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Describing discontinuous finite 3D scattering objects in Gabor coefficients: fast and accurate methods

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In relation to the computation of electromagnetic scattering in layered media by the Gabor-frame-based spatial spectral Maxwell solver, we present two methods to compute the Gabor coefficients of the transverse cross section of three-dimensional scattering objects with high accuracy and efficiency. The first method employs the analytically obtained two-dimensional Fourier transform of the cross section of a scattering object, which we describe by two-dimensional characteristic functions, in combination with the traditional Discrete Gabor Transform method for computing the Gabor coefficients. The second method concerns the expansion of the so-called dual window function to compute the Gabor coefficients by employing the divergence theorem. Both methods utilize (semi)-analytical approaches to overcome the heavy oversampling requirement for the traditional Discrete Gabor Transform methods in case of discontinuous functions. Numerical results show the significant improvement in terms of accuracy and computation time for these two methods against the traditional Discrete Gabor transform method.

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1. INTRODUCTION

The aim to further reduce the size of semiconductor devices to improve properties such as data storage [1, 2] has let to stringent demands on the lithographic production process variations [3]. Consequently, the computational characterization of electromagnetic scattering from dielectric objects embedded in a layered medium, i.e. the wafer, in an accurate and computationally efficient manner is important, since it enables non-destructive monitoring techniques, such as scatterometry, to evaluate these production process variations. The spatial spectral three-dimensional (3D) Maxwell solver presented in [4] fits this lithographic setting, because it computes the scattering of electromagnetic fields by dielectric objects in a planarly layered media. This spatial spectral 3D Maxwell solver makes use of an analytical Green function in the spectral domain for planarly layered media, which provides an efficient analytical way to compute the electromagnetic response of the layered medium, without having to include it in the computational domain. Consequently, a suitable domain of applicability for this type of solvers concerns lithographic metrology, e.g. scatterometry, due to the appearance of planarly layered media.

The spatial spectral 3D Maxwell solver is based on a volume integral equation and is characterized by its formulation in both the spatial and spectral domain simultaneously. The mixed-domain representation allows to incorporate the transverse translation symmetry induced by the layered medium such that we can use spectral-domain analytical expressions for the Green function corresponding to the layered medium. The second important characteristic is the Gabor-frame expansion, which is employed parallel to the interfaces of the layered medium. A Gabor-frame expansion is a technique to describe square-integrable functions, which can represent images, physical fields, or scattering objects, as a weighted combination of shifted and modulated window functions [5, 6]. This expansion allows fast and analytical Fourier transformations in the form of scalar multiplications. Consequently, the volume integral equation is solved in both the spatial and spectral domain simultaneously due to the Gabor-frame expansion: the field-material interaction is computed in the spatial domain and the Green function operation is computed in the spectral domain. The latter allows to compute a single matrix-vector product in a $O(N \log(N))$ steps where $N$ is the total number of unknowns in the problem, thus by using iterative methods an efficient solver is obtained. Overall, the Gabor-frame expansion is a crucial component within this solver.

In case of the spatial spectral 3D Maxwell solver, the Gabor coefficients of scattering objects are needed as part of the pre-processing stage for computing the scattered electromagnetic field. A Gabor coefficient is the appropriate weighting coefficient of a window function in a Gabor frame [7]. So, it can be seen as the Gabor-frame counterpart of the well-known Fourier coefficient. The computation of these Gabor coefficients for arbi-
tarily shaped 3D object turns out to be computationally intense. To address this issue in a more general sense, we assume that the scattering objects are piecewise homogeneous and we sample it in the stacking direction of the layered medium, which is indicated by the \( z \) direction here. This results in a number of transverse cross sections, i.e. \( xy \)-slices, for each scattering object. Each cross section of an object can be viewed as a discontinuous two-dimensional (2D) characteristic function that acts as a piecewise homogeneous permittivity distribution with respect to the background medium. The Gabor coefficients of these specific characteristic functions are required for the solver. Fig. 1 provides a graphical example of such a characteristic function. This figure is fairly similar to a binary image, since the characteristic function in this example has a value equal to one inside the domain of the scattering object in an \( xy \)-slice and zero outside. Naturally, this characteristic function can be scaled to represent any piecewise homogeneous permittivity distribution or contrast.

There are various methods [5, 8, 9] to compute the Gabor coefficients by applying a so-called Discrete Gabor Transform (DGT). A DGT utilizes a Zak transform to convert the original function into a quasi-periodic version of it [8]. Subsequently, the DGT employs Discrete Fourier Transformations (DFTs) to numerically approximate the Gabor-coefficient integrals on an uniform grid [8]. For infinitely smooth functions, the DFT algorithms exhibit exponential convergence [10]. However, it is reported in [p. 209, 11] that applying the DGT algorithm of [8] on a discontinuous one-dimensional (1D) function already requires heavy oversampling of a factor of a thousand or more to obtain the Gabor coefficients with 3 digits of accuracy. This heavy oversampling is very time-consuming. Quite similarly, [10] indicates that DFT-based integration on discontinuous 1D functions converges as \( O(N^{-1}) \) in terms of accuracy if \( N \) represents the number of samples. This is coupled to an equidistant sampling grid, which does not provide the means to accurately capture discontinuities in a computationally efficient manner. A faster and more accurate way to compute the Gabor coefficients of the cross sections of scattering objects would significantly reduce the computation time required for the pre-processing stage and it would improve the general applicability of the spatial spectral solver.

To achieve this goal, we introduce two methods for the fast and accurate computation of Gabor coefficients of a cross section of a scattering object defined as a discontinuous 2D characteristic function with a domain in the form of an arbitrary simple polygon. The first method utilizes the 2D Fourier transformation of a discontinuous 2D characteristic function to overcome the slow convergence of the current DGT approaches in the spatial domain, by computing the Gabor coefficients in the spectral domain. The second method is based on expanding the so-called dual window using a Gabor-frame expansion. This expansion allows to incorporate semi-analytical methods for accurate and efficient computation of the Gabor coefficients. These two methods are subsequently subjected to a benchmark consisting of these two methods, supplemented with the original DGT [8]. This benchmark is used to evaluate the computation of Gabor coefficients for two different scattering objects by the three methods, in terms of accuracy versus number of function evaluations and in terms of accuracy versus computation time. Lastly, we demonstrate the performance gain on a grating example consisting of 36 scattering objects in combination with the spectral spectral 3D Maxwell solver while using the spectral transformation method. We show that the computation of the Gabor coefficients of the scattering objects is no longer the main bottleneck for the computation time for such a case.

2. GABOR COEFFICIENTS OF A SCATTERING OBJECT

The starting point is describing the cross section of a scattering object by a discontinuous 2D characteristic function \( f(x) \) as

\[
f(x) = \begin{cases} 
1 & x \in D \\
0 & x \in \mathbb{R}^2 \setminus D 
\end{cases}
\]  

where domain \( D \) represents a simple polygon for which we want to expand this function in Gabor frames. The vector \( x \) is defined as \( x = (x, y) \). We utilize a polygon description similar to [12], which means that only the vertices of a polygon are used to describe the domain \( D \), its boundary gradient, and the boundary normals. The description of a polygon with \( L \) vertices is defined by the sequence of the coordinates of its vertices, i.e. \( x_i = (x_i, y_i) \), for \( i = 1, 2, \ldots, L \) that are traversed in a counter-clockwise fashion. Fig. 1 shows an example following this definition, given that only the vertices were used to construct the complete polygon by connecting the subsequent vertices with a line segment. Noteworthy, this polygon description is independent of the discretization used on the cross section of a scattering object to sample it, which means that the polygon description provides sub-pixel resolution.

We continue by introducing the Gaussian window function [8] that we use for the Gabor frames, i.e.

\[
\tilde{g}(x) = \sqrt{2} \exp \left( -\frac{x^2}{\alpha^2} - \frac{y^2}{\beta^2} \right).
\]

\( X \) and \( Y \) control the spatial width of the window function in the \( x \)-direction and \( y \)-direction, respectively. It is possible to use other window functions for the Gabor frame [13]. However, we only focus on the frequently used Gaussian window function, since it enables exponential decay for the dual window [14, 15]. The Gaussian window function is used to define the 2D Gabor frames as

\[
\tilde{g}_{mn}(x) = \tilde{g}(x - m\alpha X, y - m\beta Y) \cdot \exp \left( j\beta n_1 K_x x + j\beta n_2 K_y y \right),
\]

where \( \alpha \) and \( \beta \) are the spatial frequencies in the \( x \) and \( y \) directions, respectively. \( K_x \) and \( K_y \) are the wavenumbers in the \( x \) and \( y \) directions, respectively. \( n_1 \) and \( n_2 \) are the sub-pixel coordinates in the \( x \) and \( y \) directions, respectively.

Fig. 1. An example of a cross section of a scattering object in the form of a characteristic function given the definition of Eq. (1), while using a polygon description similar to [12].
where the indices $m = (m_x, m_y)$ and $n = (n_x, n_y)$ represent spatial shifts and modulations in the subscripted directions, respectively. The following modulation parameters are expressed as $K_x = 2\pi / X$ and $K_y = 2\pi / Y$. The oversampling parameters satisfy $\alpha_x \beta_x < 1$ and $\alpha_y \beta_y < 1$ [8]. Another important function within the theory of Gabor frames is the so-called dual window $\eta(x)$, which is necessary to compute the Gabor coefficients [8][pp. 55-69, 11]. The link between the dual window $\eta$ and its shifted and modulated version $\eta_{mn}$ is

$$
\eta_{mn}(x) = \eta(x - m_y \alpha_y X, y - m_y \alpha_y Y) \cdot \exp\left(j \beta_x m_y K_x x + j \beta_y m_y K_y y \right).
$$

(4)

Methods for obtaining this dual window can be found in the literature [8][pp. 55-69, 11]. The choice for $\eta(x)$ fixes the Gabor coefficients to a unique choice.

The Gabor frames in Eq. (3) allow to represent the cross section of a scattering object by a discontinuous 2D characteristic function as

$$
f(x) = \sum_m \sum_n c_{mn} \eta_{mn}(x),
$$

(5)

where $c_{mn}$ represent the Gabor coefficients of $f(x)$. These coefficients are obtained by

$$
c_{mn} = \int_{R^2} f(x) \eta^{*}_{mn}(x) dx,
$$

(6)

where $*$ denotes complex conjugation. Equation Eq. (6) can also be rewritten as

$$
c_{mn} = \frac{1}{|D|} \int_{D} \eta^{*}_{mn}(x) dx,
$$

(7)

when $f(x)$ is a characteristic function on domain $D$ as defined in Eq. (1).

3. SPECTRAL TRANSFORMATION METHOD

It is desirable to employ the computational efficiency of the DGT [8] for the expansion in Gabor frames of a scatterings object by discontinuous 2D characteristic functions as in Eq. (1), i.e. a computational complexity scaling as $O(N \log N)$, with $N$ the number of Gabor coefficients. However, the accuracy of the DFT-based numerical integration by trapezoidal rule with equidistant sampling convergences as $O(N^{-1})$ in case of a discontinuous function, where $N$ represents the number of function samples [10]. Moreover, Theorem 5.1 of [16] states that the accuracy of the trapezoidal rule can be analyzed by means of the Poisson summation formula of the Fourier transform of the function to be integrated, which is in this case a discontinuous 2D function. The Fourier transform of a discontinuous 2D characteristic function has an asymptotic decay of $O(|k|^{-1})$ with $k = (k_x, k_y)$. Consequently, the Fourier transform of the discontinuous 2D characteristic function does not decay to zero rapidly enough to yield fast convergence of the trapezoidal rule.

However, owing to the analytically available Fourier transform of the Gabor window, we can also apply this DGT method on the Fourier transform of the discontinuous 2D characteristic function, such that we obtain the spectral version of the Gabor coefficients. This approach ensures that the accuracy of the trapezoidal rule is coupled to the Poisson summation of the discontinuous 2D characteristic function itself, which has a clearly defined finite support by assumption. This ensures that the impact due to aliasing reduces to zero, since sampling outside domain $D$ always gives a function evaluation equal to zero. The remaining conversion of the spectral Gabor coefficients to the spatial Gabor coefficients is an almost trivial operation, which yields Gabor coefficients in the spatial domain without loss of accuracy [17]. The required analytical Fourier transformation of a discontinuous 2D characteristic function with a domain $D$ in the form of a simple polygon is described in [12, 18].

We now describe the steps to obtain the spatially defined Gabor coefficients with this method. Our starting point is denoting the spectral equivalent of Eq. (6) and the scalar multiplication necessary for performing a Fourier transformation on the Gabor coefficients. The spectral Gabor coefficients can be computed by

$$
\hat{c}_{mn} = \int_{R^2} \hat{f} (k) \hat{\eta}^{*}_{mn}(k) dk.
$$

(8)

where $k = (k_x, k_y)$. The hat symbol on each function is employed to indicate the spectral counterpart, e.g.

$$
\mathcal{F}_k [\hat{f} (k)](x) = f(x),
$$

(9)

where the symbol $\mathcal{F}_k [\cdot](x)$ represents a Fourier transformation from the spatial to the spectral domain evaluated at $x$. The subscripts $m$ and $n$ in the spectral domain represent spectral shifts and modulations, respectively. A Fourier transformation for converting the spectral Gabor coefficients to the spatial Gabor coefficients can be achieved by using the following Gaussian window function in the spectral domain

$$
\hat{g}(k) = \sqrt{2XY} \exp\left(-\frac{k_x^2}{X_k^2} - \frac{k_y^2}{Y_k^2}\right),
$$

(10)

while we define

$$
\hat{g}_{mn}(k) = \hat{g}(k_x - m_x \alpha_x K_x, k_y - m_y \alpha_y K_y) \cdot \exp\left(-j \alpha_x m_x K_x x - j \alpha_y m_y K_y y\right),
$$

(11)

Accordingly, the Fourier transform for our Gabor frame has the following form

$$
\hat{c}_{mn} = c_{mn} \exp\left[-j 2\pi (\alpha_x \beta_x m_x \alpha_y + \alpha_y \beta_y m_y \nu_y)\right].
$$

(12)

The current form of Eq. (8) allows to apply the DGT algorithm as in [8], such that afterwards we can use Eq. (12) to obtain the spatial Gabor coefficients. However, this complete procedure requires to have the spectral equivalent of the discontinuous characteristic function as in Eq. (1). The initial step to obtain the spectral version of this characteristic function is by defining the cross section of a scattering object of interest by its vertices as previously mentioned in Section 2. This ensures that we obtain the corresponding characteristic function with domain $D$ [12].

The following step is to define the Fourier transformation of this characteristic function, which is equal to

$$
\hat{f}(k) = \int_D \exp(j k \cdot x) dx.
$$

(13)

In [18] a way is provided to transform this 2D integral into a sum of line integrals along the edges of the polygon by using Gauss’s divergence theorem. This transforms Eq. (13) into

$$
\hat{f}(k) = -\int_{\partial D} \hat{f}(k \cdot \nu) \frac{\exp[j (k \cdot x)]}{\nu \cdot k} d\ell,
$$

(14)

where $\nu = (\nu_x, \nu_y)$ represents the outward pointing normal vector of the contour, $\partial D$, of polygon-shaped domain $D$. This boundary contour is traversed in the counter-clockwise direction.
The polygon description induces that Eq. (14) has a boundary contour defined by the line segments between the vertices. We employ the following parametrization for a line segment $\ell_{i}$ between the vertices $x_{i}$ and $x_{i+1}$ by $x_{i+1}(t) = [x_{i+1}^{1}(t), y_{i+1}^{1}(t)]$

$$x_{i}^{1}(t) = x_{i+1}^{1} \cdot t + x_{i}^{1} \cdot (1-t), \quad (15)$$

where $t \in [0, 1]$. This parametrization of the line segments changes Eq. (14) into

$$\tilde{f}(k) = -\sum_{i=1}^{l} \int_{0}^{1} j(k \cdot v_{i+1})(x_{i+1} - x_{i}) \exp \left( j(k \cdot x_{i}) \right) \frac{\exp \left[ j(k \cdot x_{i+1} - x_{i}) \right]}{j(k \cdot k) \left( k \cdot (x_{i+1} - x_{i}) \right)} dt$$

$$= -\sum_{i=1}^{l} \int_{0}^{1} j(k \cdot v_{i+1})(x_{i+1} - x_{i}) \exp \left( j(k \cdot x_{i}) \right) \left[ \frac{\exp \left[ j(k \cdot x_{i+1} - x_{i}) \right]}{j(k \cdot k) \left( k \cdot (x_{i+1} - x_{i}) \right)} \right] dt. \quad (16)$$

The previously defined normal vector $v$ becomes $v_{i+1}$, since the normal for each line integral only depends on the vertices $x_{i}$ and $x_{i+1}$. We note that the final result in Eq. (16) has a term-wise removable singularity when $k \cdot (x_{i+1} - x_{i}) \to 0$. Additionally, the result has a somewhat more complicated removable singularity for the entire sum at $k = 0$, which can be handled readily by inserting the total area of the cross section of the scattering object.

We continue by giving an example of the execution of this procedure for computing the Gabor coefficients of a cross section of a scattering object as a 2D discontinuous characteristic function. The initial step can be found in Fig. 2a, which displays the same cross section as seen in Fig. 1, for which we have defined all vertices of this polygonal cross section such that we can compute its Fourier transform as displayed in Fig. 2b. This Fourier transform is the input for the algorithm in [8]. This algorithm essentially performs a DGT or a so-called fast convolution to compute the Gabor coefficients. This fast convolution is used to perform the necessary Zak transforms by DFTs on both the characteristic function and the dual window. The resulting Gabor coefficients by the DGT algorithm are Fourier transformed as in Eq. (12) in order to be used to reconstruct the original shape in the spatial domain. This reconstruction is displayed in Fig. 2c. The ringing effect in Fig. 2c originates from reconstructing a discontinuous function from a finite number of Gabor coefficients [4, 17, 19] and it is analogous to the Gibbs phenomenon observed in reconstructing a discontinuous function from a finite number of Fourier coefficients [20].

We have not yet mentioned that the spectral transformation method is flexible in the sense that it does not depend on the particular choice for the window function and its dual. The main requirement for this method is that a choice for a particular dual window function has been fixed beforehand. In practice, we prefer the use of the Gaussian window function, since it exhibits exponential decay for the dual windows in case of oversampling [15, 19], i.e.

$$|\eta(x)| < C_{1} \exp(-|x|), \quad (17)$$

and

$$|\eta(k)| < C_{2} \exp(-|k|), \quad (18)$$

The parameters $\lambda_{1,2} > 0$, as expressed in [Proposition 1, Eq. (3.4) 14], are linked to the decay of the window function and the oversampling parameters. Further, $C_{1,2}$ are constants. Note that $\lambda_{1,2}$ are defined as $a$ in [Proposition 1, Eq. (3.4) 14]. We changed this notation, since the letter $a$ is already reserved in this paper for the spatial oversampling. It is shown as an example in [21] that the dual window of a Gaussian window function has decay properties similar to $\exp (-\pi|x|/\beta_{x})$ in case of $(\alpha_{x}\beta_{x})^{-1} = q$ for a given even positive integer $q$. The exponential decay of the dual windows induces exponential convergence in Eq. (8) by the trapezoidal rule approximation. This exponential convergence of the trapezoidal rule is important to arrive at an efficient method for computing the Gabor coefficients. Therefore, we give a proof concerning this exponential convergence in the Appendix.

4. DUAL WINDOW EXPANSION METHOD

Analytical integration techniques provide the advantage of computational accuracy. However, the dual window as obtained in [8][pp. 55-69, 11] is only available in sampled form, instead of given as an analytical expression. This means that we cannot directly perform (semi)-analytical techniques on Eq. (7) to obtain the Gabor coefficients. Therefore, we expand the dual window $\eta(x)$ in terms of the original window functions of the Gabor frame [22], since the Gaussian window function is an analytical function and the Gabor frame is complete. This decomposition of the dual window results in

$$\eta(x) = \sum_{rs} c_{rs} S_{rs}(x), \quad (19)$$

where $c_{rs}$ represents a Gabor coefficient of the dual window. We combine Eq. (7) and Eq. (19) to obtain

$$c_{mn} = \sum_{rs} c_{rs} I_{m+n+r,-(n+s)} \cdot \exp \left[ 2\pi j(s_{x}m_{x}\alpha_{x}\beta_{x} + s_{y}m_{y}\alpha_{y}\beta_{y}) \right]. \quad (20)$$

The $I_{m,n}$ symbol represents the integral that needs to be computed, which is given by

$$I_{m,n} = \int_{D} S_{mn}(x) dx. \quad (21)$$

The added comma in Eq. (20) is used to emphasize that the spatial shift of the Gaussian window function is set by $m + r$, while the modulation is subjected to $-n - s$. So, the dual window expansion method for obtaining the Gabor coefficients boils down to efficiently integrating modulated Gaussian window functions projected onto the polygon-shaped domain $D$. It is important to note for computational efficiency that the summation over $r$ and $s$ in combination with variations in $m$ and $n$ results in the exact same integral several times for different combinations of these parameters. So, to minimize the workload it is required to define all unique $m_{x} + r_{x}, n_{x} + s_{x}, m_{y} + r_{y}, n_{y} + s_{y}$ values in Eq. (21), given the Gabor coefficients in Eq. (20). A remaining step to perform is to determine the integral in Eq. (21).

A. Rectangular integration domain

An analytical solution is available for the special case of a rectangular domain aligned with the x- and y-directions. The relevant integral and its solution in case of this specifically defined domain can be found in [Eq. (2.33.1), 23], in terms of error functions. This solution relies on Fubini’s theorem [24] to rewrite the 2D integral as the multiplication of two independent 1D integrals, owing to the separability of the 2D Gaussian window function into the product of two Gaussian window functions in each of
We now continue by showing how to compute $z$. The definitions are only given for the components with subscript $i$. The error function is denoted by erf.

The definitions are only given for the components with subscript $x$. The same definitions also hold for the components with subscript $y$, but it requires to replace all $x$ subscripts by $y$ and by substituting window width $X$ by $Y$. The error function is denoted by erf.

For numerical stability of the expressions, it is important to note that an implementation of the analytical solution benefits from rewriting the error function in terms of the Faddeeva function if the imaginary part of the argument becomes dominant. This is related to the diverging behavior of the error function in the complex plane for arguments from $\frac{3\pi}{4}$ to $\frac{5\pi}{4}$ and from $-\frac{3\pi}{4}$ to $-\frac{5\pi}{4}$. The necessary conversion from the error function to the Faddeeva function [25] is given by

$$\text{erf}(z) = \begin{cases} 1 - e^{-z^2} w(jz) & \text{Re}(z) \geq 0 \\ e^{-z^2} w(-jz) - 1 & \text{Re}(z) < 0, \end{cases}$$

where $z$ represents an arbitrary complex number and the Faddeeva function is denoted by $w(z)$.

### B. General polygonal integration domain

We now continue by showing how to compute $I_{m+r,-(n+s)}$ in Eq. (22) in case of a general $L$-sided polygon. The main idea here is to again employ Gauss’s theorem to transform Eq. (21) into a sum of line integrals along its piecewise-linear boundary. We start from the proposed splitting

$$I_{m+r,-(n+s)} = \oint_{\partial \Omega} P(x,y) + Q(x,y) d\ell,$$  \hspace{1cm} (26)

where

$$P(x,y) = -\frac{Y}{4} \exp \left[ h_y - h_{dx}(x) \right] \text{erf}[h_{cy}(y)],$$ \hspace{1cm} (27)

$$Q(x,y) = \frac{X}{4} \exp \left[ h_x - h_{dy}(y) \right] \text{erf}[h_{cx}(x)],$$ \hspace{1cm} (28)

with $h_{dx}(x) = \frac{\pi}{\sqrt{2}} (x - \alpha_s (m_s + r_s)X)^2 + j\beta_s K_s (n_s + s_s) x$.

Yet again, switching the subscript $x$ with $y$ gives the expression for $h_{dy}(y)$. We continue by applying the same parametrization as in Eq. (15) to $x$ and $y$ coordinates along each line segment $\ell_i$ between vertices $x_i$ and $x_{i+1}$. However, we scale all coordinates as $X_i^{j+1} = [X^{-1} x_i^{j+1}(t), Y^{-1} y_i^{j+1}(t)]$. We combine Eq. (26) and the scaled version of Eq. (15), such that we obtain

$$I_{m+r,-(n+s)}^{poly} = \sum_{i=1}^{M} \int_{0}^{1} P[X^{-1} x_i^{j+1}(t), Y^{-1} y_i^{j+1}(t)] + Q[X^{-1} x_i^{j+1}(t), Y^{-1} y_i^{j+1}(t)] dt.$$ \hspace{1cm} (30)

We are not aware of a closed form for Eq. (30). To compute the remaining line integrals we employ numerical quadrature methods.

### 5. BENCHMARK RESULTS

We start this section regarding the benchmark tests and results by describing the general implementation details.

#### A. Implementation details

We use MATLAB 2019a on an Intel core i7-8850H processor with 16 GB of RAM. We use the implementation for the error function for complex arguments from [26] and the Faddeeva function from [27]. The parameters for the Gabor frame are specified in Table 1. The dual window for the comparison tests was calculated as described in [11]. We use the same dual window for all methods within this comparison. This means that we also
decompose the computed dual window into Gabor coefficients, which is possible by using the DGT algorithm of [8] on the dual window itself. Using the same dual window ensures that all methods converge to the same Gabor coefficients.

B. Numerical integration scheme

We start by examining which numerical integration scheme is the most suitable for computing the integral in Eq. (30), in the sense of minimizing the relative error while requiring the least number of samples. We tested various numerical integration schemes on a cross section of a square scattering object, since we have an analytical reference solution for this, see Section 4A. The integrals are computed for $m_x + r_x, m_y + r_y \in \{ -10, \ldots, 10 \}$ and $n_x + s_x, n_y + s_y \in \{ -15, \ldots, 15 \}$ for a discontinuous characteristic function with a square domain $D$ centered at the origin of the $xy$-plane with an edge length equal to 1. The definition of the error is set as

$$E_l = \sqrt{\frac{\sum_{n|r_{-}}(n+s)}{\sum_{n|r_{-}}(n+s)+I_{\text{rect}}}^2} \left[ I_{\text{mention}} - I_{\text{rect}} \right].$$  \hspace{1cm} (31)

Fig. 3 shows the error as in Eq. (31) as a function of the number of samples, for several numerical integration schemes. Gauss-Legendre quadrature is the method that reaches machine-precision with the smallest number of samples for each line segment of the boundary of the scattering object. Therefore, we use Gauss-Legendre quadrature for the upcoming benchmark in case of computing the integrals in Eq. (30).

C. Rectangular scattering object

The first type of characteristic function in the benchmark represents a rectangular scattering object. So, this characteristic function is defined by having a square domain $D$. The Gabor coefficients corresponding to this type of characteristic function were calculated with the vertices in $xy$-coordinates given by $(-0.5; -0.5), (0.5; -0.5), (0.5; 0.5), and (-0.5; 0.5)$. Next to that, the Gabor coefficients of the characteristic function of a square domain were also computed for an edge length of $\sqrt{10}$ and 10. This allows us to get more insight into the effectiveness of the Gabor coefficient methods with respect to area scaling.

An important advantage of this type of 2D characteristic functions is that the dual window expansion method combined with a rectangular domain $D$ provides an analytical solution. Therefore, we use the Gabor coefficients obtained by this specific method as our reference in this part of the benchmark.

The Gabor coefficients of this type of characteristic function are calculated for $m_x, m_y, n_x, n_y \in \{ -10, \ldots, 10 \}$. The expansion coefficients of the dual window are computed for $r_x, r_y, s_x, s_y \in \{ -40, \ldots, 40 \}$. Such a large number of dual window expansion coefficients ensures that the absolute difference between the original dual window and the reconstructed dual window in Gabor frames is smaller than $10^{-14}$. However, we only use these coefficients ranging from -20 up to 20. This truncation is such that we only compute the Gabor coefficients of the object for $m_x, m_y, n_x, n_y \in \{ -10, \ldots, 10 \}$. The accuracy of a computational method is defined by the error

$$E = \sqrt{\frac{\sum_{mn}|c_{mn}^\text{ref} - c_{mn}|^2}{\sum_{mn}|c_{mn}^\text{ref}|^2}}.$$

The reference Gabor coefficients are defined as $c_{mn}^\text{ref}$. The Gabor coefficients obtained by the computational methods are denoted as $c_{mn}$. Fig. 4a displays the error defined in Eq. (32) as a function of the number of samples taken for the rectangular scattering object and its scaled versions. This figure provides the insight that the dual window expansion with Gauss’s theorem requires the least number of samples regardless of the size for this type of characteristic function to reach near machine-precision error. The main reason for needing fewer samples with respect to the other methods is because it concerns a 1D numerical integration scheme, which only requires samples on the boundary of domain $D$, whereas the other two methods are 2D numerical integration schemes, which implies that the entire 2D domain $D$ has to be sampled. Consequently, the dual window expansion method requires less memory during the computation process, which is advantageous. The dual window expansion method claimed 111 MB of RAM, whereas the spectral transformation method and the method from [8] required approximately 7.4 GB at its finest sampling. This clearly demonstrates that the dual window expansion method with Gauss’s theorem is the preferred method if minimizing the memory usage is critical. This specific method also shows a linear scaling in terms of required number of samples when the test characteristic function with a square domain $D$ also increases linearly in edge length. The smallest version of this type of characteristic function requires 164 samples to reach an error of $10^{-14}$, while the enlarged versions require 524 samples and 1604 samples to reach a comparable error. This specific increase in the number of samples is close to the expected scaling factor of $\sqrt{10}$.

Fig. 4a also shows that the spectral transformation method becomes increasingly more accurate if the number of function evaluations increases. This improvement in performance is most notable when using more than $10^5$ function evaluations. An over-sampling factor of approximately 26 already provides an error.
Fig. 4. (a) The error as expressed in Eq. (32) regarding the rectangular cross section of the scattering object while increasing the number of samples in a log-log plot. (b) The error as expressed in Eq. (32) regarding the rectangular scattering object as a function of computation time in a log-log plot.

at the level of machine precision for the spectral transformation method. This is much less than the reported oversampling factor of $10^6$ for 3 digits accuracy when using the spatial approach from [8] for discontinuous 2D functions [pp. 209 11] (extrapolated from an oversampling of 1000 in 1D). It is also interesting to note that the scaling of the domain $D$ does not have a major impact on the error for the spectral transformation method. A further observation from Fig. 4a is that the spatial method from [8] clearly performs the worst. The smallest error achieved with this method is just below $10^{-2}$.

Fig. 4b displays the results regarding the computation time with respect to the error level achieved for each test object. These results are obtained by measuring the computation time of the results as shown in Fig. 4a. A first thing to note in Fig. 4b is that the spectral transformation method behaves similarly regardless of the size of the scattering object. The same observation can be made for the method of [8]. This is because they both use the same sample points, irrespective of the size of the object.

D. Polygonal scattering object

Up to this point, we only considered rectangular scattering objects, which are described by a cross section in the form of a characteristic function with a rectangular domain. These characteristic functions were chosen because of the availability of an analytical reference. We now continue with a more complicated scattering object with a cross section in the form of a compass cross with an area of approximately 1, see Fig. 5a. Consequently, we require a new reference to evaluate the performance as in Eq. (32) of the various methods for computing the Gabor coefficients. This new reference is constructed by using the Gabor coefficients of a heavily oversampled version of the spectral transformation method, i.e. approximately $10^7$ samples, which we verify by a comparison with the Gabor coefficients computed by the dual window expansion method with Gauss’s theorem with a total number of 8016 samples. This results in an error as in Eq. (32) of approximately $1.7 \cdot 10^{-14}$ between the two sets of
Fig. 5. (a) A scattering object in the form of a compass cross. The grey square markers display the vertices of the object, whereas the remaining part of this figure displays the results of reconstructing the characteristic function of this scattering object by the spectral transformation method with a total of $6.8 \cdot 10^6$ samples. (b) The error as expressed in Eq. (32) regarding the compass cross scattering objects as a function of computation time on a double logarithmic scale.

computed Gabor coefficients. We perform the exact same procedure for obtaining the reference Gabor coefficients for the same cross section when it is scaled by $\sqrt{10}$ in both the $x$-direction and $y$-direction.

This time we do not show the accuracy in terms of the number of samples, since the method for obtaining the reference Gabor coefficients already expresses that the dual window method with Gauss’s theorem is superior, i.e. $8016$ samples versus $10^7$ samples. Fig. 5b displays the results regarding the computation time with respect to the error achieved. Both the spectral transformation method and the dual window method require approximately the same computation time to achieve near machine-precision accuracy in case of the scattering object with unit area. The reason for an increased computation time of the dual window expansion method with respect to the scattering object with a rectangular domain $D$ is that the number of line segments is increased from 4 to 16. Note that the spectral transformation also requires more computation time in case of the compass cross, as compared to the other type of scattering object, which is related to the sampling of all line segments in view of Eq. (16). It can also be observed that the spectral transformation method performs similarly, regardless of the area of the compass cross. In contrast, the dual window expansion method with Gauss’s theorem requires more computation time to reach near machine-precision accuracy if the area increases. So, the compass cross examples show that both methods suffer from increased computation time if the number of line segments of the boundary of domain $D$ increases.

6. GRATING RESULTS

To demonstrate the spectral transformation method in a practical example, we compute the electromagnetic scattering from a dielectric grating consisting of 36 repeating scattering objects, as described in [pp. 168-174, 11]. Fig. 6 depicts a part of the scattering setup, including the dimensions of the scattering objects. The scattering objects are placed on top of a dielectric half-space with a relative permittivity of $\epsilon_r = 20.21 - 1.8j$, with free space ($\epsilon_r = 1$) as the top half-space. The scattering objects each have a relative permittivity of $\epsilon_r = 2.25$. The incoming field is a plane wave with a wavelength of 425 nm in free space, which has a propagation direction normal to the $xy$-plane and polarized along the $x$-direction. We use the following Gabor-frame settings. The spatial width of the window functions is set to $X = Y = 500$ nm while all the oversampling parameters such as $\alpha_x$ are set to $\sqrt{2/3}$. The nonzero Gabor coefficients are defined on the sets $m_x \in \{-40, \ldots, 40\}$, $m_y \in \{-4, \ldots, 4\}$, and $n_x, n_y \in \{-7, \ldots, 7\}$. The Gabor coefficients of all 36 scattering objects are computed via the spectral transformation method and via the original implementation for the spatial spectral 3D

![Image](image_url)
Maxwell solver, which is based on the DGT method of [8]. This enables a comparison in computation time for obtaining the scattering characteristics of this grating problem by means of the spatial spectral 3D Maxwell solver in [11]. The discretization in the z-direction consists of 21 piecewise linear basis function with a stepsize of 5 nm. Note that we use a local normal vector field formulation as defined [18] for the scattering objects in case of the spectral transformation method and the original implementation to ensure a more accurate field-material interaction in the volume integral equation. Consequently, each scattering object is actually a superposition of four triangular-shaped objects, which results in a combination of 2D characteristic functions in the $xy$-plane as shown in Fig. 7. The scaling of each characteristic function becomes a function of permittivity and normal vector, which this figure does not display.

Fig. 8 displays the magnitude of the total electric field as $|\mathbf{E}(k_x, k_y)| \cdot k_0^2$ at top of the scattering objects, where $k_0 = 2\pi/\lambda$, the free-space wavenumber. This figure only displays the magnitude of the total electric field for $k_x$ and $k_y$ inside the Ewald circle, which means that it only shows components that are present in the far field. The relative error between the total electric field computed by the spatial spectral 3D Maxwell solver with the original implementation for the Gabor coefficients and the spectral transformation method is $7.2 \cdot 10^{-4}$. This means that we maintain a three-digits accuracy with respect to JCMWave, as mentioned in [pp. 168-174, 11]. Table 2 displays the corresponding computation times necessary for the pre-processing phase, scattering objects and for solving the domain integral equation for the initial implementation and for the spectral transformation method. The pre-processing phase concerns the computation of the Gabor coefficients of all scattering objects and other things such as initializing the layered Green function. We used a single core of an Intel Xeon Gold 6148 with a base frequency of 2.4 GHz to obtain the computation times as shown in Table 2. Additionally, the computation time for the scattering objects by both methods are obtained by computing the Gabor coefficients for a single cross-section of each of the scattering objects, all cross-sections of each object are the same in the $z$-direction. This table shows that the scattering objects are a major part of the pre-processing phase in terms of computation time, even in case of the spectral transformation method. Noteworthy is the time improvement owing to the spectral transformation method that ensures that solving the integral equation becomes the most time-consuming part instead of computing the Gabor coefficients of the scattering objects. Overall, the spectral transformation method significantly reduces the computation time for the Gabor coefficients.

### Table 2. Computation times for the pre-processing phase, computing the Gabor coefficients of the scattering objects, and for solving the domain integral equation with the spatial spectral 3D Maxwell solver [11], while using two methods for computing the Gabor coefficients of the scattering objects. Note that the computation time for the scattering objects is also part of the pre-processing phase.

<table>
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<td>Solving integral</td>
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<td>962 [s]</td>
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7. CONCLUSION

We presented two fast and accurate methods to describe the discontinuous permittivity distribution with respect to the cross-section of finite 3D scattering objects with a polygonal shape in terms of Gabor coefficients, for the computation of electromagnetic scattering in layered media from these scattering scattering objects. The use of (semi)-analytical techniques in these
two methods helped to overcome the slow convergence that normally plagues the Discrete Gabor Transform. The polygon description within these two methods enables a broad range of geometries for the scattering objects. The benchmark tests displayed a significantly improved performance for these two methods in terms of the number of function evaluations, total computation time, and accuracy in obtaining the Gabor coefficients for scattering objects with respect to the method from [5]. With the spectral transformation method, the time required for computing the scattering objects, which was originally the main bottleneck for the simulation, was approximately 27 times faster. As a result, the total computation time to calculate the electromagnetic scattering behavior was approximately 4.5 times faster for a relevant scattering setup.

APPENDIX: EXPONENTIALLY CONVERGING GABOR COEFFICIENTS BY THE SPECTRAL TRANSFORMATION METHOD

We consider the exponential convergence observed for the Gabor coefficients when Gaussian window functions are employed in combination with the spectral transformation method. We utilize the work in [16] in the form of using parts of Theorem 5.1.

The ball in \( \mathbb{R}^2 \) is defined as

\[
B_R(0) = \{ x \in \mathbb{R}^2 \mid |x| < R \}. \tag{33}
\]

**Theorem 1.** Suppose \( \hat{f}(k) \) is the Fourier transform of a discontinuous 2D characteristic function with domain \( D \) in the form of a simple polygon contained in a ball with radius \( R \) centered around the origin, i.e. \( D \subset B_R(0) \). Then, for an oversampled Gabor frame with standard Gaussian window and Moore-Penrose based dual window function, the error in the Gabor coefficients converges exponentially for the trapezoidal rule.

**Proof.** We start from Eq. (8) and rewrite it as

\[
\hat{c}_{mn} = \int_{\mathbb{R}^2} \hat{f}(k) \hat{\eta}^*(k - M) \exp \left( iN \cdot k \right) dk, \tag{34}
\]

where we introduced \( M = (\beta_x m_x K_x, \beta_y m_y K_y) \) and \( N = (\alpha_x n_x X, \alpha_y n_y Y) \). We first check an initial requirement of Theorem 5.1 in [16] before continuing, i.e. the function to be integrated decays to zero when \( |k| \to \infty \). In our case, the Fourier transform of the 2D characteristic function decays as \( |k|^{-1} \) to zero [28] and the decay to zero of the spectral dual window in case of oversampling is exponential given the Gaussian window function [14, 15]. Consequently, the product of these two functions also decays exponentially to zero.

One could view Eq. (34) as the integral for computing the Fourier coefficients of the point-wise multiplication \( \hat{f}(k) \hat{\eta}^*(k - M) \). Consequently, we continue by applying a domain transformation on this point-wise multiplication, i.e.

\[
\hat{f}(k) \hat{\eta}^*(k - M) = \mathcal{F}_x [ \int_{\mathbb{R}^2} f(x') \cdot \hat{\eta}^*(x - N - x') \exp \left( iM \cdot (x - x') \right) dx'] (k). \tag{35}
\]

The symbol \( \mathcal{F}_x [ \cdot ] (k) \) represents the Fourier transformation from spatial to spectral domain evaluated at \( k \). Note that the shift in Eq. (35) for the spectrally defined dual window has become a modulation for the spatially defined dual window. Here we used the relation between the spatial domain dual window and spectral domain dual window functions, i.e.

\[
\mathcal{F}_x [ \hat{\eta}_{mn} (k)] (x) = \eta_{mn} (x). \tag{36}
\]

We continue with the insight that the spectral Gabor coefficients are also equal to

\[
I = \epsilon_{mn} = \int_{\mathbb{R}^2} f(x') \hat{\eta}^*(x - N - x') \exp \left( iM \cdot (x - x') \right) dx',
\]

where \( x = 0 \). This originates from the fact that the evaluation of the Fourier transform at the origin corresponds to the area of the function before applying a Fourier transformation. Thus, this specific integral, \( I \), is our reference with respect to the approximation of Eq. (34) by the trapezoidal rule. The approximation accuracy of the trapezoidal rule is expressed in [16] by the Poisson summation formula in the following form

\[
I_h = \sum_{l \in \mathbb{Z}^2} \int_{\mathbb{R}^2} f(x') \hat{\eta}^*(x_l - N - x') \exp \left( iM \cdot (x_l - x') \right) dx',
\]

where \( I = (l_x, l_y) \) with \( l_x, l_y \in \mathbb{Z} \), \( x_l = (2\pi l_x/h, 2\pi l_y/h) \), and \( h > 0 \) is the stepsize for both the \( x \)-direction and \( y \)-direction of the trapezoidal rule. Consequently, the difference between the reference solution and the trapezoidal approximation is equal to

\[
I - I_h = \sum_{l \in \mathbb{Z}^2, l \neq 0} \int_{\mathbb{R}^2} f(x') \hat{\eta}^*(x_l - N - x') \exp \left( iM \cdot (x_l - x') \right) dx'. \tag{37}
\]

We continue by obtaining an upper bound for the convolution integral in Eq. (37). This can be achieved by

\[
\left| \int_{\mathbb{R}^2} f(x') \hat{\eta}^*(x_l - N - x') \exp \left( iM \cdot (x_l - x') \right) dx' \right| \leq \int_{\mathbb{R}^2} |f(x')||\eta(x_l - N - x')|dx'. \tag{38}
\]

This way we can neglect the modulation part induced by \( M \). We continue by assuming that domain \( D \) of the object is close to the origin of the Cartesian system, since translations of multiples of \((X, Y)\) boil down to scalar multiplications within Gabor frames. We use a ball \( B_R(0) \), which contains the complete domain \( D \) in its interior. This allows to further bound Eq. (38) as

\[
\int_{B_R(0)} |f(x')||\eta(x_l - N - x')|dx' \leq \int_{B_R(0)} |\eta(x_l - N - x')|dx', \tag{39}
\]

where we used that \( |f(x')| \leq 1 \). The right-hand side of the inequality in Eq. (39) can be further estimated as

\[
\int_{B_R(0)} |\eta(x_l - N - x')|dx' \leq C \exp(-\lambda_1 |x_l - N - x'|)dx', \tag{40}
\]

owing to the decay in the dual window, see Eq. (17). We obtain the following inequality by combining Eq. (37) and Eq. (40), while using the reverse triangle inequality multiple times, i.e.

\[
|x_l - N - x'| \geq ||x_l - N| - |x'||,
\]

\[
|I - I_h| \leq 4C \sum_{l \in \mathbb{Z}^2, l \neq 0} \int_{B_R(0)} \exp(-\lambda_1 |x_l - N| - |x'||)dx', \tag{41}
\]

with \( D = \mathbb{R}^2 \setminus \{(0,0)\} \). Equation Eq. (41) only provides exponential decay as a function of the uniform sampling of the trapezoidal rule in case \( |x_l| > |N| + |x'| \) for all \( x' \) in the integration domain. The integral bounds in Eq. (41) induce \( |x'| \leq R \). This
means that we have to ensure that $|x| > |N| + R$ for $(l_x, l_y) \in \mathbb{D}$. Consequently, the requirement for $h$ to ensure that $|x| > |N| + R$ for $(l_x, l_y) \in \mathbb{D}$ becomes

$$h < \frac{2\pi}{R + |N|}. \quad (42)$$

Utilizing the bound on $h$ from Eq. (42) allows us to bound the integral in Eq. (41) by its maximum value multiplied by the area integral, i.e.

$$|I_h - I| \leq 4\pi CR^2 \exp \left[\lambda_1(R + |N|)\right] \max_{l \in \mathbb{D}} \exp\left(-\frac{2\pi\lambda_1}{h}l\right), \quad (43)$$

with $l = |l| = \sqrt{l_x^2 + l_y^2}$. The triangle inequality $l \leq l_x + l_y$ allows us to rewrite the geometric series in Eq. (43) to

$$\sum_{(l_x, l_y) \in \mathbb{D}} \exp\left(-\frac{2\pi\lambda_1}{h}l\right) \leq \sum_{l_x=0}^{\infty} \exp\left(-\frac{2\pi\lambda_1}{h}l_x\right) \sum_{l_y=0}^{\infty} \exp\left(-\frac{2\pi\lambda_1}{h}l_y\right). \quad (44)$$

Consequently, we evaluate the sum of these two geometric series such that we can rewrite Eq. (43) to

$$|I_h - I| \leq 4\pi CR^2 \exp \left[\lambda_1(R + |N|)\right] \left(\frac{1}{\left[1 - \exp\left(-\frac{2\pi\lambda_1}{h}\right)\right]^2} - 1\right).$$

Hence, the integral in Eq. (34) is computed with exponentially converging accuracy by the trapezoidal rule, since the last inequality shows an upper bound in the form of an exponentially decaying function.

Note that the upper bound as shown in the last inequality can be converted to a more practical version by truncating the geometric series in Eq. (44) to a finite number of $l_x$ and $l_y$ components. This truncated version of the upper bound would be more similar to the end result of the proof of Theorem 5.1 in [16].

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**Data availability.** Data underlying the results presented in this paper are not publicly available due to project restrictions at this time but may be obtained from the authors upon reasonable request.

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