Three-dimensional Modelling of the Earth's Mantle

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Abstract. Recently, Uyeshima and Schultz devised an accurate forward solution for EM induction in a 3D heterogeneous sphere based on a staggered-grid finite difference method. In the present paper we consider the means by which this may be accelerated substantially. This is an essential step if this method is to be used as the basis of a practical 3D inversion for the electrical conductivity of the Earth's mantle. Uyeshima and Schultz solved the forward system, a large sparse complex symmetric matrix, by iterative relaxation methods. Uyeshima and Schultz solved the problem by employing Mackie and Madden's minimum residual accelerated (MRA) method, a form of conjugate gradients (CGs). However, since this method is strictly valid only for real, symmetric (and thus Hermitian) and positive-definite matrices, it does not necessarily guarantee the convergence of the relaxation process for arbitrary models. To recover a Hermitian system of equations, we reposed the solution such that the biconjugate gradient (BiCG) method could be used. BCG is valid even for complex symmetric matrices. A variant of the biconjugate gradient method, BiCGSTAB, was finally employed to stabilise the relaxation process. This resulted in an approximate halving of the number of iterations required per relaxation. Further acceleration was obtained by parallelizing the problem over multiple frequencies with frequency sorting in ascending order. It was found crucial for efficient parallelization to make good use of the previous solution, i.e. substituting that solution as the initial solution for each subsequent frequency. This reduced substantially the unnecessary initial overheads of each relaxation. Examination of the accelerated code showed that the new solutions retained the accuracy that characterised the original Uyeshima and Schultz solution. The new 3D solution is shown to be accelerated by an order of magnitude relative to the original solution, thus making feasible 3D inversions of global mantle conductivity.

1 Introduction

There are on-going efforts to establish EM induction counterparts to global seismic tomographic and normal modes models of the Earth's mantle. The importance of this arises from the independent view of deep Earth conditions afforded by constraints on the electrical and elastic parameters that are provided by the two methods. The electrical conductivity of the mantle reflects the temperature, melt fraction, compositional variability (e.g Fe content) and presence of volatiles, especially water and hydrogen. Conductivity also provides a view of mineral phase transitions. Joint interpretation of seismic and EM data sets promises to more strongly constrain the geotherm, composition and state of the Earth's mantle. In addition, the discrepancies of the two may give rise to development of new interdisciplinary research fields.

Radially symmetric earths, however, have often been assumed in global induction studies (e.g., Banks 1969) in spite of the fact that there is no 1D earth model that is compatible with temporal variations of long-period magnetic fields of all the existing geomagnetic observatories (Schultz and Larsen 1990). Lizarralde et al. (1995) found the presence of a high conductive zone centred at around 200 km depth in the northeast Pacific mantle, which is significantly more conductive than the mantle beneath the Canadian shield (Schultz et al., 1993) and similar in conductivity to that beneath the Basin and Range (Egbert and Booker 1992). Such information is consistent with an upper mantle in which large-scale lateral conductivity contrasts are required.

It has been argued in support of 1D interpretations that 3D EM induction effects are difficult to model because of the sparse spatial and temporal distribution of observatory sites, and that 3D computations are both more expensive and less accurate than existing 1D or 2D methods.

Fujii and Schultz (1998) have produced a set of unbiased EM response functions using data derived from the global network of geomagnetic observatories. In contrast to previous attempts to model time variations of the global-scale geomagnetic field through spherical harmonic analysis or similar expansions, a statistically robust empirical orthogonal function (EOF) method was used. While conventional methods suffer from a breakdown in the orthogonality of the basis functions when the spatial distribution of data is irregular (e.g. that of the geomagnetic observatory nework), the EOF approach does not (e.g. Egbert 1997, Fujii and Schultz, submitted). Fujii and Schultz also identified the significant effects of the statistical auroral oval current systems on EM response functions in the period band of 2d - 2y. Such response functions are typically calculated under the assumption that the source fields are due predominantly to the magnetospheric equatorial ring current. These new responses make use of both ring current and auroral current systems and provide an improved global distribution of data suitable for 3D interpretation.

Moreover, marked progress has been achieved in the development of fast and accurate forward solvers in heterogeneous spherical domains, i.e. the geometry required for global 3D EM induction studies. Recently, semi-analytical solutions have been developed for particular 3D situations within a spherical domain (Avdeev et al. 1997; Martinec 1998). Tarits et al. (1995) and Martinec (1999) developed spherical 3D EM forward solvers based on spectral methods. Weiss and Everett (1998) applied their spherical method to a realistic land-sea conductivity distribution. An on-going project of COmparison and validation of global SYnthetic electromagnetic techniques (COSY-B) is being carried out using the semi-analytical solutions as reference models. Among many competing codes, the Staggered-Grid Finite Difference (SGFD) forward solver by Uyeshima and Schultz (2000) has been proved at least as accurate as those using integral equations or Martinec's (1998) semi-analytical solutions using spherical harmonic expansion. This success motivated us to accelerate the code for practical application of the solver into a form suitable for 3D EM inversions.

2 Biconjugate Gradient Solution

Within the frequency band of EM soundings used for investigating the electrical conductivity of the mantle (approximately 2d -2y), we take Maxwell's equations in the quasi-static apporoximation in which displacement currents are neglected. The EM fields are taken to vary harmonically with time. The magnetic permeability is assumed to be equal to its free space value. Both the electric (**E**) and magnetic (**H**) fields are divergence-free. Following the 13-point SGFD by Uyeshima and Schultz (2000), we solved the quasi-static Maxwell's equations in spherical coordinates.

Uyeshima and Schultz's (2000) spherical solver was derived from a Cartesian geometry 3D SGFD solution developed by Mackie and Madden (1993, 1994). The Mackie and Madden's solver with incomplete Cholesky pre-conditioning is computationally efficient, and with accuracy equivalent to integral equation solutions (Mackie et al. 1993). Regardless to the physical shape of the target domains, the forward problem involves solving a matrix equation, involving a large sparse complex symmetric matrix $\mathbf{A}$, $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{x}$ is the solution vector containing either $\mathbf{E}$ or $\mathbf{H}$ and a $\mathbf{b}$ is a constant vector that stores boundary values of the fields. One advantage of SGFD is that solving for either $\mathbf{E}$ or $\mathbf{H}$ yields equivalent results, which is not usually the case in non-staggered FD approximations.

In the present study, the EM induction problem was solved for $\mathbf{H}$ by specifying the tangential components of $\mathbf{H}$ at the top of the spherical computational domain (i.e. at the location of the external source current systems) and at the bottom surface that bounds the internal volume of the heterogeneous sphere (i.e. at the top of the computational core of the model Earth).

According to Martinec (1999), this corresponds to solving a Dirichlet boundary value problem for the magnetic diffusion equation. The bottom surface was placed beneath the depth of the Core Mantle Boundary (CMB), 2890 km, where the tangential components of the magnetic field were set to nil. The source field was taken to originate from the Earth's magnetospheric equatorial ring current. This was approximated by a P10 harmonic of unit strength placed at a radial distance from the Earth's surface of 10RE, where RE is the Earth's radius. The electrical conductivity of intervening air layers was set to 10^{-10} S/m. At this 10RE, distance, secondary magnetic fields induced by the presence of the conducting Earth are damped out so they may be considered negligible (Uyeshima and Schultz 2000, Appendix). A major difficulty arises from the stiffness of the matrix solution. Since the coefficient matrix **A** has complex diagonal elements while all of the off-diagonal elements are real-valued, the matrix is non-Hermitian. **A** is also indefinite and very ill conditioned. The large condition number mainly stems from the large conductivity contrast between the insulating air layers and the conducting Earth.

Fast and accurate solution even for ill-conditioned sparse matrix systems have been made possible by the development of iterative relaxation methods, such as conjugate gradients. Mackie and Madden (1993) solved their 3D Cartesian forward problem by the MRA method, a variant of CG. Strictly speaking, however, the convergence properties of the MRA method have been established only for real, symmetric (and thus Hermitian) positive-definite matrices, which is not the case here. This implies that MRA is not necessarily guaranteed to converge for arbitrary models. This is an undesirable property if the solution is to be employed as the core of a practical 3D inverse method.

In order to recover a Hermitian system of linear equations, we reposed the problem so that a Bi-Conjugate Gradient (BiCG) method of matrix solution could be employed. This is valid for complex symmetric matrices (Smith, 1996). The BiCG method is Lanczos's (1952) generalization of the CG method that recovers the following Hermitian system of linear equations at the cost of doubling the number of equations to be solved. The increased number of computations per relaxation can be reduced by exploiting the symmetry of the coefficient matrix **A**. Jacobs (1981) showed that a BiCG method with a complex symmetric matrix can be converted into a method similar to the normal CG method. The key difference between the two is that all the Hermitian transposes **h** in the CG method should be replaced by simple transposes **t** in the BiCG method.

Static divergence correction (SDC) was introduced by Smith (1996) to ensure the divergence-free nature of the electric field. Even though conservation of the null divergence of the EM fields is intrinsic to SGFD, finite values of **divE** and **divH** sometimes emerge if the inductive effect is weak. Typical manifestations of the phenomenon can be seen when the angular frequency or the electrical conductivity get very small. Smith (1996) corrected for this by introducing an electric gauge in solving for **E** at low frequencies. Since **divH** is equally affected, especially in very resistive media, Mackie and Madden (1994) introduced a magnetic gauge in solving for **H** in the air layers. This is seen to prevent the relaxation process from converging to local minima rather than global solutions. The magnetic gauge correction was confirmed as very effective in the present study, greatly enhancing the convergence speed.

There are faster variants of the BiCG method, i.e., Conjugate Gradient-Squared (CG-S; Sonneveld 1989) or BiConjugate Gradient STABilized (BiCGSTAB; Van der Vorst 1992), the latter of which is generally said to be the fastest. We reposed the solution by using BiCGSTAB. The MRA, BiCG and BiCGSTAB solvers were compared for the same 3D model and the same stopping criteria. The BiCGSTAB solver has a stable convergence property, and exhibits the steepest convergence slope of any of the methods. Even though the BiCGSTAB algorithm requires two costly backward and forward substitutions per iteration, the reduction in number of iterations makes the BiCGSTAB solver the fastest. For instance, the computation needed 364s, 541s and 334s CPU time on a single 625 MHz Digital Alpha EV56 processor (1.2 GFLOPS peak speed) for the MRA, BiCG and BiCGSTAB solvers, respectively.

The accuracy of the three SGFD solvers (BiCG, MRA and BiCGSTAB) was examined using several combinations of models and quasi-analytical 3D solutions. The three solvers gave nearly identical results for the 3D models examined. The specified accuracy was reached by changing the convergence threshold. The SGFD solutions were also compared with Martinec's (1998) semi-analytical solution (Uyeshima and Schultz 2000, Fig.8), which showed superiority of the BiCG solution to the semi-analytical solution in accuracy. However, it is probable that the semi-analytical solution suffered from severe truncation errors. The infinite spherical harmonic expansion in Martinec's (1998) formulation was truncated at 12 degrees, which was coarser than our FD grid.

3 Further Acceleration over Multiple Frequencies

Selection of an initial solution vector for a particular relaxation can be arbitrary. However, it was found that a good guess is crucial to guide the relaxation to rapid convergence. Use of the previous solution as the initial solution for the next frequency eliminates the unnecessary overheads of the initial relaxation steps, and has a remarkable effect on accelerating convergence for a multiple frequency forward solution. The total number of iterations over 16 frequencies was reduced by 51.5 % for this particular model.

The order in which the frequencies are arranged, e.g. ascending or descending, has a significant impact on computational overheads. Ascending order, viz., beginning with the lowest frequency, yields superior results. This situation is analogous to nested iteration by multigrid methods. The lower frequencies correspond to the coarser grids and hence starting with the lowest frequency yields a good long wavelength solution. By refining the mesh, i.e. considering higher frequencies subsequently, the relaxation converges rapidly.

Further gains in execution speed were achieved by parallelizing the solver over multiple frequencies. The full range of n frequencies over which forward solutions were required was subdivided into a set of **m** frequency bins to which sets of adjacent frequencies were allocated, where **m** was typically set to equal the number of available processors. Within a given bin, the frequences were sorted in ascending order. The forward solution computation for each frequency bin was then distributed to a different processor. The relaxation method noted before was used within each computational node, i.e. the converged solution for frequency **k-1** was used as the starting solution for the relaxation at frequency **k**. This computationally parallel approach was tested for solutions with up to 16 frequencies on a symmetric multiprocessor (SMP) machine with 8 processor nodes operating under the MPI parallel programming model. We observed approximately linear scaling with number of processors.

4 Discussion

While the equatorial magnetospheric ring current (typically approximated by the P10 spherical harmonic term) is one of the most useful sources in the global induction studies, we must make use of different source current systems operating over a wide variety of frequencies if we are to realize the potential of whole mantle EM tomography. Since the upper mantle is known to be abundantly heterogeneous, high frequency (and non-zonal) sources such as Sq are necessary to delineate regional conductivity anomalies. Zonal sources are insufficient to resolve adequately purely 3D bodies. The new BiCGSTAB solver has been tested for the zonal outer boundary conditions alone at present. Sources with more complexity should be included in the near future.

Although EM induction in the ocean is negligible for periods longer than a few days, Sq responses at some geomagnetic observatories are obviously affected by the presence of the ocean. We need to model topography/bathymetry if we are to increase the variety in the source field. Our answer for this problem is to make numerical meshes as fine as possible to represent the complicated land-sea distribution. In cases when the approach becomes too memory intensive and thus becomes impractical, introduction of a thin sheet subdomain on the surface of the heterogeneous spherical Earth model may be a good tactic to circumvent the problem.

In our present algorithm, the BiCGSTAB relaxation is alternated SDC every **J** iterations. Since SDC changes the original Krylov space spanned by an initial residual **r0**, the BiCGSTAB relaxation has to be resumed by recomputing **r0**. However, we observed a strong dependence of the convergence speed on the number of the BiCGSTAB relaxations before commencement of SDC. Selection of appropriate values for **J** remains an area of current research, particularly when considering inversion for 3D earth structure.

Automatic mesh migration is an important issue for successful and practical inversions. With finite memory storage, it is often required in practise to maximize the ability to resolve abrupt spatial gradients in the fields in the vicinity of large conductivity contrasts. Uyeshima and Schultz (2000) developed an auto mesh generator that generates vertical grids finer than 1/4 skin depth within a conductivity cell. They found it greatly enhanced the accuracy of their MRA solver. Making the grid spacing smaller than 1/4 skin depth is presently a good rule of thumb to employ, though the skin depth is not necessarily a sufficient measure of scale lengths.

The boundary value problem for EM induction in heterogeneous spheres is now thus solved by the BiCGSTAB method. Although the method needs further improvement, it may be applied to various geophysical problems. One possibility is to apply this approach to compute the screening effect of the geomagnetic secular variations by the mantle. This can be done by assigning the inner boundary condition, i.e., the tangential magnetic field at the CMB, while the outer boundary condition is set to null instead. Calculation of the mantle screening effect may provide estimates of the lower mantle conductivity, which is indispensable to extending EM 3D imaging methods into the lower mantle. Our preliminary result shows that it is very difficult to reproduce the observed degree 2 pattern of geomagnetic decadal variations (Yokoyama, 1993) simply by assigning a very heterogeneous upper mantle. This implies that there exists a long wavelength anomaly of the Earth's electrical conductivity in the D" layer as seen in global seismic models (Romanowicz, 1998).

5 Conclusions

Stabilized biconjugate gradient solutions using a staggered grid finite difference solver were found to be more robust and computationally more rapid than our former 3D EM forward solver (Uyeshima and Schultz 2000). This is because the BiCGSTAB method requires fewer iterations per relaxation and has recovered the Hermitian system of linear equations.

Further acceleration was achieved over multiple frequencies by using the converged solution for a given frequency as the initial solution of the system of equations for subsequent frequencies. Additional acceleration was realised by dividing the total range of frequencies into bins and distributing the forward solution calculation for each bin to a separate processor in a parallel computing environment. Sorting of frequencies into ascending order was found to further speed the solutions. Future 3D inversion of global mantle conductivity structure will be facilitated by this approach since a total speedup of more than an order of magnitude in computational time has been obtained relative to the previous MRA solution.

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6 Reference

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