Abstract—We present a corrective subcell averaging technique that improves on the accuracy of the volume-averaged finite-difference time-domain (FDTD) method in the presence of dispersive material interfaces. The method is based on an alternative effective-medium formulation that captures field discontinuities at interfaces as electric and magnetic surface currents. In calculating the spectra of strongly dispersive Mie scatterers we demonstrate that the derived FDTD algorithm is both highly efficient and able to approximately restore second order accuracy.

I. INTRODUCTION

Half a century after its invention by Kane Yee [1] the finite-difference time-domain (FDTD) method remains a popular choice for simulating the propagation of electromagnetic waves and their interaction with electronic media [1], [2]. The simplicity of the algorithm and its low computational footprint contrasted by the use of non-conformal grids, which, if field discontinuities are not properly accounted for, reduce accuracy from second to first order [3], [2]. This not only negates the advantage of the staggered grid Yee-algorithm but also impacts on the computational cost when modeling systems that exhibit geometric features on sub-wavelength scales due to poor convergence.

The problem of restoring accuracy of the FDTD scheme in the presence of interfaces was first studied in the microwave regime [4], [5], [6]. Since then a variety of effective-permittivity (EP) models have been suggested for the treatment of field discontinuities at material interfaces, which can broadly be classified as either contour-path (CP) or volume-averaged (VA) methods [7], [8], [9], [10], [11]. Fundamentally, defining the effective permittivity $\tilde{\varepsilon}_\infty$ as volume-average (VA) of the permittivity $\varepsilon_\infty$ over one Yee-cell $\varepsilon_\infty = \langle \varepsilon_\infty \rangle$ is compatible with the standard FDTD scheme but does not constitute an accurate VP model as discontinuities of the electric field at interfaces are not accounted for. In this context the VP model proposed by Farjadpour et al. [12] is of particular importance. Based on the continuity of the parallel electric and normal displacement field components, the effective permittivity tensor is derived as $\tilde{\varepsilon}_\infty^{-1} = (\varepsilon_\infty^{-1})^{\parallel} + (\varepsilon_\infty^{-1})^{\perp}(I - P)$, where $P = n \otimes n$ performs a vector-projection onto the face-normal of the interface. The application of this non-diagonal and anisotropic permittivity tensor requires interpolation of the Yee-centered $\mathbf{D}$-field to the cell-center and subsequent interpolation of the cell-centered $\mathbf{E}$-field back onto the Yee-grid, a procedure that effectively equates to a smoothing operation with extended spatial stencil [13]. Nonetheless, as numerical evidence suggests, the spectral accuracy increases to approximately second order, reducing the computational cost for problems that involve non-dispersive dielectrics (e.g., photonic crystal applications). In 2007, Deinega et al. [14] suggested an approach that extends this method to the linear dispersive regime. Their algorithm uses the decomposition $\mathbf{E} = E_\parallel + \mathbf{n}(E_{1,1} + E_{1,2})$, where $E_{1,1} = \mathbf{n} \cdot \mathbf{E}$ and $E_\parallel = \mathbf{E} - \mathbf{n}(\mathbf{n} \cdot \mathbf{E})$, to split the electric field into four independent components, which drive the polarization currents at the interface. While the split-field approach applies to the general case it is noteworthy that splitting the electric field into normal and parallel components is not always necessary. For example, Lee et al. [15] derive a model that uses an effective conductivity tensor in the quasi-static limit without splitting the fields, while Liu et al. [16] employ a rotation of the coordinate system in conjunction with modified material responses to avoid an explicit computation of the four split-field components. The resulting algorithms are computationally more efficient yet less general in the sense that they do not apply to arbitrary dispersive material responses. Furthermore, as in [12], it remains unspecified how these algorithms interface with the standard Yee-centered algorithm that could be efficiently employed across regions where permittivities are smooth.

Here, we present an alternative VP approach (see Fig. 1) that solves the EP curl equations on the Yee-grid using the standard volume-averaged FDTD algorithm but replaces the electric field with an approximate field $\mathbf{E}$ that is continuous across non-dispersive interfaces. The field discontinuities at dispersive media interfaces need then to be captured as corrective electric and magnetic currents $\delta J_{\parallel}$ and $\delta K_{\parallel}$, which are induced by a surface charge field $\rho$. Based on this idea we first formulate an effective medium theory and then show how this EP model translates into a FDTD scheme that offers...
II. CORRECTIVE-CURRENT SUBCELL SMOOTHING

Our starting point are the split-field equations derived by Deinega et al. \cite{14} (equations (3)-(6) therein). Without loss of generality we write the scalar permittivity as \( \varepsilon(\omega) = \varepsilon_{\infty} + \chi(\omega) \) and transform the equations into time-domain. Using a slightly different notation, we write

\[
\begin{align*}
\langle \varepsilon_{\infty} \rangle \partial_t \mathbf{E}_{||} &= (\nabla \times \mathbf{H})_{||} - f_1 J_1[\mathbf{E}_{||}] - f_2 J_2[\mathbf{E}_{||}] \\
\varepsilon_{\infty,1} \partial_t E_{\perp,1} &= f_1 (\nabla \times \mathbf{H})_{\perp} - J_1[\mathbf{E}_{\perp,1}] \\
\varepsilon_{\infty,2} \partial_t E_{\perp,2} &= f_2 (\nabla \times \mathbf{H})_{\perp} - J_2[\mathbf{E}_{\perp,2}]
\end{align*}
\]

where \( J_{1/2}[\mathbf{E}] = \partial_t \mathbf{P}_{1/2}[\mathbf{E}] \) are functionals of \( \mathbf{E} \), describing the (isotropic) polarization current response. The symbols ‘\( \perp \)’ and ‘\( \parallel \)’ denote vector-projections relative to the interface with face-normal \( \mathbf{n} \) and the notation \( J_{1/2} = \mathbf{n} \cdot J_{1/2} \) is introduced for brevity where quantities with a \( \perp \) suffix are always scalars (for example \( E_{\perp} = \mathbf{n} \cdot \mathbf{E} \)) and quantities with a \( \parallel \) are always vectors (for example: \( \mathbf{E}_{\parallel} = \mathbf{E} - (\mathbf{E} \cdot \mathbf{n}) \mathbf{n} \)). In adopting vector-notation we do not impose restrictions on the numbers of dimensions (i.e., the equations are valid for the two- and three-dimensional case). The above formulation of Ampre’s law implicitly assumes an averaging over a volume-cell that is intersected by a boundary between media 1 and 2 with cell-filling ratios \( f_1 \) and \( f_2 \) (\( f_1 + f_2 = 1 \)). Angled brackets are used throughout this work to denote volume averages of the form \( \langle \varepsilon_{\infty} \rangle = f_1 \varepsilon_{\infty,1} + f_2 \varepsilon_{\infty,2} \).

The derivation of \( (1) \) is straightforward but their translation into an efficient and stable finite-difference scheme is not. To retain second order accuracy, the field components in the curl expression \( \nabla \times \mathbf{H} \) should be calculated on the Yee-grid while the projections onto parallel and normal projections require interpolation to the cell-center. After calculating the updates of the \( \mathbf{E}_{||} \), \( \mathbf{E}_{\perp,1} \) and \( \mathbf{E}_{\perp,2} \) components at the cell-center the \( \mathbf{E} \)-field thus needs to be reconstructed and redistributed onto the Yee-grid. However, a direct implementation proves impractical for the following reason. The cell-centered four-field representation and the extended spatial stencil (due to interpolation between the grids) is incompatible with the standard Yee-algorithm. As a consequence the algorithm is best deployed across the whole grid irrespective of whether cells are intersected by media-boundaries or not. This introduces unnecessary smoothing operations across the whole grid, increases the computational cost and requires a reimplementation of the infrastructure typically associated with FDTD frameworks (e.g., total-field scattered-field injection, boundary conditions etc).

We here seek to derive an alternative formulation where the standard Yee scheme can be efficiently applied across the domain augmented by corrections that only apply to the comparably small number of interface cells. The basis for this corrective method is a reformulation of \( (1) \). In introducing new variables for the normal electric field and the density of the induced surface charges,

\[
E_{\perp} = E_{\perp,1} + E_{\perp,2} \\
\rho = f_2 \varepsilon_{\infty,1} E_{\perp,1} - f_1 \varepsilon_{\infty,2} E_{\perp,2}
\]

equations \( (1) \) can be cast into the form

\[
\langle \varepsilon_{\infty} \rangle \partial_t \mathbf{E}_{||} = (\nabla \times \mathbf{H})_{||} - f_1 J_1[\mathbf{E}_{||}] - f_2 J_2[\mathbf{E}_{||}] \\
\langle \varepsilon_{\infty} \rangle \partial_t E_{\perp} = (\nabla \times \mathbf{H})_{\perp} - \gamma_1 J_1[\mathbf{E}_{\perp,1}] - \gamma_2 J_2[\mathbf{E}_{\perp,2}] \\
\partial_t \rho = f_1 J_2[\mathbf{E}_{\perp,2}] - f_2 J_1[\mathbf{E}_{\perp,1}]
\]

with \( \gamma_{1/2} = \langle \varepsilon_{\infty} \rangle^{-1} \varepsilon_{\infty,1/2} \). The fact that \( \langle \varepsilon_{\infty} \rangle^{-1} \neq \varepsilon_{\infty}^{-1} \) makes it impossible to reconstruct Ampre’s law in isotropic form by directly combining the first two equations. However, we can define an approximate electric field

\[
\tilde{\mathbf{E}} = \mathbf{E}_{||} + \langle \varepsilon_{\infty} \rangle^{-1} \varepsilon_{\infty,1/2}^{-1} \mathbf{n} \mathbf{E}_{\perp}
\]

which, in the absence of dispersive currents, is continuous across material interfaces and matches \( \mathbf{E} \) at non-interface cells. Combining the first two equations of \( (3) \) in this fashion yields

\[
\langle \varepsilon_{\infty} \rangle \partial_t \tilde{\mathbf{E}} = \nabla \times \mathbf{H} - (\mathbf{J}[\mathbf{E}]) - \delta \mathbf{J}_{\perp}
\]

We note that apart from the extra current term \( \delta \mathbf{J}_{\perp} \) we now have recovered the volume-averaged curl equation for the electric field. The correction \( \delta \mathbf{J}_{\perp} = \mathbf{n} \delta \mathbf{J}_\perp \) compensates the error that arises from using volume-averaged permittivities and current densities for the normal components. Assuming an isotropic response one obtains after some algebra

\[
\delta \mathbf{J}_{\perp} = -f_1 J_1[\tilde{\mathbf{E}}] - f_2 J_2[\tilde{\mathbf{E}}] + \gamma_1 J_1[\mathbf{E}_{\perp,1}] + \gamma_2 J_2[\mathbf{E}_{\perp,2}]
\]

for the surface current correction. Its calculation requires the scalar fields \( \mathbf{E}_{\perp,1/2} \) that are obtained by projection

\[
E_{\perp,1} = f_1 \varepsilon_{\infty,1} \langle \varepsilon_{\infty} \rangle \mathbf{n} \cdot \tilde{\mathbf{E}} + f_1^{-1} \gamma_2 \rho \\
E_{\perp,2} = f_2 \varepsilon_{\infty,2} \langle \varepsilon_{\infty} \rangle \mathbf{n} \cdot \tilde{\mathbf{E}} - f_2^{-1} \gamma_1 \rho
\]

Inserting these relations into \( (6) \) yields

\[
\delta \mathbf{J}_{\perp} = f_1 (J_{1/2}[\tilde{\mathbf{E}}, \rho] - J_1[\tilde{\mathbf{E}}]) + f_2 (J_{2/2}[\tilde{\mathbf{E}}, \rho] - J_2[\tilde{\mathbf{E}}])
\]

where we defined

\[
J_{1/2}^{\ast}[\tilde{\mathbf{E}}, \rho] = \gamma_{1/2} \varepsilon_{\infty,1/2}^{-1} \langle \varepsilon_{\infty} \rangle J_{1/2}[\tilde{\mathbf{E}}] \pm f_{1/2}^{-1} \gamma_{2/1} J_{1/2}[\rho]
\]

This implies that the electric current correction can be calculated from the currents induced by \( \tilde{\mathbf{E}} \) and \( \rho \). The terms in \( (6) \) proportional to \( J_{1/2}[\tilde{\mathbf{E}}] \) are the volume-averaged normal currents, which need to be subtracted from eq. \( (5) \) before adding the correct \( J_{1/2}^{\ast}[\tilde{\mathbf{E}}, \rho] \) contributions. Applying \( (7) \) to the equation for the charge field \( \rho \) \cite{14} gives

\[
(f_1 f_2)^{-1} \partial_t \rho = \gamma_2^{-1} J_2^{\ast}[\tilde{\mathbf{E}}, \rho] - \gamma_1^{-1} J_1^{\ast}[\tilde{\mathbf{E}}, \rho]
\]
In order to complete the update of the magnetic field the correct electric field \( \tilde{E} \) needs to be recovered from \( \tilde{E} \). This is achieved by introducing a corrective magnetic current density

\[
\delta K_\parallel = \nabla \times \mathbf{n} \delta E_\perp = \nabla \times \mathbf{n} (1 - \langle \varepsilon_{\infty} \rangle) \mathbf{n} \cdot \tilde{E} \tag{11}
\]

to Faraday’s law

\[
\partial_t \mathbf{H} = -\mu_0^{-1} \nabla \times \tilde{E} - \mu_0^{-1} \delta K_\parallel \tag{12}
\]

This completes our reformulation of the effective field-corrected Maxwell’s equations. The curl equations (5), (12) together with the electric and magnetic current corrections (8) and (11) and the surface charge equation (10) form a closed set of equations. We achieved our goal of finding an effective medium formulation where the corrective current densities \( \delta J_\perp \) and \( \delta K_\parallel \) depend on \( \tilde{E} \) in a functional fashion. The corrections apply at interface cells only and vanish whenever permittivities vary smoothly across cells. The magnetic current correction \( \delta K_\parallel \) accounts for field discontinuities caused by a jump in the static permittivity across the interface, while the electric current correction \( \delta J_\perp \) captures all discontinuities induced by the dispersive material response. Notably, calculating the induced corrections requires only three additional physical fields, namely the interface charge field \( \rho \) and the associated induced normal currents \( J_{1/2}[\rho] \).

III. YEE-COMPATIBLE CORRECTIVE-CURRENT FDTD SCHEME

We now proceed to translate the equations derived in the previous section into a versatile and efficient FDTD scheme. In compliance with the standard Yee-scheme we integrate (5) and (12) in two distinct half-steps by first performing the electric field update

\[
\tilde{E}^{n+1/2} = \tilde{E}^{n-1/2} + \Delta t (1 - \langle \varepsilon_{\infty} \rangle)^{-1} \nabla \times H^n - \Delta t (1 - \langle \varepsilon_{\infty} \rangle)^{-1} (J^n [\tilde{E}^{n-1/2}] + \delta J^n_\parallel) \tag{13}
\]

and then the magnetic field update

\[
H^{n+1} = H^n - \Delta t \mu_0^{-1} (\nabla \times \tilde{E}^{n+1/2}) + \Delta t \mu_0^{-1} \delta K^{n+1/2} \tag{14}
\]

To keep the notation compact, we implicitly assume that \( \tilde{E}^{n+1/2} \) and \( H^n \) are \( 3N \)-dimensional vectors (\( N \) being the number of Yee-cells) aggregating the electric and magnetic field components on the staggered subgrids across the problem domain. In this formulation the curl-operator \( \nabla \times \) is a matrix that performs a stencil operation at each point of either the electric or magnetic subgrid. Note, that discretization turns the inverse of the volume averaged permittivity \( \langle \varepsilon_{\infty} \rangle^{-1} \) (a scalar field) into a 3N x 3N dimensional diagonal matrix, which can be precalculated by volume-averaging the permittivities at the various positions of the Yee-cube. In a similar way \( J^n [\tilde{E}^{n-1/2}] \) can be obtained by weighting the contributing current vectors \( J^n \) with the matrix of precalculated cell-filling factors \( f_i \). It is important to note that the treatment of dispersive currents requires a preceding evaluation of the response functionals \( J^n [\ldots] \) by either integrating appropriate auxiliary differential equations (e.g., for the Lorentz pole) \( \mathbb{I} \) or by using the piecewise linear recursive convolution (PLRC) method \( \mathbb{L} \).

Following the arguments laid out in the previous section it is clear that the corrective currents \( \delta J^n_\parallel \) and \( \delta K^{n+1/2} \) vanish whenever the material constants vary smoothly across cells. For these volume cells \( \tilde{E} \rightarrow \tilde{E} \) and the update equations reduce themselves to the dispersive VA FDTD method, which, as \( \langle \varepsilon_{\infty} \rangle^{-1} \) is diagonal can be efficiently integrated using the standard Yee-scheme. Within interface cells, on the other hand, \( \tilde{E} \) differs from the electric field \( \mathbf{E} \) and a corrective step is necessary to accurately account for the discontinuity of the normal field component. As shown before the discontinuity in the normal component is directly proportional to the surface charge density \( \rho \) induced at the interface. Discretizing (10) results in an update equation for \( \rho \)

\[
\rho^{n+1/2} = \rho^{n-1/2} + \Delta t (f_1 f_2) \left( \zeta_2^{-1} J_{1/2}^n - \zeta_1^{-1} J_{1/2}^n \right) \tag{15}
\]

that requires evaluation of the currents \( J_{1/2}^n \) according to (9).

In difference to the electromagnetic field components, which are evaluated on the Yee-grid, \( \rho \) is a cell-centered quantity. We therefore need to introduce operators to interpolate between the Yee- and cell-centered grids. Figure (2) illustrates the action of the Y and C interpolation operators (left and right panel) together with the projection operator \( P \) (center panel). Applied to write (9) this yields

\[
J_{1/2}^n = \zeta_1^{-1} \langle \varepsilon_{\infty} \rangle^{-1/2} (P \langle \varepsilon_{\infty} \rangle J_{1/2}^n [\tilde{E}^{n-1/2}] \pm f_1 f_2 S_{2/1} J_{1/2}^n [\rho^{n-1/2}]) \tag{16}
\]

This expression recycles the previously calculated \( J_{1/2}^n \) currents on the Yee-grid but introduces a charge-current \( J_{1/2}^n [\rho^{n-1/2}] \) that, using the same current-functional, is evaluated at the cell center. To improve smoothness of the fields under the projection/interpolation operation we multiply \( J_{1/2}^n \) with the \( \langle \varepsilon_{\infty} \rangle \) tensor, which is already available on the Yee-grid. In contrast, the coefficients \( \zeta_1/2, \varepsilon_{\infty}^{-1/2}, f_1^{-1} \) and the face-normal \( \mathbf{n} \) are parameters that are defined at the cell-center (see Fig. 3). As \( \mathbb{L} \) can be evaluated on-the-fly, the only additional physical fields that need to be stored at the cell-center are \( \rho \) and its induced currents \( J_{1/2}^n [\rho^{n-1/2}] \). With the surface charge and its currents known, it becomes possible to compute the corrections \( \delta J_\parallel \) and \( \delta K^{n+1/2} \) that enter the update equations (13) and (14). However, the order of operators (and hence the discretization) is ambiguous, and,
**Algorithm 1** Sequence of field updates (VA+CC)

- **n+1/2 (on Yee-grid):**
  - VA: update $\tilde{E}^{n+1/2} \rightarrow \tilde{E}^{n+1/2}$ w/o $\delta J_{\perp}^n$ [13]
  - CC: add correction $\delta J_{\perp}^n$ [17]
- **n+1/2 (on centered-grid):**
  - CC: update $\rho^{n+1/2} \rightarrow \rho^{n+1/2}$ [14]
  - CC: evaluate $J_{\perp}^{n+1}[\rho^{n+1/2}]$ (for next cycle)
- **n+1 (on Yee-grid):**
  - VA: evaluate $J_{\perp}^{n+1}[\tilde{E}^{n+1/2}]$ (for next cycle)
  - VA: update $H^n \rightarrow H^{n+1}$ w/o $\delta K_{||}^{n+1/2}$ [14]
  - CC: add correction $\delta K_{||}^{n+1/2}$ [18]

as the scheme is corrective, can impact on the stability of the scheme. A numerical analysis of the computational errors suggests that $J_{\perp}^{1/2}$ is best multiplied with the $\langle \varepsilon_{\infty} \rangle$ tensor before centering to the grid. This is due to the fact that the normal component of $\langle \varepsilon_{\infty} \rangle \tilde{E}$ retains smoothness across adjacent cells with different $\varepsilon_{\infty}$. Further, to maintain consistency between the Yee and cell-centered update equations [13], [14] and [15] we assign parameters as indicated by Fig. 8. This allows us to write

$$
\langle \varepsilon_{\infty} \rangle^{-1} \delta J_{\perp}^n = - \langle \varepsilon_{\infty} \rangle^{-2}(f_1 \text{YPc}(\varepsilon_{\infty})J_{\perp}^n - f_2 \text{YPc}(\varepsilon_{n}))J_{\perp}^n + \gamma n f_1 J_{1n}^n + \gamma n f_2 J_{2n}^n
$$

(17)

where volume filling factors in the first line are applied after centering onto the Yee-grid, and, for the second line, directly at the cell-center.

The discretization of the magnetic current requires both terms in (11) to be interpolated to the center before spreading them out again onto the Yee-grid. We obtain

$$
\delta K_{||}^{n+1/2} = \nabla \times \delta \tilde{E}_{\perp}^{n+1/2}
$$

(18)

with

$$
\delta \tilde{E}_{\perp}^{n+1/2} = (Y(\varepsilon_{\infty}^{-1}) - \langle \varepsilon_{\infty} \rangle^{-1}Y)\text{PC}(\varepsilon_{\infty})\tilde{E}_{\perp}^{n+1/2}
$$

(19)

Fundamentally, both the electric and magnetic current corrections can be calculated on-the-fly. As the corrections only apply to interface cells, they can be added in a separate step to the update equations. This means that the update equations of the VA FDTD scheme can be deployed across the whole grid, followed by oversampling processes that perform the current-corrections (CC) for interface cells only. The complete update sequence for the VA+CC algorithm is shown in Alg. 1.

As each step can be associated with a loop over cells, it becomes evident that the current-correction (CC) steps augment those related to the VA FDTD scheme. As the CC steps only apply to interface cells, the computational overhead of the VA+CC FDTD scheme is not significant unless the number of interface cells becomes comparable to the number of volume cells.

IV. RESULTS

To verify the accuracy of our method we compare our numerical calculations with the Mie scattering cross section of an infinitely extended strongly dispersive cylinder excited by a TM plane-wave. Although the calculations presented here are 2D, the derived equations and algorithms are also valid in 3D. The dielectric function describing the response of the cylinder consists of a single Lorentzian resonance at $\lambda_0^{-1} = 0.25R$ and a background dielectric constant of $\varepsilon_{\infty} = 4$, where $R$ is the radius of the cylinder. Figure 3 shows real and imaginary parts of the complex permittivity $\varepsilon(\lambda^{-1}) = \varepsilon'(\lambda^{-1}) + i\varepsilon''(\lambda^{-1}) = \varepsilon_{\infty} + 2.5\lambda_0^{-2}(\lambda_0^{-2} - \lambda^{-2} - i0.05\pi^{-1}\lambda^{-1})^{-1}$ together with the analytically calculated scattering cross-sections for scatterers with and without the dispersive contribution $\chi(\lambda^{-1})$ (Fig. 2d).

The numerical setup of the 2D calculation is depicted in Fig. 4. A Total-Field-Scattered-Field (TFSF) box is used to inject pulses with $E_{inc}(r,t) = E_0 A(t) \exp(-i\omega t + ik \cdot r)$ with temporal envelope $A(t)$, polarisation $E_0$ and center frequency $\omega = c|k|$ into the system in direction of $k$ (where $k \perp E_0$). To minimize the error from numerical dispersion we take into account the numerical phase velocity at the center frequency for the given angle of incidence and chose a sufficiently narrow-band excitation. The energy flux $\mathbf{E} \times \mathbf{H}$ of the scattered field is recorded at the boundary of a box located outside of the TFSF box. The computational region is terminated with perfectly matched layers (PML) which nearly completely attenuate any reflections caused by the computational boundary. After the simulation, the scattering spectrum can be retrieved by Fourier-transforming the fields recorded at a closed surface outside of the TFSF box (marked with DIAG in Fig. 5).

Figure 5 (top) shows the difference between the analytic and numerical scattering cross sections obtained by numerical simulation with a resolution of eight Yee-cells per cylinder radius. The results of the VA+CC FDTD scheme (dashed red line) are in better agreement with the analytical calculation than the VA FDTD scheme (dotted green line) throughout the
spectrum. For comparison, the result of a simple staircased FDTD scheme was included in the figure (dash-dotted blue line). By selectively disabling either the current correction $\delta J_\perp$ or $\delta K_\parallel$ and subtracting the result from the VA FDTD scheme, the contributions of the charge corrections to the spectrum were quantified (Fig. 5b). The contribution $\delta J_\perp$ shows a prominent peak at a frequency which is slightly offset to the resonance frequency of the Lorentzian (indicated by the vertical dotted line). To illustrate the spatial dependence of the corrections and the charge density we plot contour images of the charge field $\rho$ (Fig. 6b), the energy density of the electric correction $\delta J_\perp \cdot E$ (Fig. 6c), and the energy density of the magnetic correction $\delta K_\parallel \cdot H$ (Fig. 6d). Whereas the corrections associated with the charge density and electric field correction are stored at the cell center, the correction associated with $\delta K_\parallel \cdot H$ is calculated from Yee-centered quantities and therefore appears to be smeared out over several adjacent cells.

To investigate the convergence behavior of the charge correction algorithm, numerical simulations with increasing resolution $N$ were conducted for incident angles of 0° and 30°. The RMS error for each simulation was obtained, by comparing the numerical scattering cross section spectrum with the analytical result (Fig. 7b). The overall error reduction is achieved by the combined action of the corrections $\delta J_\perp$ and $\delta K_\parallel$ as shown in Fig. 7b. The VA (green diamonds) and the staircasing (blue circles) FDTD scheme produce errors that are significantly larger than those of the VA+CC scheme (red squares), whose RMS error decreases with $\propto N^{-2.0}$. For higher resolutions the decrease in error saturates, which may be attributed to error contributions from the PMLs. We therefore conclude that for this particular system VA+CC is approximately second order accurate and consistently achieves lower errors than the VA scheme.

Finally, we compare the computational cost (memory and processing time) for the different schemes. The results are summarized in Fig. 8. The staircasing scheme only requires the static epsilon $\varepsilon_{\infty}$ at each Yee-cell position of the $E$-field and the three vectorial fields $E, H, J_1$. The VA algorithm additionally stores the filling factors $f_1$ at each Yee-cell position of the $E$-field. The VA+CC scheme is identical to the VA scheme for non-interface cells requiring 15 scalar components. At interface cells the VA+CC scheme requires an additional 7 scalar components for storing $\rho, J_1[\rho], n, f_1$ and $\varepsilon_{\infty,1/2}$. The comparsion of computation time indicates an almost identical performance for the staircase and VA schemes. VA+CC delivers the same performance for volume cells but requires additional computational steps for interface cells, resulting in $\approx 50\%$ overhead in the per cell processing time. These overheads seems significant but rarely matter for practical applications as the surface to volume ratio is typically
small. For the Mie scattering simulations presented in Fig. 5 for example (8 cells per radius) the increase in computation time of the VA+CC algorithm is < 1% (compared to VA) as the interface/volume cell ratio is ≈ 0.6%.

V. CONCLUSION

In summary we presented an effective-medium theory that takes a corrective approach to the cell-averaged Maxwell’s curl equations. The theory holds for static and linear dispersive permittivities and captures the field discontinuities inside a cell in form of surface current corrections, which can be calculated by integrating a surface charge equation alongside the volume-averaged curl equations. We derived a computationally efficient FDTD algorithm that allows deploying the standard Yee-algorithm across the domain followed by surface current corrections that selectively apply at interface cells. The improvement in accuracy is quantified by calculating spectral scattering cross-sections of strongly dispersive Mie scatterers. The extracted error exponents indicate that the algorithm approximately restores second order accuracy. The work presented is relevant in the current context of nanophotonic research and may pave the way to the development of novel perturbative techniques for solving Maxwell’s equations.

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