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Computational aspects of a spatial-spectral domain integral equation for scattering by objects of large longitudinal extent

R. J. Dilz *

M. C. van Beurden †

Abstract — With a 3D spatial spectral integral-equation method for EM scattering from finite objects, a significant part of the computation time is spent on a middle region around the origin of the spectral domain. Especially when the scatterer extends to more than a wavelength in the stratification direction, a fine discretization on this region is required, consuming much computation time in the transformation to the spatial domain. Numerical evidence is shown that the information in the middle region of the spectral domain is largely linearly dependent. Therefore, a truncated singular-value decomposition is proposed to make the computation time largely independent of the discretization on this middle region. For a practical example the increased computational efficiency and the approximation error of the singular-value decomposition are shown.

1 INTRODUCTION

Previously a 2D and 3D spatial spectral integral equation methods for electromagnetic scattering from dielectric objects in multilayered media were proposed [1–3]. This approach is based on handling the field-material interaction in the spatial domain and the Green function in the spectral domain. Fourier transforms are needed to transform the contrast current density and the electric field between the spatial and spectral domain. The scattered electric field is computed from the contrast current density by a recursive set of multiplications by several parts of the Green function.

The Green function contains branch cuts and poles. To avoid these difficulties the contrast current density and scattered electric field are therefore represented on a manifold that is deformed slightly into the complex plane. This deformation decomposes each of the two transverse spectral directions into three parts, two parts containing most information and a small part to connect them. In total, this yields nine different regions. Although the connecting part is small, still a significant amount of computation time is spent on transforming information represented in the connecting part to the spatial domain. Since the connecting part contains infor-

mation about waves traveling close to the stratification direction, a fine discretization is needed especially for objects with large extent in this direction. Each basis function in this connecting part is Fourier transformed individually, although the contained information is largely redundant. We propose a singular-value decomposition to remove the redundancy and speed up these computations.

2 SPECTRAL PATH

We use the formulation for electromagnetic scattering as explained in [3, 4]. In these articles, the branch cuts and poles in the Green function are evaded by representing the contrast current density, the electric field and the Green function in the spectral domain on a path

$$\tau_\alpha(k_\alpha) \in \begin{cases} k_\alpha - jA & \text{if } k_\alpha < -A \\ (1+j)k_\alpha & \text{if } -A \leq k_\alpha < A \\ k_\alpha + jA & \text{if } k_\alpha > A, \end{cases} \quad (1)$$

with $\alpha \in \{x, y\}$. The $k_x k_y$ plane is then divided in nine regions as shown in Figure 1, where we will focus on the middle region indicated by M. In the z direction, a PWL expansion in the spatial domain is employed.

Figure 1: Subdivision of the $k_x - k_y$ plane with piecewise-constant and piecewise linear imaginary shifts

*Eindhoven University of Technology. e-mail: r.dilz@tue.nl

†Eindhoven University of Technology. e-mail: m.c.v.beurden@tue.nl

3 DISCRETIZATION ON THE MIDDLE REGION

3.1 2D: one-dimensional Taylor series

Gabor frames are used as a discretization for the contrast current density on the regions $k_\alpha < -A$ and $k_\alpha > A$. For the two-dimensional algorithms in [2, 4, 5], where the y direction is absent, a Taylor-series approximation with $N_a + 1$ terms is employed on the connecting part $-A < k_x < A$. A function $f(k_x)$ is approximated on the spectral path of Eq. (1) for $k_x \in [-A, A]$ by

$$f(\tau_x(k_x)) \approx \sum_{n=0}^{N_a} \frac{f^{(n)}(0)}{n!} \tau_x(k_x)^n. \quad (2)$$

So instead of function values on the path τ_x , the derivatives at $k_x = 0$ are kept as a representation. In the spectral domain, we multiply the contrast current density and the Green function. The result $m(k_x)$ of multiplying of two functions, say $g(k_x)$ and $h(k_x)$, where the derivatives of these functions are known, can then be calculated by the Leibnitz rule as

$$m^{(n)}(0) = \sum_{\ell=0}^n \frac{n!}{(\ell-n)! \ell!} g^{(\ell-n)}(0) h^{(n)}(0). \quad (3)$$

Since there are N_a derivatives needed, the number of operations for such a multiplication scales as $O(N_a^2)$ for the number of terms in the Taylor series. For problems without features extending more than a wavelength in the z -direction, around ten terms are required in the Taylor series. Even though this Taylor series is computationally not very efficient, it does not significantly contribute to the overall computation time, owing to the small number of terms in the truncated Taylor series.

3.2 3D: Piecewise-linear functions

For a 3D algorithm, functions are represented on complex paths τ_x and τ_y , in the k_x and k_y direction, respectively. Although a two-dimensional Taylor series would be able to represent the Green function and contrast current density on the region $(k_x, k_y) \in [-A, A]^2$, the quadratic computational complexity in the multiplication in Eq. (3) makes it unsuitable for a generalization to two dimensions. Therefore, the Taylor-series approach was replaced by a piecewise-linear (PWL) discretization for the 3D algorithm in [3]. With the PWL discretization, a function $f(\tau_x(k_x), \tau_y(k_y))$ is approximated by a list of function values $f_{n_x, n_y} =$

$f(\tau_x(n_x A/N_p), \tau_y(n_y A/N_p))$ as

$$f(\tau_x(k_x), \tau_y(k_y)) \approx \sum_{n_x=-N_p}^{N_p} \sum_{n_y=-N_p}^{N_p} \Lambda_{n_x}(k_x) \Lambda_{n_y}(k_y) f_{n_x, n_y}, \quad (4)$$

where

$$\Lambda_n(k) = \max\{0, 1 - |x N_p / A - n|\}. \quad (5)$$

With the PWL approximation, the multiplication operation simply becomes a point wise multiplication, which scales linearly with the number of basis functions instead of quadratically in Eq. (3).

4 TRANSFORMATION TO THE SPATIAL DOMAIN

4.1 Transformation of PWL functions

To transform the representation on Region M in Eq. (4) to the spatial domain as needed for the electric field, we use the Fourier integrals over the complex spectral path restricted to M, i.e.

$$L_n(x) = \int_{-A}^A \Lambda_n(k) e^{j(1+j)kx}. \quad (6)$$

Consequently, $f^M(x)$, i.e. the contribution of region M to the spatial domain, can be written as

$$f^M(x) = \sum_{n_x=-N_p}^{N_p} \sum_{n_y=-N_p}^{N_p} f_{n_x, n_y} L_{n_x}(x) L_{n_y}(y). \quad (7)$$

Now we put this into a matrix formulation. First, let $\underline{f}$ represent the size $(2N_p + 1)^2$ vector of f_{n_x, n_y} coefficients. The spatial domain is discretized via discretization operator $\mathcal{S}$ into N_s basis functions $b_m(x, y)$. For example, we denote the discretized version of the arbitrary function $t(x, y)$ as $t_m = \mathcal{S} \circ t(x, y)$, such that $t(x, y) = \sum_{m=0}^{N_s} t_m b_m(x, y)$. We use this discretization operator to calculate $L_{m, (n_x, n_y)} = \mathcal{S} \circ (L_{n_x}(x) L_{n_y}(y))$, such that

$$L_{n_x}(x) L_{n_y}(y) = \sum_{m=1}^{N_s} L_{m, (n_x, n_y)} b_m(x, y). \quad (8)$$

Where we will use the notation $\underline{L}$ for the $N_s \times (2N_p + 1)^2$ matrix, where in general $N_s \gg N_p^2$. A discretized counterpart of Eq. (7) can be computed by computing $\underline{f}^M = \underline{L} \cdot \underline{f}$, which yields a vector of length N_s . This matrix product has to be computed, which requires $O(N_s N_p^2)$ operations. Especially for large, but realistic, N_p this becomes the dominating contribution to the computation time, as will be shown in Section 5.

Figure 2: A set of $L_n(x)$ for $N_p = 20$, red signifying $n = 1$ and purple $n = 41$, and $A = 5.6 \times 10^{-3}$. These integrals are cut off at $x = \pm 6$ corresponding to the discretization used in the spatial domain.

4.2 Singular-value decomposition

In Figure 2, a set of Fourier integrals of the PWL basis, L_n , as defined in Eq.(6) are shown. Clearly, there is a lot of redundancy in this set. At a large distance from $x = 0$, these integrals $L_n(x)$ are less redundant. However, they are only required for small x where the scattering object is located. This suggests that the sum in Eq. (7) can be sped up by a truncated singular-value decomposition (SVD) [6, Chapter 2.6].

The matrix $\underline{\underline{L}}$ can be decomposed into

$$\underline{\underline{L}} = \underline{\underline{U}} \cdot \underline{\underline{\Sigma}} \cdot \underline{\underline{V}}^T, \quad (9)$$

where many entries in the diagonal $(2N_p + 1)^2$ matrix $\underline{\underline{\Sigma}}$ are negligible. The elements are said to be negligible when they are smaller than threshold ϵ , and will then be set to zero. Afterwards, $N_t \leq (2N_p + 1)^2$ significant entries in the diagonal matrix remain. Now $\underline{\underline{L}}$ can be approximated by $\underline{\underline{L}} \approx (\underline{\underline{\tilde{U}}} \cdot \underline{\underline{\tilde{\Sigma}}}) \cdot \underline{\underline{\tilde{V}}}^T$, where $\underline{\underline{\tilde{V}}}^T$ is an $N_t \times (2N_p + 1)^2$ matrix and $(\underline{\underline{\tilde{U}}} \cdot \underline{\underline{\tilde{\Sigma}}})$ is an $N_s \times N_t$ matrix.

Since there is a significant redundancy in the system, usually $N_t \ll (2N_p + 1)^2$, so computing

$$\underline{\underline{f}}^M = (\underline{\underline{\tilde{U}}} \cdot \underline{\underline{\tilde{\Sigma}}}) \cdot (\underline{\underline{\tilde{V}}}^T \cdot \underline{\underline{f}}) \quad (10)$$

requires only $O(N_t(N_p^2 + N_s))$ operations instead of $O(N_p^2 N_s)$. Since the spectral Region M is of small size, compared to the complete spectral range included in the simulation, it represents only a small amount of information compared to the number of spatial basis functions N_s . For this reason N_t does not increase very much after a certain number PWL basis function N_p as will be shown next.

5 IMPACT ON ACCURACY

The idea to apply the SVD on the region M in the spectral domain is tested by computing the scatter-

Figure 3: (a) Scattering setup, (b) the upwards-directed electric-field amplitude in the far field, $|\mathbf{E}(k_x, k_y)|$ (a.u.) from this scattering setup.

ing from a dielectric block of $400 \times 400 \times 800$ nm illuminated by an incident plane wave with wavelength $\lambda = 425$ nm as shown in Figure 3(a). The amplitude of the scattered electric field, $|\mathbf{E}|$, in the far field is plotted against the transverse part of the wavenumber (k_x, k_y) , and $k_0 = 2\pi/\lambda$ in Figure 3(b). For large N_p , the rank of the truncated SVD increases to a value that is independent of N_p and depends merely on the error level ϵ as is shown in Figure 4(a). Without the SVD, the computation time increases significantly with large N_p . However, when the truncated SVD is used, the computation time does not depend strongly on N_p as can be seen in Figure 4(b). To show how the truncated SVD influences the accuracy of the far field, we have plotted the $\mathcal{L}^2$ -norm of the relative difference in the far field data for different truncation thresholds ϵ and numbers of PWL basis function N_p . A reference was calculated with $\epsilon = 10^{-7}$ and $N_p = 40$. In Figure 4(c), it can be observed that the error with the use of the SVD can be made small, when N_p is chosen large enough. For an error level of 10^{-3} a truncation threshold $\epsilon = 10^{-2}$ is already sufficient,

Figure 4: (a) The size of the significant part of the SVD truncated at ϵ with N_p basis functions. (b) The percentage of the total computation time that is spent on region M. With SVD the computation time was between 290 and 350 seconds on a single core of a 3.1 GHz Xeon E5-2687 processor, without SVD it increased up to 950 seconds with $N_p = 25$. (c) The error in the region M discretization relative to the complete far field result as in Figure 3(b)

since region M contributes only a part of the complete electric field to which all regions in Figure 1 contribute.

6 CONCLUSION

The Fourier transformation from the spectral domain to the spatial domain of a small patch of the spectral domain can take up more than half of the computation time. A truncated singular-value decomposition was used to speed up the computation of this Fourier transform, so the time spent on this patch was reduced to less than 10%, with an error level of 10^{-3} .

Numerical evidence was shown that the rank of the singular-value decomposition and therefore the

computation time depends weakly on the fineness of the discretization on this patch in the spectral domain.

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