Scattering matrix evaluation using spatial symmetry in electromagnetic modelling

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SUMMARY

In this paper we discuss the possibility of a drastic computational reduction in forming the scattering matrix for electromagnetic modelling of 3-D conductivity structure embedded in a stratified and vertically anisotropic earth using integral equations. This reduction is facilitated by using the lateral homogeneity of the space and the symmetry property of the Green's functions to reduce the redundancy of calculating the scattering matrix by identifying classes of cell pairs which give either identical entries in the scattering matrix or entries that differ only in the sign. It is required that a conductivity structure be discretized into equal-size or equal-size-based cells. By the latter we mean that the structure is first divided into equal-sized basic cells, and some odd numbers of the basic cells may form secondary, bigger cells where the scattering currents and other field quantities may be assumed to be constant, in order to allow the symmetry reduction while keeping the dimension of the linear system as low as possible. This method of reduction is valid for arbitrary conductivity structure. The factor of reduction depends mostly on the number of cells in the lateral direction and can be up to several hundred.

Key words: EM modelling, scattering matrix, symmetry reduction.

1 INTRODUCTION

Electromagnetic modelling of 3-D conductivity structures using integral equations has been widely accepted in geophysics since its appearance in the early 1970s (Hohmann 1971, 1975; Weidelt 1975). Yet the quadratically growing requirements on computer storage and on computation time in forming the scattering matrix, and the cubic growth of matrix factorization time with the number of discretization cells have remained the major obstacles for its application for about two decades.

The computation of the scattering matrix elements usually consumes about 80 per cent of the total CPU time for models of moderate size. The cubically growing time consumption of the matrix factorization is dominant only for models with a fairly large number of cells, say over 500 cells. With the optimization efforts of Xiong (1992a) where he approached the integration of the secondary parts of the Green's tensors in the vertical direction analytically in the Hankel transform domain and thus increased the accuracy and efficiency of the numerical integrations, the computation time required by matrix formation was greatly reduced. Even so, forming the scattering matrix still takes about 50 per cent of the total CPU time for structures with moderate discretization. Also, the computation of the scattering matrix elements involves tedious numerical integrations of the Green's tensors which are merely scalar and cannot be vectorized. Thus, in the integral equation method the formation of the scattering matrix can dominate the computation time.

With the introduction of the method of system iteration (Xiong 1992a), matrix factorization time and storage requirements were markedly reduced. In the method of system iteration a conductivity structure is divided into many substructures. The direct matrix inversion is applied to each substructure only, whereas the mutual interactions among the substructures are treated as being due to equivalent sources. This method not only solves the problem of storage requirements, but also greatly reduces the computation time needed for the solution of the matrix equation. Furthermore, the method of system iteration also allows vector and/or parallel processing. Hence, the scattering matrix formation time dominates the computation for large structures, too.

We can use geometric model symmetries, if present, to mitigate these computational problems. Among others, Tripp & Hohmann (1984) (see also Tripp 1990) put forward a block diagonalization method which reduces the scattering matrix to four block diagonal matrices and reduced the computation time for matrix formation by a factor of 4. The
method also reduces the storage requirement by a factor of 16 and the matrix factorization time by a factor of 16. About the same efficiency was reached by Xiong (1992b) for plane wave excitations where only the scattering current in one quarter needs to be computed. Those reductions, however, are limited to symmetrical models only. For arbitrary models that are not symmetrical such reductions are invalid.

In this paper we show that the computation time required by the scattering matrix formation can be drastically reduced for models embedded in a layered earth. The reduction can be up to a factor of 100s, depending on the number of discretization cells in the lateral directions. This is achieved by reducing the redundancy of calculating the scattering matrix by identifying classes of cell pairs that give either identical entries in the scattering matrix or entries that differ only in the sign by using the lateral homogeneity of the space and the symmetry property of the Green’s functions.

This reduction of computation is valid for arbitrary structures. However, we need to discretize a conductivity structure into equal-size cells, or equal-size-based cells. By the latter we mean that a structure is discretized into two sets of cells, with a set being equal-sized basic cells. Some odd numbers of the basic cells may form secondary, large cells in which the scattering currents and other field quantities are assumed to be constant. Thus, the discretization of a conductivity structure should not be arbitrary, but should be comprised of basic, equal-size cells.

2 THE INTEGRAL EQUATION METHOD

Here we follow the notation and discussions of Xiong (1992a). Let us consider the model shown in Fig. 1. The earth is assumed to be vertically anisotropic with a conductivity tensor \( \sigma_n \) of a diagonal form with the entries \( \sigma_h \), \( \sigma_v \), and \( \sigma_w \), where \( \sigma_n = \sigma_h + i \omega \varepsilon_h \) and \( \sigma_v = \sigma_v + i \omega \varepsilon_v \) are the complex conductivities of the medium in the horizontal and the vertical directions, respectively.

\[
\begin{align*}
\sigma_h & \quad \sigma_v \\
\sigma_w & \quad \sigma_n
\end{align*}
\]

**Figure 1.** An arbitrary 3-D structure comprised of multiblocks embedded in a stratified vertically anisotropic earth. \( \sigma_h \) and \( \sigma_v \) are the horizontal and vertical conductivity of the earth. \( \sigma_n \) represent the 3-D conductivity structure. Dotted lines show the arbitrary discretizations of the blocks.

The scattering current, denoted by \( \mathbf{J}_s \), within an arbitrary 3-D structure embedded in the anisotropic host is defined as

\[
\mathbf{J}_s = \sigma_n \cdot \mathbf{E},
\]

with \( \sigma_n = \sigma \delta - \sigma_m \), where \( \delta \) is a unit tensor, \( \sigma \) is the conductivity of the structure which we assume to be isotropic for simplicity, and \( \mathbf{E} \) the total electric field in the structure.

The scattering current \( \mathbf{J}_s \) within a structure \( V \) satisfies the following Fredholm integral equation of the second kind:

\[
\Theta \cdot \mathbf{J}_s(r) - \int_V \mathbf{G}^E(r | r') \cdot \mathbf{J}_s(r') dv' = \mathbf{E}_n(r), \quad (2)
\]

where \( \mathbf{E}_n \) is the incident electric field in the absence of the 3-D scatterer, and \( \mathbf{G}^E \) is the electric Green’s tensor. Once \( \mathbf{J}_s \) is found from eq. (2), the electromagnetic fields everywhere can be determined by integration of the scattering current with corresponding Green’s functions.

Equation (2) is usually discretized by dividing the structure \( V \) into \( M \) cells, which yields the matrix equation,

\[
(\Gamma)(\mathbf{J}_s) = (\mathbf{E}_n), \quad (3)
\]

with

\[
\Gamma_m(r_m | r_n) = \delta_m \Theta_{mn} - \int_{V_m} \mathbf{G}^E(r_m | r_n) dv, \quad (4)
\]

where

\[
\delta_{mn} = \begin{cases} 1, & m = n, \\ 0, & m \neq n. \end{cases}
\]

The coefficient matrix \( \Gamma \) in eq. (3) is usually referred to as the scattering matrix. It is also known as the impedance matrix (Tripp & Hohmann 1984). The size of \( \Gamma \) is \( N \) by \( N \) where \( N = 3 \times M \), since we have three components for each vector quantity. The \( m \) in \( \Theta_{mn} \) indicates that the conductivity \( \sigma \) in \( \Theta \) takes the value at \( r_m \).

3 SPATIAL HOMOGENEITY AND THE SYMMETRY RELATION OF GREEN’S TENSOR

Let us consider again the model depicted by Fig. 1. The space consists of an air layer in the upper half-space, and multilayered earths of anisotropic conductivity. Note that the anisotropy is only in the vertical direction. If we ignore the 3-D conductivity structure and look vertically down at the stratified earth, the earth will be homogeneous in all lateral directions along each \( (x-y) \) plane. This lateral homogeneity of the space was used by Xiong (1992b) to study the symmetry relations of the scattering matrix to reduce the modelling problem to a quarter of a symmetrical
3-D structure only. Following the same lines as Xiong (1992b), however, we can show in what follows that most of the elements of the scattering matrix for a 3-D structure, which is discretized into equal-size cells, are related by some simple symmetry relations, which facilitate drastic reductions in computing the scattering matrix elements.

For simplicity of discussion, and without losing any generality, we consider a block structure discretized into \(N_x \times N_y \times N_z\) equal-size rectangular prismatic cells, as shown by the solid lines in Fig. 2. The conductivity in the block can be arbitrary, provided that the conductivity of each cell remains constant within the cell itself.

We now construct three more adjacent imaginary blocks using reflections to the \(X\)- and \(Y\)-axes, respectively, and a rotation of 180°. However, the imaginary blocks do not have the same size as the original one. The block generated by the reflection to the \(X\)-axis is one cell less in the \(y\) direction; the block generated by the reflection to the \(Y\)-axis is one cell less in the \(x\) direction; and the block generated by rotation is one cell less in either direction. We label the cells in the original block by \(ij\) in the lateral directions where \(i\) and \(j\) refer to the \(x\) and \(y\) directions, respectively. The cells in the vertical direction have their \(z\) locations denoted by either \(z\) or \(z'\). The imaginary cells are numbered by \((-i)j\), \((-i)(-j)\), and \((-i)(-j)\), as shown in Fig. 2. The cells with \((-1)j\) are identical to the cells denoted by \(ij\), while the cells denoted by \(i(-1)\) are identical to those denoted by \(i\).

If we translate the coordinate system \(XYZ\) to a new system \(X'Y'Z\), with the \(X'\)- and \(Y'\)-axes passing through the centres of the cells 11 and \(Z\) unchanged, we see that the cells \((-i)j\), \((-i)(-j)\), and \((-i)(-j)\) are the symmetrical imaginings of the cell \(ij\) with respect to the cell 11. For complete representations of the cell locations, we denote the cells with the cell centre vectors \(r'_{ij}\), etc.

The spatial homogeneity and the linearity of the Green's tensors with the directions of the coordinate axes allow us to deduce the symmetry relations of the components of the Green's tensors \(G(ri1|ri'_{ij})\), \(G(ri1|ri'_{ij})\), and \(G(ri1|ri'_{ij})\) with the components of \(G(ri1|ri'_{ij})\). This can be readily done by taking into account the \(X'\)- and \(Y'\)-axis directions as well as the directions of components of the Green's tensors, as discussed in Xiong (1992b). If we write down all the components of the Green’s tensors \(G(ri1|ri'_{ij})\), where \(l=(-i)j\), \((-i)(-j)\), and \((-i)\), as a function of the components of the Green's tensor \(G(ri1|ri'_{ij})\), the symmetry relation will be very obvious:

\[
G(r_{i1} | r'_{ij}) = \begin{pmatrix}
\beta_{xx}G_{xx} & \beta_{xy}G_{xy} & \beta_{xz}G_{xz} \\
\beta_{yx}G_{yx} & \beta_{yy}G_{yy} & \beta_{yz}G_{yz} \\
\beta_{zx}G_{zx} & \beta_{zy}G_{zy} & \beta_{zz}G_{zz}
\end{pmatrix} (r_{i1} | r'_{ij})
\]

Table 1 shows the values of the symmetry coefficients \(\beta\). Note the form \(G(r_{i1} | r'_{ij})\) denotes the field quantities due to the source cell at \(r_{ij}\) to be measured at \(r'_{ij}\).

| \(r_{i1} | r'_{ij}\) | \(r_{i1} | r'_{ij}\) | \(r_{i1} | r'_{ij}\) |
|----------------|----------------|----------------|
| \(\beta_{xx}\)  | \(\beta_{xy}\)  | \(\beta_{xz}\)  |
| \(\beta_{yx}\)  | \(\beta_{yy}\)  | \(\beta_{yz}\)  |
| \(\beta_{zx}\)  | \(\beta_{zy}\)  | \(\beta_{zz}\)  |

4 REDUCTION OF COMPUTATION BY THE SYMMETRY RELATIONS

4.1 Equal-size cells

If we compute all the elements of \(G(r_{i1} | r'_{ij})\), for \(i = 1, 2, \ldots, N_i\), and \(j = 1, 2, \ldots, N_j\), we can obtain the
elements of the Green's tensors from all the imaginary cells to cell 11 in Fig. 2 according to eq. (5). Now suppose we want to determine the values of \( G(r_{m1}, r_{p1}) \) with \( m \) and \( p = 1, 2, \ldots, N_x \), and \( n \) and \( q = 1, 2, \ldots, N_y \). With a translation of the coordinate system in the lateral direction by moving cell 11 to the cell at \( r_{m0} \) in the original block, we see that the value of \( G(r_{m0}, r_{p0}) \) can be easily found from the results determined by \( G(r_{m1}, r_{p1}) \), for \( i = 1, 2, \ldots, N_x \), and \( j = 1, 2, \ldots, N_y \), and eq. (5), due to spatial homogeneity of the space in the lateral direction. In this way, we can evaluate every element of the Green's tensor in the original block.

Thus, with the results of \( N_x N_y \) operations, we obtain what used to require \((N_x N_y)^2\) operations, or \((N_x N_y)(N_x N_y + 1)/2\) operations, if reciprocity is taken into account, a reduction of a factor \((N_x N_y + 1)/2\) for one \( z \) and one \( z' \) level. Here we refer to one operation as the evaluation of all the nine components of the Green's tensor which tie one cell to another.

For a structure discretized into \( N_x \times N_y \times N_z \) cells, we usually need

\[ N_x N_y N_z (N_x N_y + 1)/2 \]

operations to get the \((3 \times N_x N_y N_z)^2\) matrix elements. If we repeat the above procedure for all the cells in the vertical direction, namely, all the \( z \) and \( z' \) levels, we need only

\[ N_x N_y (N_z)^2 \]

operations to get the \((3 \times N_x N_y N_z)^2\) matrix elements in eq. (3). We can also take advantage of the reciprocity of the Green's tensors in computing the matrix elements for the different \( z \) and \( z' \) levels. However, reciprocity can only be used for \( z \neq z' \). For \( z = z' \), we cannot apply the reciprocity theorem to find the Green's tensors since all the \( N_x N_y \) operations are necessary for computing the matrix elements at one \( z \) and \( z' \) level. Thus, the total number of operations will be

\[ N_x N_y (N_z + 1)/2 \]

Therefore, the reduction of computation is a factor of

\[ \frac{N_x N_y N_z + 1}{N_z + 1} \]

This is a tremendous reduction. To illustrate the efficiency, if we discretize a body into \( 10 \times 10 \times 10 \) cells, totalling 1000 cells, the reduction of computation of the scattering matrix will be 91 times; if we have 1000 cells in the lateral direction, and only 1 cell in the vertical direction, or 500 cells in the lateral direction and 2 cells in the vertical direction, both also totalling 1000 cells, the reduction will be 500 and 333 times, respectively.

Here we considered the lateral homogeneity only. If we divide the Green's tensors into whole space and layered earth parts, the whole space parts will have an additional symmetry with respect to the vertical direction, if the entire structure lies within one layer. This will allow us to further reduce the computation needed by the whole space parts. This can be done as for Fig. 2 provided now we need a 3-D picture. The reduction for the whole space parts will be a factor of \((N_x N_y N_z + 1)/2\).

**Figure 3.** A block structure discretized into two sets of cells. The dotted lines show the basic equal-sized cells. Every three basic cells but the first and the last one form a bigger, secondary cell shown by the thin solid lines.

### 4.2 Non-equal-size cells

The only restriction for the reduction discussed in the previous section would be the requirement that all cells have the same size. The structure can be of arbitrary shape and of arbitrary conductivity. If we model an arbitrary structure by a cluster of blocks where each block is discretized into equal-size cells (Xiong 1991, 1992a), we can still use the technique discussed above to reduce the computation of all the diagonal block matrix elements associated with each of the conductivity blocks, if the cell sizes in the conductivity blocks differ from each other.

However, due to the great advantages of equal-size cells, we suggest discretizing any structure into equal-size cells to facilitate the above-discussed reduction, or discretizing a structure into two sets of cells, with the basic set of cells being equal-sized. Some odd number of cells from the basic cell set may form the basis of a secondary set of bigger cells across which the scattering currents are assumed to be constant. This would allow us to use the above-discussed reduction in forming the scattering matrix whilst keeping the dimension of the matrix equation as small as possible. Non-equal-sized cells are useful for modelling large structures in which the scattering currents vary drastically near the structure boundaries while remaining relatively invariant in body centres.

As an example, we divide a block structure into \( 8 \times 8 \times 8 \) cells, and we combine every three cells but the first and the last cells in either direction into large cells where the scattering currents are assumed to be constant, giving a final discretization of \( 4 \times 4 \times 4 \) non-equal-size cells only. Fig. 3 shows the two different discretizations. The dotted lines show the basic cells, while the thin solid lines show the secondary cells. If we define one operation as the numerical integration of the basic cell of the discretization \( 8 \times 8 \times 8 \), the accurate integration of the Green's tensor due to the secondary, large cells approximately involves as many operations as the number of basic cells which comprise the large cells. The computational saving of the large cell system will be achieved through factoring a matrix with a reduced number of matrix elements. The total number of operations
for forming the matrix equation of the secondary discretization of $4 \times 4 \times 4$ cells while including redundant calculations would involve approximately $4^3 \times 8 = 32,768$ operations. With the method of reduction, we need $8 \times 8 \times [8(8 + 1)/2] = 2304$ operations, a reduction of factor 14.

In general, if we have $N_x \times N_y \times N_z$ basic cells, and from those basic cells we build $N_x^* \times N_y^* \times N_z^*$ secondary cells, we have a matrix equation of dimension $3N_x^*N_y^*N_z^*$ instead of $3N_xN_yN_z$. The computation of the matrix elements will involve approximately $N_x^*N_y^*N_z^*N_xN_yN_z$ operations if the symmetry relations are not taken into account. Here again each operation is defined as the numerical integration of the Green's tensor contributed by a basic cell. Thus, if we use the symmetry algorithm discussed above, we will have a reduction of

$$\frac{N_x^*N_y^*N_z^*N_xN_yN_z}{N_xN_yN_z(N_x + 1)/2} = \frac{N_x^*N_y^*N_z^*}{(N_x + 1)/2}.$$  

If we drop some computations arising from the unnecessary $z$ levels, since we need only $N_z^*$ $z$ levels for the secondary cell system, the number of operations required when using the symmetry relations will be

$$N_xN_yN_zN_z^*,$$

and the reduction of computation will be a factor of

$$N_x^*N_y^*N_z^*,$$

depending on the number of the secondary cells in the lateral direction alone.

5 A NUMERICAL EXAMPLE

To illustrate the above-discussed saving of computation time, we present a numerical example. The 3-D structure is a $10 \times 5 \times 5 \text{km}^3$ conductivity block with an electric resistivity of 1 $\Omega\text{m}$ buried 0.5 km deep in a half-space of 1000 $\Omega\text{m}$. Suppose the excitation is a plane wave at a frequency of 1 Hz and seven receivers are required. Even though this model is a symmetrical one, we do not use the model symmetry in the following discussions in order to address the problem with a general scope.

Table 2 shows the computation time required by different parts of the computations for four different discretizations of 54, 128, 200, and 480 cells, respectively. The 'Factor' in the table means the factors of reduction facilitated by the method discussed above, which are the ratios of the numbers in the column under 'non-reduced' to the number in the column under 'reduced'. Here 'reduced' refers to the method with the symmetry reductions. The 'other' column contains miscellaneous computation times, primarily the time needed for computing the responses at the seven receivers and for establishing the grid values for the interpolations of the Hankel transforms required by the numerical integrations of the Green's tensors. The computation time needed by these two operations is in general linear with the number of cells and plays a minor role in the computation for about 100 or more cells. The computation times listed in Table 2 are the CPU time in seconds on a SUN SPARC 2 station.

The numerical integration of the Green's tensors of our code has been greatly optimized (see Xiong 1991, 1992a). The optimization includes the analytical integration of the secondary parts of the Green's tensors in the vertical direction in the Hankel transform domain. This also enables us to reduce the tedious 3-D interpolations of the Hankel transforms required in the numerical integrations, which used to dominate the computation, to 1-D interpolations. Despite all these optimization efforts, the computation time needed by the matrix formation still takes about 50 per cent of the total CPU time for small to moderate size models if the symmetry reduction is not used. It should be noted that the computation time required by the matrix formation also depends on the accuracy levels desired for the matrix elements. Our code defines different accuracy levels by different step lengths for the numerical integration over the cells. The results in Table 2 were computed at a moderate accuracy level which ensured that the modelling results of the conductivity structure for the discretization of 54 cells were still reliable.

With the symmetry reduction method of computation the computation time needed by the matrix formation almost vanishes as compared with the matrix factorization time or total CPU time. The reduction factors of the matrix formation are almost exactly as predicted by the theory in the previous section. As the numbers of cells increase, the factors of reduction become slightly smaller than their theoretical values. This reduced efficiency is due to the fact that identifying the $\beta$ values in eq. (5) involves an additional computation time. If we ignore this portion of the computation time, the factors of reduction are the same as their theoretical values.

So far we have limited out computational trials to 480 cells. However, using straightforward estimators, we may estimate how much time would be required by each part of the computation for a large number of cells. Suppose we have 2000 cells. Since the computation time required by matrix formation grows quadratically with the number of cells, the non-reduced method requires about 86 111 s while the symmetry reduction method requires 1302 s. The computation time needed for the reduced method depends, of course, on the discretization. The matrix factorization time would be then 346 630 s, since it grows cubically with the number of cells. Note that the matrix factorization time listed in Table 2 is the time required by direct matrix inversion. If the method of system iteration is used, however, the computation time for solving the matrix equation would be greatly reduced. If, as discussed in Xiong (1992a), the computation time for solving a matrix equation of 2000 cells can be reduced by about nine times, only about 38 514 s will be needed to solve the matrix equation, compared with the 86 111 s in matrix formation if symmetry...
reduction is not used. Thus, the reduction in matrix formation time is also significant for large bodies.

6 CONCLUSIONS

Using the spatial homogeneity and thus the symmetry relations of the Green's tensors we have drastically reduced the computation time of the scattering matrix in electromagnetic modelling with the integral equation method. As shown by the example, what used to dominate the computation now becomes a small fraction of the total computation time.

This great reduction allows us to compute the elements of the scattering matrix to a high accuracy at small cost, which facilitates a thorough, detailed numerical analysis of the accuracy of our modelling schemes. The quantitative analysis of the accuracy of the modelling schemes has been untouched so far, partly due to the high costs.

The requirements that a 3-D structure be discretized into equal-size cells or equal-size-based cells in order to realize the reduction using symmetries implies that the discretization of a conductivity structure should obey certain laws and should not be arbitrary. Only in an organized way can we achieve great efficiency.

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