an extended Lorentz oscillator model associated with, for example, the electric polarization in the time and space domain as,

\[
\frac{\partial^2 P_y}{\partial t^2} + \left( \alpha_{0,e} - \alpha_{2,e} \frac{\partial^2}{\partial x^2} \right) \frac{\partial P_y}{\partial t} + \left( \xi_{2,e} \frac{\partial^2}{\partial x^2} \right) P_y = \epsilon_0 \left( \beta_{0,e}^2 - \beta_{2,e} \frac{\partial^2}{\partial x^2} \right) E_y, \quad \text{(9)}
\]

where the second subscript “e” on the Lorentz parameters specifies values associated with the electric polarization.

Next, for improved numerical accuracy let us consider first-order time and space derivatives only, by adding auxiliary differential equations (ADEs). Considering the tight-asymmetric (TA) cell with the TE GSTCs and tangential susceptibility only, the resulting system of equations is then comprised of: 1) a set of equations describing the electric polarization from (9) using a first order construction,

\[
\frac{\partial P_y'}{\partial t} + \alpha_{0,e} P_y' - \alpha_{2,e} \frac{\partial}{\partial x} P_y + c_0^2 P_y = \epsilon_0 \left( \beta_{0,e}^2 E_y,av - \beta_{2,e} \frac{\partial}{\partial x} E_y,av \right),
\]

\[
P_y' - \frac{\partial P_y}{\partial x} = 0, \quad P_y' - \frac{\partial P_y'}{\partial x} = 0 \quad \text{(10b)}
\]

\[
P_y' - \frac{\partial P_y}{\partial x} = 0, \quad P_y - \frac{\partial E_{y,av}}{\partial x} = 0; \quad \text{(10c)}
\]

2) a complimentary set of equations for the magnetic polarization,

\[
\frac{\partial M_x'}{\partial t} + \alpha_{0,m} M_x' - \alpha_{2,m} \frac{\partial}{\partial x} M_x + c_0^2 M_x = \epsilon_0 \left( \beta_{0,m}^2 H_x,av - \beta_{2,m} \frac{\partial}{\partial x} H_x,av \right)
\]

\[
M_x' - \frac{\partial M_x}{\partial x} = 0, \quad M_x' - \frac{\partial M_x'}{\partial x} = 0 \quad \text{(10e)}
\]

\[
M_x' - \frac{\partial M_x}{\partial x} = 0, \quad H_x,av - \frac{\partial H_x,av}{\partial x} = 0; \quad \text{(10f)}
\]

and, finally, 3) four equations describing the field updates for the special cells and the GSTCs,

\[
-\Delta E_y = -\frac{\partial M_x}{\partial t}, \quad \frac{\partial E_y}{\partial t} = \frac{1}{\epsilon_0} \left( \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) \quad \text{(10g)}
\]

\[
\Delta H_x = \frac{\partial P_y}{\partial t}, \quad \frac{\partial H_x}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_y}{\partial z} \quad \text{(10h)}
\]

One important difference compared to the temporal-dispersive-only case in [12] is that now, due to spatial dispersion, we have to solve a coupled system of equations, where all points along the surface must be solved at the same time self-consistently. A second consideration about the system of equations in (10) is that the number of additional ADEs (unknowns) is equal to \(n_d - 1\) for each of the polynomials in (8), where \(n_d\) is the highest-order derivative in each of the extended Lorentz terms. In the current example, since all the terms are expanded up to the second order, there are three additional ADEs (variables) for each polarization term.

Discretizing (10) using Forward-Euler for time derivatives and spatial Forward-Euler for \(E\) and \(P\) and spatial Backward-Euler for \(H\) and \(M\) terms results in the system of equations
cases inside the simulation setup of Fig. 1(a). The first one

\[ \mathbf{X}^{n+1} = \begin{bmatrix} E_{x,i,k}^{n+1} & E_{y,i,s}^{n+1} & H_{x,i,s}^{n+1} & H_{x,i,k}^{n+1} \\ P_{y,i}^{n+1} & P_{x,i}^{n+1} & P_{x,i}^{n+1} & P_{x,i}^{n+1} \\ E_{y,i}^{n+1} & M_{x,i}^{n+1} & M_{x,i}^{n+1} & M_{x,i}^{n+1} \\ M_{x,i}^{n+1} & M_{x,i}^{n+1} & M_{x,i}^{n+1} & M_{x,i}^{n+1} \end{bmatrix} \]

\[ \text{where } \mathbf{A} \text{ are the coefficient matrices, } \mathbf{B} \text{ are the forcing term matrices that depend on past values of the unknowns in } \mathbf{X}, \]

and \( \mathbf{C} \) are matrices that are forcing terms that depend on field terms not part of the unknowns. Each entry within these matrices is presented in Supplementary Material S2 in equations (S2-S8).

After these matrices have been computed for every point on the surface, they need to be assembled in the coupled system of equations (8). Moreover, for each cell, the complete set of equations, considering the spatial coupling due to spatial dispersion, is represented as

\[ \begin{bmatrix} A_{i,-1}^{n+1} & A_{i}^{n+1} & A_{i+1}^{n+1} \\ B_{i,j}^{n} & B_{i,j}^{n+1} & B_{i,j+1}^{n+1} \end{bmatrix} \begin{bmatrix} X_{i,i}^{n+1} \\ X_{i,i}^{n} \end{bmatrix} = \begin{bmatrix} X_{i,i}^{n+1} \\ X_{i,i}^{n} \end{bmatrix} + \mathbb{C} \]

where \( \mathbb{A} \) are the coefficient matrices, \( \mathbb{B} \) are the forcing term matrices that depend on past values of the unknowns in \( \mathbb{X} \),

and \( \mathbb{C} \) are matrices that are forcing terms that depend on field terms not part of the unknowns. Each entry within these matrices is presented in Supplementary Material S2 in equations (S2-S8).

For testing the proposed method, we present two simulation cases inside the simulation setup of Fig. 1(a). The first one consists of a single tangential TDSD electric susceptibility

\[ \text{case with no magnetic response, and the second case is that of both electric and magnetic surface susceptibility in a Huygens' configuration. For simplicity, these choices of susceptibilities attempt to approximate a single dipole dispersive cell and a Huygens structure that, as shown in [1], may require terms up to the sixth-order in } k. \text{ A more practical scenario will be presented in Sec. V with a more robust implementation of the GSTC-FDTD method that easily supports higher-order terms.} \]

The extended Lorentz parameters for the first case are presented in Tab. I, consisting of terms up to the second-order in the polynomial representation of (8).

The simulation setup consists of a 2.5 \( \times \) 2.5 \( \mu m \) region with the metasurface placed at \( z = 1.25 \mu m \). The region is terminated with CPMLs along the \( z \) direction and PBCs along the \( x \) direction. Simulation parameters are: \( \Delta x = \Delta z = 12.5 \) nm \((\lambda_0/98)\), \( \Delta t = 14.74 \) as (Courant stability factor of 1/2) running for a total of 700 fs. The source is a Gaussian pulsed plane wave, centered at 245 THz, with a bandwidth of 10 THz and angle of incidence varying from 0° to 60°, and placed at \( z = 0.75 \mu m \). The angle is limited to up to 60° to avoid disturbances caused by the constant phase shift imposed by the PBCs. The reflected and transmitted fields are measured at 2\( \Delta z \) away from the source, in free space, within bulk Yee-cells, and their spectrum is de-embedded to the face of the metasurface. Time monitors in the reflection region measure both incident and reflected fields.

Results for Case 1 are shown in Fig. 2. Figure 2 (a) shows two rows of panels representing analytical transmission and reflection data for a case of time dispersion only (top row), where the susceptibility is taken to be constant \((k_z = 0)\) across different angles of incidence \((\theta)\) and a second case, with time and space dispersion (TDSD), where now the electric susceptibility is varying according to the coefficients shown in I. It is clear that for this custom case, SD becomes important for the correct description of T and R. Moreover, Fig. 2 (b) compares the results of the GSTC-FDTD-TDSD method with analytical analytical results obtained from (6). One of the clear characteristics is the location of the deep minimum in transmission shifting from 240 THz to 250 THz as \( C_2 \) shifts the location of the Lorentz resonance as the angle of incidence increases. Figure 2(c) shows snapshots of the real part of the electric field for different angles of incidence over the simulation region, and the corresponding temporal waveforms in the transmission and reflection regions, showing

### Table I

<table>
<thead>
<tr>
<th>Case 1: Custom TDSD Electric Susceptibility Parameters</th>
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<tbody>
<tr>
<td>Tangential Electric Susceptibility ( (\chi_{\text{ee}}^{\text{mm}}) )</td>
</tr>
<tr>
<td>( \alpha_0 ) ( (x 10^{12}) )</td>
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<tr>
<td>7.5398</td>
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### Table II

<table>
<thead>
<tr>
<th>Case 2: Custom TDSD Electric and Magnetic Susceptibility Parameters</th>
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<tbody>
<tr>
<td>Tangential Electric Susceptibility ( (\chi_{\text{ee}}^{\text{mm}}) )</td>
</tr>
<tr>
<td>( \alpha_0 ) ( (x 10^{12}) )</td>
</tr>
<tr>
<td>7.5398</td>
</tr>
</tbody>
</table>

| Tangential Magnetic Susceptibility \( (\chi_{\text{mm}}^{\text{mm}}) \) |
| \( \alpha_0 \) \( (x 10^{12}) \) | \( \alpha_2 \) \( (x 10^{12}) \) | \( \beta_0 \) \( (x 10^{12}) \) | \( \beta_2 \) \( (x 10^{12}) \) | \( \zeta_0 \) \( (x 10^{12}) \) | \( \zeta_2 \) \( (x 10^{12}) \) |
| 7.5398 | 75.3982 | 3.0121 | 7.5303 | 1.4451 | 5.0579 |
Fig. 2. (a) Analytical comparison of transmission and reflection magnitudes (dB) and phases (deg) for a uniform metasurface made of a custom electric susceptibility function defined by the parameters in Tab I. The top panels show the analytical data for time dispersive susceptibility ($\chi(\omega, k_z)$), and the bottom panels show data for a time and space dispersive scenario ($\chi(\omega, k_z)$). (b) Transmission and reflection where solid lines are analytical data obtained from (6), and marked dot-dashed lines are the results obtained from the GSTC-FDTD-TDSD algorithm. Line markers denote the angle of incidence. (c) The amplitude of the real part of the electric field over time. Image panels show field snapshots over the simulation region for three different angles of incidence and three different time instants. The insets show the source plane location (white solid line), the metasurface location (white dashed line), and the location of the reflection and transmission point monitors (white ‘x’ markers).
strong temporal distortion and broadening.

Case 2 consists of a case where both tangential TDSD electric and magnetic susceptibility parameters are equal at all angles, resembling a Huygens cell characterized by co-located orthogonal electric and magnetic resonance responses [7], [26], [27]. The parameters are presented in Tab. II. The simulation setup is the same as that of Case 1, and results are shown in Fig. 3. Figure 3(a) shows the comparison between constant susceptibilities across angles of incidence in the top row and their SD counterpart in the bottom row. The effects of SD are clearly depicted by the huge differences in the T and R profiles compared to the time-dispersive-only case. In Fig. 3(b), we observe a good match between the GSTC-FDTD-TDSD method and the analytical results from (6) for various incidence angles. In this case, the surface becomes more transmissive (or better matched) at oblique angles due to optimum interactions of collocated electric and magnetic resonances. However, the response still presents a spatially dispersive profile controlled by the higher-order terms in \( k_x \) and manifesting as variation with the angle of incidence. This phenomenon is also depicted in the field plots over time and angle of Fig. 3(c), where the transmitted fields present a lower amplitude at 20° compared to higher angles. These two examples thus successfully illustrate the proposed GSTC-FDTD platform with TD-SD incorporated, along with the importance of including SD in the analysis compared to a purely non-SD case.

So far, the cases analyzed were limited to second-order terms in \( k_x \), which produces second-order derivatives in (9). General metasurface cells may require higher order dependence of surface susceptibilities on the incidence angles or equivalently on \( k_x \). In those cases, a need for higher-order terms would require the extension of the system of coupled equations. This is a main drawback of this method; if higher-order terms are required, the whole system of equations becomes larger, new ADEs must be added, and the condition of the matrix \( A \) in (14) (a measurement of how sensitive the matrix is to changes in the input data and roundoff errors in the solution process [28]), increases by several orders of magnitude, even after performing matrix scaling and permutation [29], [30]. This can lead to close to singular matrices or even cases where solutions might diverge. As an approach to solve this limitation and make the method easier to expand for higher-order terms in \( k_x \), in the next section, we propose a Mixed GSTC-FDTD-TDSD that solves (10) in the spatial frequency domain at each time-step.

V. MIXED FINITE-DIFFERENCES

Spatial-Frequency/Time-Domain Method

As mentioned in the previous section, for the solution of (10) for higher-order terms in \( k_x \) and even larger surfaces, it was observed that \( A \) in (14) can become badly conditioned, making the solution unstable, and very sensitive to small changes in the Lorentz parameters and roundoff errors during the solution process. As an attempt to improve these issues, we present in this section a mixed finite differences spatial-frequency/time-domain method (Mixed GSTC-FDTD-TDSD) that solves the surface equations (10) in the spatial frequency domain at every time step.

We start by converting (10) to the spatial frequency domain using the spatial Fourier transform along the surface direction (i.e., \( x \) dimension). The spatial derivatives are no longer needed explicitly as they can be replaced in the spatial frequency domain by a \( k_x \) factor. We thus obtain a reduced set of equations defining the polarizations,

\[
\begin{align*}
\frac{\partial M_x'}{\partial t} + \gamma_m(k_x)M_x' + \omega_0^2\gamma_m(k_x)M_x &= \mu_0\omega_0^2\epsilon_{p,m}(k_x)H_{x,av} \\
\frac{\partial P_y'}{\partial t} + \gamma_e(k_x)P_y' + \omega_0^2\epsilon_{s,0,c}(k_x)P_y &= \epsilon_0\omega_0^2\epsilon_{p,s}(k_x)E_{y,av} \\
P_y' - \frac{\partial P_y'}{\partial t} = 0, & \quad M_x' - \frac{\partial M_x}{\partial t} = 0,
\end{align*}
\]
Fig. 3. (a) Analytical comparison of transmission and reflection magnitudes (dB) and phases (deg) for a uniform metasurface made of custom electric and magnetic susceptibility functions defined by the parameters in Tab II. The top panels show the analytical data for time dispersive susceptibilities ($\chi_0(\omega)$), and the bottom panels show data for a time and space dispersive scenario ($\chi_0(\omega, k_z)$). (b) Transmission and reflection where solid lines are analytical data obtained from (6), and marked dot-dashed lines are the results obtained from the GSTC-FDTD-TDSD algorithm. Line markers denote the angle of incidence. (c) The amplitude of the real part of the electric field over time. Image panels show field snapshots over the simulation region for three different angles of incidence and three different time instants. The insets show the source plane location (white solid line), the metasurface location (white dashed line), and the location of the reflection and transmission point monitors (white ‘x’ markers).
and the GSTCs and surface fields,
\[
-\Delta E_y = -\frac{\partial M_x}{\partial t}, \quad \Delta E_y = \frac{1}{\epsilon_0} \left( \frac{\partial H_x}{\partial z} - j k_x H_z \right)
\]
\[
\Delta H_x = \frac{\partial P_y}{\partial t}, \quad \Delta H_y = \frac{1}{\mu_0} \frac{\partial E_x}{\partial z}
\]  
(15b)
where calligraphic quantities correspond to the spatial frequency representatives of their spatial field counterparts (i.e., $E \rightarrow \mathcal{F} E$). Equation (16) is the discretized version of (15) using FE for time derivatives, BE for $z$-space derivatives on $H_x$ and FE for $z$-space derivatives on $E_y$. The physical cells in [1] contain constant electric polarization terms, $P_{y,0}$ and $M_{x,0}$ that are independent of the Lorentz oscillator model and can be added using superposition to the total polarization terms, $P_y$ and $M_x$,
\[
P_y = P_{y,1} + P_{y,0}
\]
\[
M_x = M_{x,1} + M_{x,0}
\]
The two non-dispersive terms are then related to the average fields on the surface using standard constitutive relations,
\[
\mathcal{P}_{y,0} = \epsilon_0 \chi_{ee,0} \mathcal{E}_{y,ax}
\]
\[
M_{x,0} = \mu_0 \chi_{mm,0} \mathcal{H}_{x,ax},
\]
which conforms to the following discretized scheme:
\[
\mathcal{P}_{y,0}^{n+1} = \epsilon_0 \chi_{ee,0} \mathcal{E}_{y,ax}^{n+1} + \frac{1}{2} \chi_{ee,0} \mathcal{E}_{y,ax}^{n+1} \mathcal{H}_{x,1,k_x+1}^{n+1} + \mathcal{H}_{y,1,k_y+1}^{n+1}
\]
\[
M_{x,0}^{n+1} = \mu_0 \chi_{mm,0} \mathcal{H}_{x,ax}^{n+1} + \frac{1}{2} \chi_{mm,0} \mathcal{H}_{x,ax}^{n+1} \mathcal{H}_{y,1,k_y+1}^{n+1} + \mathcal{H}_{y,1,k_y+1}^{n+1}.
\]
It is worth noting that the overall susceptibility description across frequency and all angles of incidence must still follow Kramers-Kronig relations for a stable causal response. Furthermore, we can incorporate all these equations in and write its final matrix form as shown in (17).

It is worth mentioning that in this particular system of equations, the index $i$ refers to the discrete values of $k_{x,i}$ in the spatial frequency domain, defined as
\[
k_x = \left[ \cdots, k_{x,i}, \cdots \right] = 2\pi \left[ -\frac{1}{2dx}, \cdots, \frac{1}{dx} - \frac{1}{2} \right],
\]
where $n_{x,MS}$ is the number of samples along the surface, $1/dx$ is the spatial sampling frequency, and $(1/dx - 1/2)/(n_{x,MS} - 1)$ is the size of the spatial frequency bin. For a scenario where the surface length and space-step provide a coarse value of $k_{x,i}$, the spatial frequency bins in the $k_x$ domain become large, and spectral leakage occurs. In this case, spectral power goes to a spectral bin that does not precisely correspond to the $k_x$ value where the field is, in fact, incident, leading to two problems: wrong evaluation of the susceptibility transfer function and leakage of the spectral power to a spatial frequency bin that is outside the propagation range ($-k_0, k_0$).

A solution adopted in this work is to take advantage of the periodic boundary conditions imposed at the edges of the metasurface and, at each time step, and replicate the whole fields along the surface by $N_{FFT}$ times. Thus, increasing the resolution in the spatial frequency domain, as in (18) the new number of samples becomes $n_{x,MS} \rightarrow N_{FFT} n_{x,MS}$. Therefore, reducing the size of the spatial frequency bins and preventing both problems while overall improving the accuracy of the solution once the resulting fields are converted back to the space domain via the inverse spatial FFT and further used by regular Yee-cell update equations for appropriate field propagation.

Finally, the solution at each time step $n\Delta t$ is obtained with the following steps:

1) Update bulk $H$ nodes using regular Yee-cell update equations;
2) Compute the spatial Fourier transform of $H_x^{n+\frac{1}{2}}$, $E_y^{n+1}$, and $H_z^{n+\frac{1}{2}}$ after replicating them by $N_{FFT}$ times;
3) Solve for the unknowns in (17) for $-k_0 \leq k_z \leq k_0$;
4) Compute the inverse spatial Fourier transform of $H_x^{n+\frac{1}{2}}$, $E_y^{n+1}$, and $H_z^{n+\frac{1}{2}}$;
5) Update the remaining bulk $E$ nodes using regular Yee cell update equations.

The second method, therefore, generalizes the SD response of the surface beyond 2nd order spatial derivatives at the expense of performing Fast Fourier Transforms of the surface fields at each time step.

### A. Numerical Demonstrations

The Mixed GSTC-FDTD-TDS method will be validated using analytical transmission and reflection equations from (6). The examples discussed use the surface susceptibilities data extracted from physical cells in [1] for the electric dipole unit cell and the Huygens’ unit cell. The overall simulation setup is depicted in Fig. 1(a).

The electric dipole data is shown in Tab. III with the non-spatially dispersive magnetic polarization term, $\chi_{mm}^x$ modeled...
\[
\begin{align*}
\mathcal{E}_{y|_{k+1}} - \mathcal{E}_{y|_{k}} &= \frac{M_{x|_{i}} + \frac{1}{2} - M_{x|_{i}} - \frac{1}{2}}{\Delta t}, \quad \mathcal{H}_{y|_{i}} = \frac{H_{x|_{i}} + \frac{1}{2} - H_{x|_{i}} - \frac{1}{2}}{\Delta t}, \quad \mathcal{P}_{y|_{i}} = \frac{P_{y|_{i}} + \frac{1}{2} - P_{y|_{i}} - \frac{1}{2}}{\Delta t} \\
\mathcal{E}_{y|_{k+1}} - \mathcal{E}_{y|_{k}} &= \frac{M_{x|_{i},k+1} + \frac{1}{2} - M_{x|_{i},k+1} - \frac{1}{2}}{\Delta t}, \quad \mathcal{H}_{y|_{i}} = \frac{H_{x|_{i},k+1} + \frac{1}{2} - H_{x|_{i},k+1} - \frac{1}{2}}{\Delta t}, \quad \mathcal{P}_{y|_{i},k+1} = \frac{P_{y|_{i},k+1} + \frac{1}{2} - P_{y|_{i},k+1} - \frac{1}{2}}{\Delta t} \\
\mathcal{E}_{y|_{k+1}} - \mathcal{E}_{y|_{k}} &= \frac{M_{x|_{i},k} + \frac{1}{2} - M_{x|_{i},k} - \frac{1}{2}}{\Delta t}, \quad \mathcal{H}_{y|_{i},k} = \frac{H_{x|_{i},k} + \frac{1}{2} - H_{x|_{i},k} - \frac{1}{2}}{\Delta t}, \quad \mathcal{P}_{y|_{i},k} = \frac{P_{y|_{i},k} + \frac{1}{2} - P_{y|_{i},k} - \frac{1}{2}}{\Delta t}
\end{align*}
\]

(16)
Fig. 4. (a) Analytical comparison of transmission and reflection magnitudes (dB) and phases (deg) for a uniform metasurface made of electric dipole cells with susceptibilities defined by the parameters in Tab III and a magnetic susceptibility modeled using a temporally-dispersive-only Drude model with \( \omega_p = 4.9119 \times 10^9 \) rad/s and \( \gamma = 0.98 \times 10^9 \) rad/s. The top panels show the analytical data for time dispersive susceptibilities \( (\chi(\omega, \mathbf{k})) \), and the bottom panels show data for a time and space dispersive scenario \( (\chi(\omega, \mathbf{k}_z)) \). (b) Transmission and reflection where solid lines are analytical data obtained from (6), and marked dot-dashed lines are the results obtained from the Mixed GSTC-FDTD-TDSD algorithm. Line markers denote the angle of incidence. (c) The amplitude of the real part of the electric field over time. Image panels show field snapshots over the simulation region for three different angles of incidence and three different time instants. The insets show the source plane location (white solid line), the metasurface location (white dashed line), and the location of the reflection and transmission point monitors (white ‘x’ markers).