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Accelerating an EM integral equation forward solver for global geomagnetic induction using SVD based matrix decomposition method

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SUMMARY

We develop an SVD based recursive decomposition of the system matrix of an EM integral equation forward solver for global geomagnetic induction, on top of an FFT reduction of the system to a block-diagonal form. With this approach, the memory cost and computational complexity of Krylov subspace iterative solutions are significantly reduced, making the accelerated forward solver suitable for 3-D inversions. We explore different implementation schemes to assess the effectiveness of this method.

Keywords: 3-D forward modeling, integral equation, matrix decomposition, fast algorithm

INTRODUCTION

Frequency-domain integral equation (IE) based electromagnetic (EM) forward solvers, known for their high accuracy and numerical stability, flexible discretization, as well as compact computational domain with exact boundary conditions for open domain problems, find their applications in geomagnetic induction at both local and global scales (Wannamaker, 1991, Fainberg et al *et al.*, 1990, Avdeev *et al.*, 2002, Koyama, 2001, Kuvshinov *et al.*, 2002, Singer, 2008, Sun & Egbert, 2012; among others). However, a known drawback of such methods is the large computational complexity, since EM Green's functions, central to the IE formulation, are global operators that, after discretization, result in full system matrices. Fortunately, certain properties of typical EM Green's functions allow efficient storage and fast application (multiplication) of such operators, leading to fast implementation of iterative solutions, e.g., Krylov subspace methods, to the IE. One such property is the shift invariances of the Green's functions defined on regular grids under invariant background geometries, e.g., shift invariances in lateral dimensions for horizontally layered structures under cartesian geometry, and rotational invariance under spherically layered geometry. Such invariances allow applications of the Green's functions to be implemented as linear or circular convolutions using fast Fourier transform (FFT). However, when such invariances are not available either due to shift-variant grids or shift-variant background geometries, FFT cannot be directly applied. In such more general cases, another property, the diagonal dominance of the Green's functions, is often employed. The diagonal dominance is the result of a general phenomenon that EM field responses of a collection of sources reduce with distance. This is especially true for quasi-static interactions in lossy media, as is the case in geomagnetic induction. When the sources a sufficiently separated from the observations, the observed EM field has a much smaller degree of freedom than the total number of possible configurations of the sources. The field can thus be computed from a reduced number of equivalent sources with reduced computational complexity and memory requirement. Acceleration methods based on such considerations are numerous, see Chew *et al.* (1997) for a review. Two such methods widely used in IE EM forward modeling include: fast multipole algorithm (FMA) and varieties (Rokhlin, 1990, Lu & Chew, 1994), which develop analytic local and multipole expansions of Green's functions of known analytic forms; and matrix decomposition algorithm (MDA) and varieties (Michielssen & Boag, 1994, Rius *et al.*, 2008), which develop expansions of the Green's functions using numerical linear algebra techniques. While the multi-level variety of FMA is asymptotically slightly faster than the multi-level MDA for very large scale EM scattering problems, the matrix decomposition methods are more straightforward to apply to existing implementations of IE solvers, and should work very effectively for quasi-static EM induction problems involving lossy media.

In this work, we apply a singular value decomposition (SVD) based matrix decomposition method, similar to that developed by Rius *et al.* (2008), to an IE forward solver for global geomagnetic induction. The Green's function of a spherically layered Earth, when discretized on a regular spherical coordinates grid of $N_\theta \times N_\phi \times N_r$, where N_θ, N_ϕ and N_r are numbers of samples in colatitudinal, longitudinal and radial dimensions, respectively, is rotationally invariant with respect to the longitude ϕ. Applying FFT in the longitudinal direction transforms the discrete Green's function operator into a block-diagonal form of N_ϕ diagonal blocks. Each diagonal block is a full matrix of $N_\theta N_r \times N_\theta N_r$. An SVD based recursive matrix decomposition procedure is then applied to each of these diagonal blocks, leading to a recursively decomposed form of the Green's function with maximal compression.

CONCEPT

To illustrate the concept, let us consider integral equation formulation of global geomagnetic induction in a form

$$\mathbf{E} = \mathbf{E}_0 + \mathbb{G}(\Delta\sigma \mathbf{E}) \,, \tag{1}$$

where $\mathbf{E}$ is the unknown total electric field in the computational domain, i.e., the three-dimensional (3-D) conductive Earth, $\mathbf{E}_0$ is the known "unperturbed" electric field, i.e., the electric field if the conductivity anomaly $\Delta\sigma = 0$, and $\mathbb{G}$ is the second-order tensor Green's function of the background, typically a spherically layered Earth. A fixed-point iterative solution to (1) may be given by

$$\mathbf{E} = \sum_{n=0}^{\infty} \mathbf{E}_n \,, \tag{2}$$

where

$$\mathbf{E}_n(\mathbf{r}) = \int d^3r' \, \mathbb{G}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_n(\mathbf{r}') \,, \tag{3}$$

where the field point $\mathbf{r} = (r, \theta, \phi)$, the source point $\mathbf{r}' = (r', \theta', \phi')$, $\mathbb{G}(\mathbf{r}, \mathbf{r}')$ is the kernel of the Green's function $\mathbb{G}$ without ambiguity, and $\mathbf{J}_n(\mathbf{r}) = \Delta\sigma(\mathbf{r})\mathbf{E}_{n-1}(\mathbf{r})$. The simplest discrete version of (3) is

$$\begin{aligned} \mathbf{E}_n(r_i, \theta_j, \phi_p) = \sum_{k,l,q} & \mathbb{G}(r_i, \theta_j, \phi_p, r_k, \theta_l, \phi_q) \\ & \cdot \mathbf{J}_n(r_k, \theta_l, \phi_q) r_k^2 \sin\theta_l \Delta r \Delta\theta \Delta\phi \,, \end{aligned} \tag{4}$$

where $\Delta r, \Delta\theta, \Delta\phi$ are spacings of the uniform numerical grid. To implement (2) numerically, recursive computations of (4) is the most time-consuming part. Fast and efficient implementation of (4) thus becomes critical.

Due to rotational invariance of a sphericall layered Earth, $\mathbb{G}$ is shift invariant in ϕ, i.e., $\mathbb{G}(r_i, \theta_j, \phi_p, r_k, \theta_l, \phi_q) = \mathbb{G}(r_i, \theta_j, r_k, \theta_l, \phi_p - \phi_q)$. Applying FFT with respect to ϕ to (4) leads to

$$\begin{aligned} \tilde{\mathbf{E}}_n(r_i, \theta_j, s_m) = \sum_{k,l} & \tilde{\mathbb{G}}(r_i, \theta_j, r_k, \theta_l, s_m) \\ & \cdot \tilde{\mathbf{J}}_n(r_k, \theta_l, s_m) \,, \end{aligned} \tag{5}$$

where the tilde'd quantities are FFT's of the original quantities, indexed by the discrete (spatial) frequency $s_m \in \{0, 1, ..., N_\phi - 1\}$, and the metric factor $r_k^2 \sin\theta_l \Delta r \Delta\theta \Delta\phi$ maybe absorbed into either $\tilde{\mathbb{G}}$ or $\tilde{J}_n$.

To efficiently store the matrix $\tilde{\mathbb{G}}(s_m)$ and compute the matrix-vector multiplication given by (5), we observe diagonal dominance of $\tilde{\mathbb{G}}(s_m)$ and decompose it recursively, as illustrated in Figure 1.

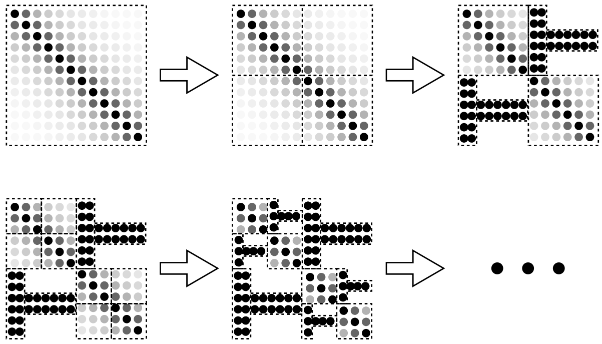

Figure 1. Illustration of recursive decomposition of a diagonally dominant matrix.

The matrix $\tilde{\mathbb{G}}$ is first divided evenly into four sub-blocks, two diagonal and two off-diagonal. Due to diagonal dominance of $\tilde{\mathbb{G}}$, the off-diagonal blocks are numerically rank deficient and may be approximated by the first few terms of their SVD representations. The truncation errors are easily quantified by the sum of squares of the truncated singular values, leading to a quantification of errors in terms of squares of the sub-blocks' Frobenius norms summable over sub-blocks. Specifically, if the maximal allowed error in terms of Frobenius norm of the matrix $\tilde{\mathbb{G}}$ is ϵ, each of the four sub-blocks is allowed to have an error of $\epsilon/2$, the total error is thus $\sqrt{4(\epsilon/2)^2} = \epsilon$. The off-diagonal sub-blocks are approximated by truncating their SVD at levels corresponding to a truncation error of $\epsilon/2$, in terms of the square root of the sum of squares of the truncated small singular values. The on-diagonal sub-blocks are again diagonal dominant, and similar procedures may be recursively applied (maintaining a total error of $\epsilon/2$ for each sub-block) until the diagonal sub-blocks become too small or the off-diagonal sub-blocks become rank sufficient. This procedure leads to a compression of the original matrix $\tilde{\mathbb{G}}$, in terms of both storage and computational complexity of matrix-vector multiplication, with a prescribed error ϵ in terms of Frobenius norm. Note that in theory, the compression ratio with regard to memory efficiency is the same as that with regard to computational efficiency, since for each matrix-vector multiplication, each element in the compressed form of the original matrix is multiplied exactly once. Different domain decomposition schemes, not restricted to a 2×2 subdivision, as well as different error distributions among sub-blocks may be explored to find the "optimal" choice of schemes.

AN EXAMPLE

To illustrate the procedures described in the preceding section, we consider a simplified example of induction from an inhomogeneous spherical shell of inner radius 0.5 and outer radius 1, discretized on a regular spherical grid of $N_\theta \times N_\phi \times N_r$, where $N_\theta = 128$, $N_\phi = 256$ and $N_r = 32$. Figure (2) shows a cross-section of the 3D numerical grid through the $0°$ longitude.

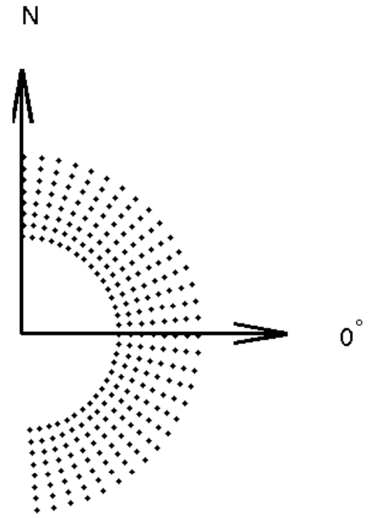

Figure 2. The cross-section of the numerical grid at $0°$ longitude.

For simplicity, we use a scalar Green's function assumed to be inversely proportional to the separation distance between the source and the field points to describe the induction. Such a Green's function is certainly rotational invariant under the spherical geometry. After applying FFT as described in (5), the leading term of the diagonal blocks, $\tilde{\mathbb{G}}(0)$, is shown in Figure (3), where the singular diagonal elements were regularized using simple extrapolation. The total number of elements in $\tilde{\mathbb{G}}(0)$ is around 1.6×10^7, and the total storage is around 128 MB. After applying the recursive matrix decomposition at a relative error of 0.1%, the total number of elements becomes around 2.4×10^6, and the corresponding storage is reduced to around 18 MB: a 7 fold compression ratio. At relative error of 1%, the compression ratio becomes around 10. In contrast, if a straightforward cutoff of smaller off-diagonal matrix elements are applied, for 1% error, less than 1% of all matrix elements are eliminated; For a compression ratio of around 10, a near 40% error is incurred!

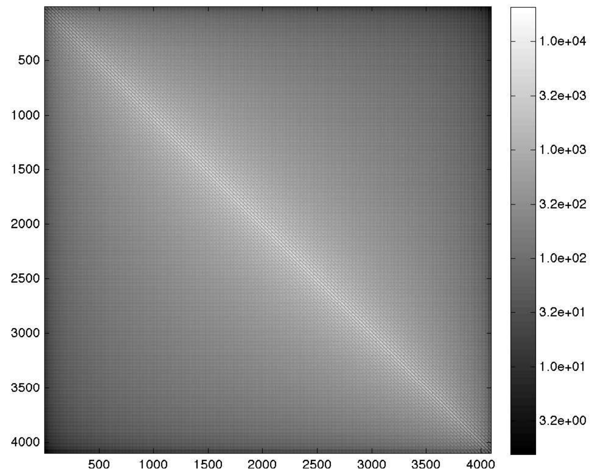

Figure 3. The leading diagonal block of the FFT'ed Green's function in logarithm scale.

CONCLUSION

We have developed a simple and effective compression method for the EM Green's function encountered in global geomagnetic induction. This method is based on recursively approximating the off-diagonal sub-matrices of the diagonal-dominant tensor Green's function using SVD based low rank approximations. A simplified illustrative example reveals a 7 fold compression with only 0.1% error in terms of Frobenius norm. A compressed Green's function is particularly efficient in a gradient-search based 3-D inversion of global induction, where a Krylov subspace based forward solver involving iterative application of the Green's function as well as its adjoint has to be performed repeatedly.

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