Computation of Scattering from Rough Surfaces using Successive Symmetric Over Relaxation and Eigenvalue Deflation

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***Abstract*—The problem of computing 2D EM wave scattering from rough surfaces is addressed using an integral equation formulation discretised using the method of moments. Successive Symmetric Over-Relaxation (SSOR) is applied to the governing matrix equations along with eigenvalue deflation which is designed to separately account for the effect of those eigenvectors of the iteration matrix that have eigenvalues greater than 1. Numerical results are presented applying the method to a variety of scattering profiles and examining the resultant convergence performance.**

***Index Terms*—Rough surface scattering, method of moments, stationary iterative methods, eigenvalue deflation**

I. Introduction

The computation of the scattering of electromagnetic waves from randomly rough surfaces is a classic problem. Approximate analytic solutions date back many years and include the well-known Beckman Kirchhoff theory [1]. The move towards the use of higher frequencies, specifically millimetre wave and TeraHertz, in communication systems has seen a renewed interest in this problem. This is because physical surfaces that could be practically viewed as effectively smooth at lower frequencies must be considered to be rough as the wavelength diminishes and surface features on the scale of the wavelength become important centres of scattering. Consequently, in a ray tracing context for example, one must upgrade the simple specular reflection interaction that would occur with a smooth surface with a more complicated diffuse scattering model. Recent work in this area has focused on the use of Beckmann-Kirchhoff theory [2] and effective roughness models [3]. Both of these approaches are effective, but approximate.

An alternative approach is to use an approach based on a numerical solution of Maxwell's equations which potentially offers a near-exact analysis. The method of moments applied to a surface integral equation offers a very compact formulation as only the rough boundary needs to be discretised but, like all full-wave solutions, is computationally expensive. There are two main sources of computational overhead. Firstly, for practical sized problems the resultant matrix equation cannot be solved directly and must be solved by a suitable iterative method. Each step of an iterative solution requires $\mathcal{O}\left(N^2\right)$ computations where N is the number of basis functions used to discretise the problem. This has been addressed in recent decades by the use of acceleration schemes such as the Fast Multipole Algorithm [4] or the Spectral Acceleration Method [5], both of which reduce this computational cost to $\mathcal{O}\left(N \log N\right)$. A second issue, which is the focus of this paper, is the number of such iterations needed to ensure acceptable convergence of the solution. While Krylov subspace based solvers such as Bi-CG or GMRES have traditionally been applied on account of their reliability when applied to general scattering problems, the use of stationary solvers based on matrix-splitting have been shown to be highly effective when applied to problems such as rough surface scattering [6]. Such methods are often colloquially referred to as "forward-backward" methods in the literature on account of their intuitive interpretation as propagating a solution forward and backward along the physical extent of a scatterer and when effective can converge in much fewer iterations than Krylov methods. However, they suffer from uncertain convergence characteristics as the convergence properties are dependent of the spectral radius (maximum eigenvalue) of the iteration matrix. If this spectral radius is greater than one the method will diverge.

The technical contribution of this paper is the introduction and investigation of a technique, eigenvalue deflation, for generalising the stationary iterative algorithm to ensure that it converges even when the associated spectral radius is greater than one. The paper is organised as follows. Section II describes the integral equation formulation used and the matrix splitting technique used, namely Successive Symmetric Over Relaxation (the mathematical term for "forward-backward"). Section III outlines the process of eigenvalue deflation, a strategy to identify, and separately treat, eigenvectors with eigenvalues greater than one, thereby ensuring convergence. Section IV validates the formulation and presents results and we summarise relevant conclusions in section V.

II. Formulation and SSOR

We consider a 2D scattering problem comprising a TM^z polarised incident wave impinging on an irregular boundary between region 1 (free space) and region 2 which is homogeneous material with permittivity, permeability and conductivity given by $\epsilon = \epsilon_r \epsilon_0$, $\mu = \mu_0$ and σ respectively. Time variation of $e^{j\omega t}$ is assumed and suppressed where ω is the angular

frequency. The electric fields in region 1 and region 2 can be expressed via potential integrals in terms of the tangential electric and magnetic fields on the boundary, known as the magnetic and electric current respectively and given by

$$\vec{K} = \hat{n} \times \vec{E} \quad (1)$$
$$\vec{J} = \hat{n} \times \vec{H}. \quad (2)$$

Forcing continuity across the boundary yields the electric field integral equation [7]. Representing each unknown current by a weighted sum of N pulse basis functions and applying the method of moments yields the following dense matrix equation

$$\mathbf{Z}\mathbf{x} = \mathbf{v}. \quad (3)$$

$\mathbf{Z}$ is a dense $2N \times 2N$ matrix containing interactions between the basis functions. It can be considered as an array of four $N \times N$ matrices namely

$$\mathbf{Z} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}, \quad (4)$$

where $\mathbf{A}, \mathbf{B}, \mathbf{C}$ and $\mathbf{D}$ describe interactions between discretised electric and magnetic current basis functions radiating in either region 1 (free-space) or region 2 (dielectric material). $\mathbf{x}$ is a $2N \times 1$ vector containing the amplitudes of the basis functions. These are unknown and can be thought of informally as sampled values of the electric and magnetic currents

$$\mathbf{x} = \begin{bmatrix} \mathbf{j} \\ \mathbf{k} \end{bmatrix}, \quad (5)$$

while $\mathbf{b}$ is a $2N \times 1$ vector containing information about the incident field

$$\mathbf{b} = \begin{bmatrix} \mathbf{E}^i \\ \mathbf{0} \end{bmatrix}. \quad (6)$$

To apply Successive Symmetric Over-relaxation (SSOR) we first re-arrange (3). Rather than $\mathbf{x}$ containing first N sampled electric currents followed by N sampled magnetic currents we interleave the unknowns to yield

$$\tilde{\mathbf{Z}}\tilde{\mathbf{x}} = \tilde{\mathbf{v}}, \quad (7)$$

where each $\tilde{\mathbf{Z}}_{mn}$, for $m, n = 1 \dots N$, is a 2×2 matrix given by

$$\tilde{\mathbf{Z}}_{mn} = \begin{bmatrix} A_{mn} & B_{mn} \\ C_{mn} & D_{mn} \end{bmatrix}. \quad (8)$$

Each $\tilde{\mathbf{x}}_n$, for $n = 1 \dots N$, is a 2×1 column vector of unknowns associated with surface discretisation (basis domain) n.

$$\tilde{\mathbf{x}}_n = \begin{bmatrix} j_n \\ k_n \end{bmatrix}, \quad (9)$$

while each $\tilde{\mathbf{v}}_n$, for $n = 1 \dots N$, is a 2×1 column vector containing incident field information at basis domain n.

$$\tilde{\mathbf{v}}_n = \begin{bmatrix} E^i_n \\ 0 \end{bmatrix}. \quad (10)$$

The SSOR[1] proceeds by splitting the interleaved matrix $\tilde{\mathbf{Z}}$ into diagonal, lower and upper sub-matrices as

$$\tilde{\mathbf{Z}} = \tilde{\mathbf{D}} + \tilde{\mathbf{L}} + \tilde{\mathbf{U}}, \quad (11)$$

choosing an initial estimate for the solution $\tilde{\mathbf{x}}^{(0)}$, and iterating a solution according to

$$\tilde{\mathbf{x}}^{(k+1)} = \mathbf{M}\tilde{\mathbf{x}}^{(k)} + \mathbf{G}\tilde{\mathbf{v}}, \quad (12)$$

where $\mathbf{M}$ is the *iteration matrix* given by

$$\mathbf{M} = \left(\tilde{\mathbf{D}} + \tilde{\mathbf{U}}\right)^{-1} \tilde{\mathbf{L}} \left(\tilde{\mathbf{D}} + \tilde{\mathbf{L}}\right)^{-1} \tilde{\mathbf{U}}, \quad (13)$$

and

$$\mathbf{G} = \left(\tilde{\mathbf{D}} + \tilde{\mathbf{U}}\right)^{-1} \tilde{\mathbf{D}} \left(\tilde{\mathbf{D}} + \tilde{\mathbf{L}}\right)^{-1}. \quad (14)$$

The effectiveness of the SSOR depends on ρ the spectral radius of $\mathbf{M}$, that is the largest magnitude of its eigenvalues λ_m

$$\rho = \max |\lambda_m| \dots \text{ for } m = 1 \dots 2N. \quad (15)$$

It will converge if $\rho < 1$ and its convergence is more rapid the smaller ρ is. Equations (12) and (13) are useful in explicitly identifying the reliance of the algorithm on the value of ρ. However in practice one would not implement the SSOR in this fashion for large problems (due to the implied necessity to compute and store large matrices and their inverses). Instead the update can be computed on a component by component basis as follows

$$\tilde{\mathbf{x}}_m^{\left(k+\frac{1}{2}\right)} = \tilde{\mathbf{Z}}_{mm}^{-1} \left(\tilde{\mathbf{v}}_m - \mathbf{f}_m^{\left(k+\frac{1}{2}\right)} - \mathbf{b}_m^{(k)} \right) \quad (16)$$
$$\text{for } m = 1 \dots N$$
$$\tilde{\mathbf{x}}_m^{(k+1)} = \tilde{\mathbf{Z}}_{mm}^{-1} \left(\tilde{\mathbf{v}}_m - \mathbf{f}_m^{\left(k+\frac{1}{2}\right)} - \mathbf{b}_m^{(k+1)} \right) \quad (17)$$
$$\text{for } m = N \dots 1$$

where the vectors $\mathbf{f}_m^{(k)}$ and $\mathbf{b}_m^{(k)}$ are estimates of forward and backward scattered field at location m respectively

$$\mathbf{f}_m^{(k)} = \sum_{n<m} \tilde{\mathbf{Z}}_{mn} \tilde{\mathbf{x}}_n^{(k)} \quad (18)$$
$$\mathbf{b}_m^{(k)} = \sum_{n>m} \tilde{\mathbf{Z}}_{mn} \tilde{\mathbf{x}}_n^{(k)} \quad (19)$$

The SSOR is applied to a number of scattering problems in section IV to validate the method and to indicate its effectiveness. However the process as described above will fail if the spectral radius of the iteration matrix ρ is greater than one, which occurs as the roughness of the surface becomes more pronounced. However, in such cases the problem is generally confined to a small number of eigenvectors, and the SSOR will remain effective in computing the contribution to the solution due to the remaining eigenvectors. Eigenvalue deflation, outlined in the next section, is a way of effectively splitting the problem, identifying a small dimensional subspace spanned by the "problem" eigenvectors (with eigenvalues greater than 1) and projecting away from this subspace to an orthogonal

[1]Strictly speaking the SSOR with relaxation parameter set to 0. A more general implementation applies a non-zero relaxation parameter.

subspace within which SSOR can be effectively applied to the remaining eigenvalues. The contribution from the "problem" eigenvectors can be included directly via the inversion of a low dimension matrix and a solution is iteratively updated by coupling between the subspaces.

III. Eigenvalue deflation

This section follows the treatment as described in [8]. Assuming that there are r "problem eigenvectors" with eigenvalues greater than 1, we can form an orthonormal basis for the space $\mathcal{P}$ spanned by these eigenvectors [2]. This is denoted as $\mathbf{Y}$, a $N \times r$ matrix of orthonormal unit vectors. $\mathbf{P}$ and $\mathbf{Q}$ are projections onto $\mathcal{P}$ and onto the space orthogonal to it respectively and are defined by

$$\mathbf{Q} = \mathbf{I} - \mathbf{Y}\mathbf{Y}^T \quad (20)$$

$$\mathbf{P} = \mathbf{Y}\mathbf{Y}^T. \quad (21)$$

Defining the new unknown vectors $\mathbf{u}$ and $\mathbf{q}$ as

$$\mathbf{u} = \mathbf{Y}^T\tilde{\mathbf{x}} \quad (22)$$

$$\mathbf{q} = \mathbf{Q}\tilde{\mathbf{x}}, \quad (23)$$

allows the SSOR process to be re-cast as a coupled iteration between them according to

$$\mathbf{W}\mathbf{u}^{(k+1)} = \mathbf{Y}^T\left(\mathbf{G}\tilde{\mathbf{v}} + \mathbf{M}\mathbf{u}^{(k)}\right) \quad (24)$$

$$\mathbf{q}^{(k+1)} = \mathbf{Q}\left(\mathbf{G}\tilde{\mathbf{v}} + \mathbf{M}\mathbf{q}^{(k)} + \mathbf{M}\mathbf{Y}\mathbf{u}^{(k+1)}\right), \quad (25)$$

where W is a $r \times r$ matrix given by

$$\mathbf{W} = \mathbf{I}_r - \mathbf{Y}^T\mathbf{M}\mathbf{Y}, \quad (26)$$

and

$$\mathbf{I}_r = \mathbf{Y}^T\mathbf{Y} \quad (27)$$

is an $r \times r$ identity matrix. $\mathbf{u}$ contains the part of the solution which depends on the r "problem" eigenvectors spanning $\mathcal{P}$ where r is assumed small compared to $2N$. At each iteration it is updated by solving a $r \times r$ systems. The vector $\mathbf{q}$ contains information in the space orthogonal to $\mathcal{P}$ and is updated using a SSOR iteration.

A. Implementation

The eigenvalue deflation approach requires that we have knowledge of the so-called r "problem" eigenvectors whose eigenvalues have absolute value greater than 1. For practical problems this is of course not feasible as exact computation of the eigenvalues of the iteration matrix $\mathbf{M}$ is too expensive. Instead these r eigenvectors must be approximated. The simplest way to do this is apply the SSOR iteration (given by (16) and (17)) to the starting estimate $\tilde{\mathbf{x}}^{(0)}$ *at least* r times. At each iteration the difference between the updated solution vector and the previous solution estimate is noted, that is the update vector defined by

$$\mathbf{\Delta}^{(k+1)} = \tilde{\mathbf{x}}^{(k+1)} - \tilde{\mathbf{x}}^{(k)}. \quad (28)$$

[2]The practical implementation of this is discussed in section III-A.

As the SSOR iteration matures these difference vectors will be dominated by the dominant eigenvectors of $\mathbf{M}$, that is the eigenvectors with the largest eigenvalues. Consequently, applying a Gram-Schmidt orthonormalisation process to the most recent r of them will create an approximation to the matrix of basis vectors $\mathbf{Y}$ needed to compute the updates defined by (24) and (25). This approximation will improve with the number of initial SSOR iterations performed. It should be noted that precise knowledge of r, the number of problem eigenvectors, is not required in advance. A conservative approach can be taken, choosing r in excess of what it is likely to be. There is no penalty incurred as the worst outcome is that some non-problematic eigenvectors (with eigenvalues less than one) are deflated that would otherwise be treated using SSOR. Indeed it is possible to update r as the algorithm progresses, initially estimating some eigenvalues to deflate and periodically adding a batch to this set as the algorithm matures and more information is available [8].

IV. Results

A. Validation - Example One

Consider a tapered plane wave radiating at 2GHz and impinging on a flat boundary ($y = 0$) between free space and a lossless medium of relative permittivity $\epsilon_r = 3$. The boundary runs from $-16\lambda_d < x < 16\lambda_d$ where λ_d is the wavelength in the material. The electric field is polarised in the z direction, is incident from $\theta_i = \frac{\pi}{4}$ and at a point $\vec{\rho} = x\hat{i} + y\hat{j}$ is given by

$$\vec{E}^i(\vec{\rho}) = e^{-jk_0(x\sin\theta_i - \cos\theta_i y)(1+\psi(\vec{\rho}))}e^{-\frac{(x+y\tan\theta_i)^2}{g^2}}\hat{k}, \quad (29)$$

where

$$\psi(\vec{\rho}) = \frac{2\frac{(x+y\tan\theta_i)^2}{g^2} - 1}{(k_0 g\cos\theta_i)^2}. \quad (30)$$

The parameter g controls the tapering width [9] and was set to $4\lambda_d$. The purpose of the tapering is to smoothly reduce the incident field to zero at the edges of the surface in order to reduce unwanted edge diffraction effects. The pulse basis function domain size was chosen to be $\lambda_d/10$ yielding $N = 512$ and a $\tilde{\mathbf{Z}}$ matrix of size 1024. It can be shown (by direct computation) that for this scenario the SSOR iteration matrix has spectral radius equal to 0.400366 and the SSOR algorithm will therefore converge without the need for eigenvalue deflation. Fig. 1 shows the electric and magnetic current on the boundary computed by direct inversion of (3) and by SSOR iteration (given by (16) and (17)). In addition we show the electric and magnetic currents computed by application of Fresnel reflection coefficients [10]. The match between direct inversion and SSOR is excellent. The rapid convergence of the SSOR should be noted. Defining the residual error by

$$\chi^{(k)} = \frac{\|\tilde{\mathbf{Z}}\tilde{\mathbf{x}}^{(k)} - \tilde{\mathbf{v}}\|}{\|\tilde{\mathbf{v}}\|} \quad (31)$$

Fig. 2 shows the incident and scattered fields above the boundary. The scattered fields clearly comprise a specular

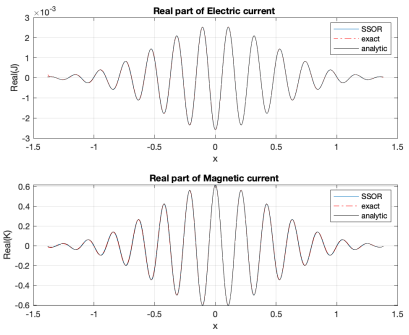

Fig. 1. Real part of electric and magnetic currents on flat boundary between free space and medium with $\epsilon_r = 3$. Tapered incident field is centred on (0,0) and is impinging at 45 degree angle to normal.

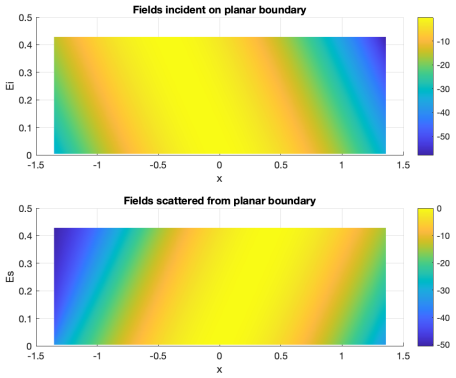

Fig. 2. Incident fields (above) and scattered fields (below) in dB in the space above flat boundary between free space and medium with $\epsilon_r = 3$. Tapered incident field is centred on (0,0) and is impinging at 45 degree angle to normal.

reflected component with no diffuse scattering. it was noted that a residual error of $\chi = 10^{-3}$ was achieved after 7 SSOR iterations (or 7 full forward-backward sweeps).

B. Results - Example Two

Having validated the matrix formulation and basic SSOR implementation the application of eigenvalue deflation to the computation of scattering from a randomly rough surface with Gaussian correlation function is now examined. Fig. 3 shows a single realisation of a 1D random rough surface. The RMS height is given by $h_{RMS} = 0.6\lambda_d$ while the correlation length is given by $l_c = 0.8\lambda_d$. The same tapered plane wave was applied as in example one and the material properties and surface length was also the same. Again the $\tilde{\mathbf{Z}}$ matrix was of size 1024. In this case the SSOR iteration matrix has spectral radius equal to 2.666687 and there are 4 eigenvalues greater than 1 (as per Fig. 4). Hence SSOR will diverge and instead eigenvalue deflation was used. We set $r = 5$ and used 20 initial iterations of SSOR to form a basis. The rapid convergence of the SSOR with eigenvalue deflation algorithm is highlighted in Fig. 5 which shows the relative error, $\chi^{(k)}$, versus iteration number. Figure (6) shows the incident and scattered fields

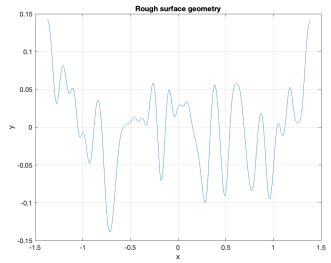

Fig. 3. Problem geometry for example two. Rough surface with Gaussian correlation. RMS height is $h_{RMS} = 0.6\lambda_d$ and correlation length is $l_c = 0.8\lambda_d$.

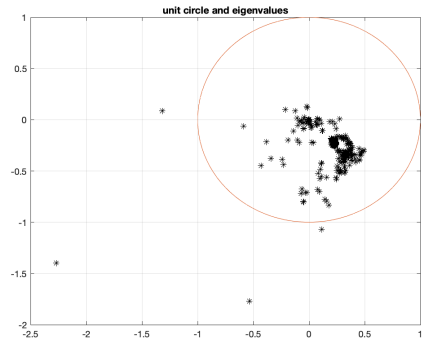

Fig. 4. Eigenvalues of SSOR iteration matrix for example 2. There are four eigenvalues greater than 1 which must be deflated

above the boundary, highlighting the diffuse scattering pattern created.

C. Results - Example Three

The final example involves scattering from a surface with three rectangular corrugations. A tapered incident wave with $\theta_i = \frac{\pi}{3}$ and $g = 0.5$ is used. The material has relative permittivity $\epsilon_r = 4 - 0.1\jmath$. The matrix size in this case is 3944, the spectral radius of the iteration matrix is 1.634878, while there are 4 eigenvalues greater than 1, as seen in Fig. 7. Eigenvalue deflation was applied with r initially set to $r = 5$. The initial estimate for $\mathbf{Y}$ was based on update vectors obtained from running 5 iterations of the SSOR (given by (16) and (17). In this case two further batches of eigenvector approximations were added after a further 5 and 10 iterations ((24) and (25)) gradually bringing r up to a final value of 15. In this application a relative error $\chi = 10^{-3}$ was achieved after 29 iterations. Fig. 8 shows the total fields outside and inside the corrugations.

V. Conclusions and Future Work

This paper has addressed the problem of computing 2D EM wave scattering from rough surfaces using an integral equation formulation discretised using the method of moments. Numerical results have demonstrated how eigenvalue deflation can allow one to apply SSOR even when the spectral radius of the iteration matrix is greater than one. The "problem"

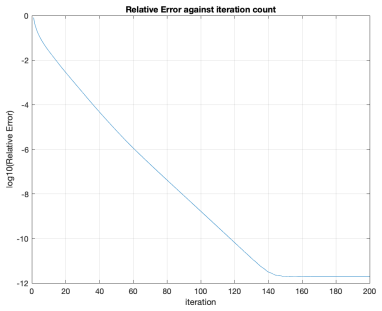

Fig. 5. Relative residual error $\chi^{(k)}$ for example two. Relative error of 10^{-3} achieved after 25 iterations.

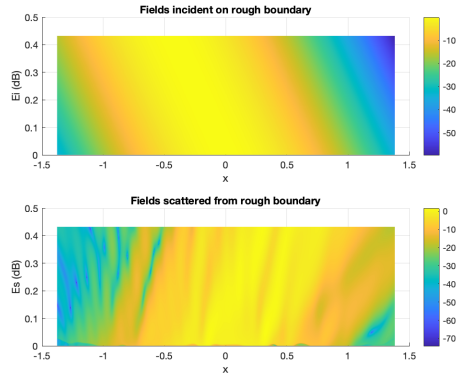

Fig. 6. Incident fields (above) and scattered fields (below) in dB in the space above rough boundary between free space and medium with $\epsilon_r = 3$. Tapered incident field is centred on (0,0) and is impinging at 45 degree angle to normal.

eigenvectors (with eigenvalues greater than one) form a low-dimensional sub-space which can be projected away from when performing the SSOR iterations. One need not know the eigenvector information beforehand as dominant eigenvectors can be approximated during the algorithm run-time. The method is compatible with acceleration methods such spectral acceleration (which has not been applied in this

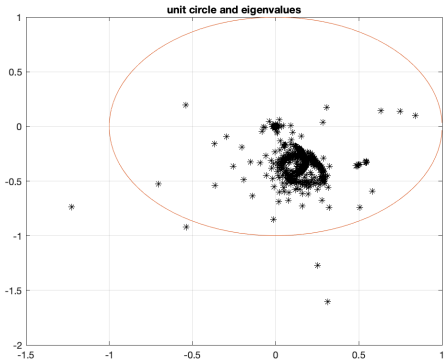

Fig. 7. Eigenvalues of SSOR iteration matrix for example 3. Spectral radius is 1.634878 and there 4 eigenvalues outside the unit circle

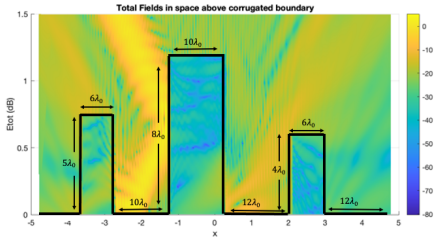

Fig. 8. Total fields in dB in the space above corrugated boundary between free space and medium with $\epsilon_r = 4 - 0.1j$. Tapered incident field with $g = 0.5$ is centred on (0,0) and is impinging at $\theta_i = \frac{\pi}{3}$. Boundary between regions shown by black lines (note scale different on horizontal and vertical axes).

paper) as vectors are updated on a component by component basis. The method is also compatible with the use of suitable preconditioning to reduce the spectral radius before applying SSOR. Again, this was not applied in this paper but will form the basis of future work along with a study of what the most effective strategy for identifying and approximating the necessary eigenvectors, in order that the method can be most effectively applied to larger, and more general, problems.

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