Contraction integral equation method in three-dimensional electromagnetic modeling

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[1] The integral equation method has been proven to be an efficient tool to model three-dimensional electromagnetic problems. Owing to the full linear system to be solved, the method has been considered effective only in the case of models consisting of a strongly limited number of cells. However, recent advances in matrix storage and multiplication issues facilitate the modeling of horizontally large structures. Iterative methods are the most feasible techniques for obtaining accurate solutions for such problems. In this paper we demonstrate that the convergence of iterative methods can be improved significantly, if the original integral equation is replaced by an equation based on the modified Green's operator with the norm less or equal to one. That is why we call this technique the Contraction Integral Equation (CIE) method. We demonstrate that application of the modified Green's operator can be treated as a preconditioning of the original problem. We have performed a comparative study of the convergence of different iterative solvers applied to the original and contraction integral equations. The results show that the most effective solvers are the BIGGSTAB, QMRCGSTAB, and CGMRES algorithms, equipped with preconditioning based on the CIE method. *INDEX TERMS:* 0644 Electromagnetics: Numerical methods; 0619 Electromagnetics: Electromagnetic theory; *KEYWORDS:* electromagnetic, modeling, integral equation, contraction

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1. Introduction

[2] Many geoelectrical structures can be modeled by a set of 3-D inhomogeneities embedded in a horizontally layered medium. The integral equation (IE) method is well known as one of the most accurate techniques for modeling these kind of problems [*Weidelt*, 1975; *Hohmann*, 1975; *Wannamaker et al.*, 1984; *Xiong*, 1992]. The IE method consists of several independent steps making it ideal for easy parallelization providing high performance.

[3] The major obstacle in the full integral equation solution is handling the coefficient matrix with a full structure. For models consisting of more than a couple of thousands of cells, the storage of the coefficient matrix is practically impossible, not to mention the horrendous cost of its direct inversion.

[4] There have been several attempts to overcome the storage and computational cost problem for large matrix inversion. *Xiong* [1992] applied a block iterative scheme to solve the electromagnetic forward problem. In that algorithm only a reasonably small submatrix of the original coefficient matrix is stored at a time. *Portniaguine et al.* [1999] applied the compression algorithm, which is based on a special linear transformation of the full coefficient matrix, such that most elements of the resulting matrix become nearly zero. Thus, thresholding those entries to zero results in significant storage reductions.

[5] Iterative schemes form an alternative to the direct matrix inversion. For example, they have been playing a significant role in forward electromagnetic modeling based on differential methods. There are several studies concerning the finite difference or finite element methods dealing with convergence issues of iterative techniques [*Mackie et al.*, 1994; *Alumbaugh and Newman*, 1995; *Smith*, 1996; *Varentsov*, 1999; *Coggon*, 1971; *Jin*, 1993; *Rätz*, 1999; *Druskin et al.*, 1999]. However, only a few iterative methods solving integral equations have been tested [*Samokhin*, 1993; *Habashy et al.*, 1993; *Singer and Fainberg*, 1995; *Zhdanov and Fang*, 1997; *Avdeev et al.*, 1997; *Zhdanov et al.*, 2000].

[6] In papers by *Pankratov et al.* [1995], *Zhdanov and Fang* [1997], *Zhdanov et al.* [2000], and *Avdeev et al.*

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[2002], an alternative form of the electromagnetic integral equation was used based on the modified Green's operator with a norm less than one. Based on this contraction operator we consider the Contraction Integral Equation (CIE), which can be treated as a preconditioned conventional integral equation. The preconditioners are diagonal operators determined by the conductivity distribution within the geoelectrical model, facilitating inexpensive manipulations. Existing codes based on the solution of the conventional integral equation can be easily improved by applying preconditioning matrices described in this paper.

[7] In contrast to the series representations used by *Pankratov et al.* [1995], *Zhdanov and Fang* [1997], *Zhdanov et al.* [2000], and *Avdeev et al.* [2002], within the framework of CIE formulation any existing iterative solver can be easily applied. Iterative techniques tested for the conventional IE and CIE methods include a) the Successive Iteration (SI) method, b) the Conjugate Gradient Normal Equation Residual (CGNR) method, c) the Biconjugate Gradient (BICG) method, d) the Biconjugate Gradient Stabilized (BICGSTAB) method, e) a quasi-minimal residual variant of the BiCGSTAB (QMRCGSTAB), and f) the Complex Generalized Minimum Residual (CGMRES) algorithms. Also, we examine the effect of an initial model choice for the iterative solution by introducing a simple strategy for multiple frequency modeling.

[8] The model used in the numerical experiments is a relatively complex 3-D structure consisting of several conductive structures of different sizes, conductivity contrasts and depths. This model has been originally selected within the framework of the COMMEMI project [*Zhdanov et al.*, 1997; *Varentsov et al.*, 2000].

[9] As a result of this work we conclude that the convergence rate of the iterative methods applied to the CIE solution is much better than for the conventional IE method. The most effective solvers are the BIGGSTAB, QMRCGSTAB and CGMRES algorithms (equipped with preconditioning based on the CIE method).

2. Integral Equation Method in Electromagnetic Modeling

[10] To make the presentation clearer, we begin our paper with a short review of the conventional integral equation method. Consider a 3-D geoelectric model with background (normal) complex conductivity $\tilde{\sigma}_b$ and local inhomogeneity D with an arbitrarily varying complex conductivity $\tilde{\sigma} = \tilde{\sigma}_b + \Delta\tilde{\sigma}$, which can be, in a general case, frequency dependent (Figure 1). We assume that $\mu = \mu_0 = 4\pi \times 10^{-7} H/m$, where μ_0 is the free-space magnetic permeability. The model is excited by an electromagnetic field generated by an arbitrary source. This field is time harmonic as $e^{-i\omega t}$. Complex conductivity includes the effect of displacement currents: $\tilde{\sigma} = \sigma - i\omega\varepsilon$, where σ and ε are the electrical conductivity and dielectric permittivity, respectively. The electromagnetic fields in this model can be presented as a sum of background (normal) and anomalous fields:

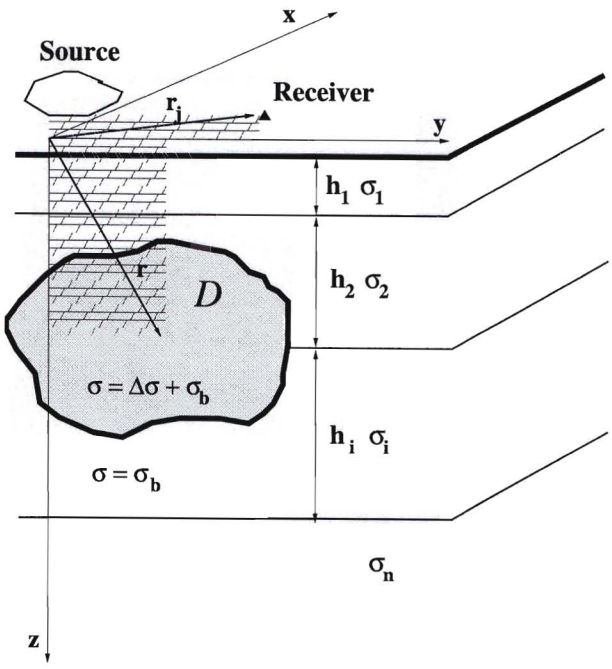

Figure 1. 3-D geoelectric model consisting of a local body with arbitrary conductivity situated in a horizontally layered half-space.

$$\mathbf{E} = \mathbf{E}^b + \mathbf{E}^a, \quad \mathbf{H} = \mathbf{H}^b + \mathbf{H}^a, \tag{1}$$

where the background field is a field generated by the given sources in the model with a background distribution of conductivity $\tilde{\sigma}_b$, and the anomalous field is produced by the anomalous conductivity distribution $\Delta\tilde{\sigma}$.

[11] The anomalous field can be expressed as an integral over the excess currents in inhomogeneous domain D [*Weidelt*, 1975; *Hohmann*, 1975]:

$$\mathbf{E}^a(\mathbf{r}_j) = \mathbf{G}_E[\Delta\tilde{\sigma}(\mathbf{r})\mathbf{E}] = \int\int\int_D \widehat{\mathbf{G}}_E(\mathbf{r}_j \mid \mathbf{r})\Delta\tilde{\sigma}(\mathbf{r}) \cdot [\mathbf{E}^b(\mathbf{r}) + \mathbf{E}^a(\mathbf{r})]\,dv, \tag{2}$$

$$\mathbf{H}^a(\mathbf{r}_j) = \mathbf{G}_H[\Delta\tilde{\sigma}(\mathbf{r})\mathbf{E}] = \int\int\int_D \widehat{\mathbf{G}}_H(\mathbf{r}_j \mid \mathbf{r})\Delta\tilde{\sigma}(\mathbf{r}) \cdot [\mathbf{E}^b(\mathbf{r}) + \mathbf{E}^a(\mathbf{r})]\,dv, \tag{3}$$

where $\mathbf{G}_E$ and $\mathbf{G}_H$ are the electric and magnetic Green's operators; $\widehat{\mathbf{G}}_E(\mathbf{r}_j|\mathbf{r})$ and $\widehat{\mathbf{G}}_H(\mathbf{r}_j|\mathbf{r})$ are the electric and

magnetic Green's tensors defined for an unbounded stratified conductive medium with a background conductivity $\widetilde{\sigma}_b$. They can be found as the solution of the following differential system [*Tang*, 1979; *Felsen and Marcuvitz*, 1994]:

$$\nabla \times \widehat{\mathbf{G}}_H = \widetilde{\sigma}_b \widehat{\mathbf{G}}_E + \widehat{\delta}, \tag{4}$$

and

$$\nabla \times \widehat{\mathbf{G}}_E = i\omega\mu_0 \widehat{\mathbf{G}}_H, \tag{5}$$

where $\widehat{\delta}$ is the tensor delta function

$$\widehat{\delta} = \begin{bmatrix} \delta(\mathbf{r}_j - \mathbf{r}) & 0 & 0 \\ 0 & \delta(\mathbf{r}_j - \mathbf{r}) & 0 \\ 0 & 0 & \delta(\mathbf{r}_j - \mathbf{r}) \end{bmatrix}. \tag{6}$$

The $\nabla\times$ operator affects one column of the tensor at a time. It has been demonstrated that the solution of equation (4) and (5) for the horizontally layered background model is reduced to the Hankel transform of some elementary functions [*Anderson*, 1979; *Xiong*, 1989; *Zhdanov and Keller*, 1994; *Cheryauka and Zhdanov*, 2001]. A detailed specification is given by *Wannamaker et al.* [1984].

[12] Expression (2) becomes a singular vector Fredholm integral equation of the second kind with respect to the anomalous electric field $\mathbf{E}^a$, if we consider the points $\mathbf{r}_j$ within the domain D with anomalous conductivity:

$$\mathbf{E}^a(\mathbf{r}_j) = \mathbf{G}_E\left[\Delta\widetilde{\sigma}(\mathbf{r})\left(\mathbf{E}^b(\mathbf{r}) + \mathbf{E}^a(\mathbf{r})\right)\right], \mathbf{r}, \mathbf{r}_j \in D. \tag{7}$$

We can also represent the same integral equation with respect to the total field:

$$\mathbf{E}(\mathbf{r}_j) = \mathbf{E}^b(\mathbf{r}_j) + \mathbf{G}_E[\Delta\widetilde{\sigma}(\mathbf{r})\mathbf{E}(\mathbf{r})], \mathbf{r}, \mathbf{r}_j \in D. \tag{8}$$

Once the unknown electric field is found inside D, we use (2) and (3) to find the response of the anomaly at any receiver position $\mathbf{r}_j$. Since the most resource intensive step in the algorithm is the solution of (7) or (8), the main effort in this paper is devoted to the rapid solution of this problem.

3. Contraction Integral Equation (CIE) Method

[13] The integral equation (7) in a different operator form is:

$$\mathbf{E}^a = \mathbf{A}^a(\mathbf{E}^a), \tag{9}$$

where the nonlinear operator $\mathbf{A}^a$ is defined as

$$\mathbf{A}^a(\mathbf{E}^a) = \mathbf{G}_E\left(\Delta\widetilde{\sigma}\mathbf{E}^b\right) + \mathbf{G}_E(\Delta\widetilde{\sigma}\mathbf{E}^a). \tag{10}$$

The simplest technique to attempt to solve the operator equation (9) is the method of successive iterations:

$$\mathbf{E}^{a,k} = \mathbf{A}^a\left(\mathbf{E}^{a,k-1}\right), \quad k = 1, 2, \ldots \tag{11}$$

This method is also known as Born or Neumann series. It converges only if $\mathbf{A}^a$ is a contraction operator, which means that $\|\mathbf{A}^a(\mathbf{E}^{a,1} - \mathbf{E}^{a,2})\| < \|\mathbf{E}^{a,1} - \mathbf{E}^{a,2}\|$, for arbitrary $\mathbf{E}^{a,1}$ and $\mathbf{E}^{a,2}$. Here $\|\ldots\|$ is the L_2 norm.

[14] Also, the total field equation (8) can be represented in a similar form:

$$\mathbf{E} = \mathbf{A}^t(\mathbf{E}), \tag{12}$$

where

$$\mathbf{A}^t(\mathbf{E}) = \mathbf{E}^b + \mathbf{G}_E(\Delta\widetilde{\sigma}\mathbf{E}). \tag{13}$$

Unfortunately, $\mathbf{A}^a$ and $\mathbf{A}^t$ are contraction operators only for weak scatterers, where the size of the anomalous domain is much smaller than the wave-length inside the body, and the conductivity contrast $\Delta\widetilde{\sigma}/\widetilde{\sigma}_b$ is small [*Habashy et al.*, 1993].

[15] Based on the iterative dissipative method developed by *Singer and Fainberg* [1995], *Pankratov et al.* [1995], and *Zhdanov and Fang* [1997] applied some linear transformations to Green's operator $\mathbf{G}_E$ such that its norm is smaller than 1 for any conductivity distribution and frequency, i.e., the method of successive iterations becomes always convergent. The specific form of this linear transformation is motivated by the energy inequality for the anomalous electromagnetic field, which expresses a fundamental physical fact, that the energy flow of the anomalous field outside the domain with the anomalous conductivity is always non-negative.

[16] As a result, the original equations (7) or (8) can be converted into a contraction operator-based equation. Following the notations of *Zhdanov and Fang* [1997], the anomalous field equation (7) can be rewritten as

$$a\mathbf{E}^a + b\mathbf{E}^b = \mathbf{G}^m\left[b\left(\mathbf{E}^a + \mathbf{E}^b\right)\right], \tag{14}$$

where

$$a = \frac{2Re\widetilde{\sigma}_b + \Delta\widetilde{\sigma}}{2\sqrt{Re\widetilde{\sigma}_b}}, \; b = \frac{\Delta\widetilde{\sigma}}{2\sqrt{Re\widetilde{\sigma}_b}}, \tag{15}$$

and operator $\mathbf{G}^m(\mathbf{x})$ is defined as a linear transformation of the original electric Green's operator:

$$\mathbf{G}^m(\mathbf{x}) = \sqrt{Re\widetilde{\sigma}_b}\mathbf{G}_E\left(2\sqrt{Re\widetilde{\sigma}_b}\mathbf{x}\right) + \mathbf{x}. \tag{16}$$

Equation (14) can be rewritten with respect to the product of a and the total electric field $\mathbf{E}$, using simple algebraic transformations:

$$\widetilde{\mathbf{E}} + (b - a)\mathbf{E}^b = \widetilde{\mathbf{E}} - \sqrt{Re\widetilde{\sigma}_b}\mathbf{E}^b = \mathbf{G}^m\left[ba^{-1}\widetilde{\mathbf{E}}\right], \tag{17}$$

where $\widetilde{\mathbf{E}}$ is the scaled electric field

$$\widetilde{\mathbf{E}} = a\mathbf{E} \tag{18}$$

Equation (17) can also be presented in the form

$$\widetilde{\mathbf{E}} = \mathbf{C}\left(\widetilde{\mathbf{E}}\right) = \mathbf{G}^m\left[ba^{-1}\widetilde{\mathbf{E}}\right] + \sqrt{Re\widetilde{\sigma}_b}\mathbf{E}^b. \tag{19}$$

In this equation operator $\mathbf{C}\left(\widetilde{\mathbf{E}}\right)$ is a contraction operator for any lossy media [*Zhdanov and Fang*, 1997]:

$$\left\|\mathbf{C}\left(\widetilde{\mathbf{E}}^{(1)} - \widetilde{\mathbf{E}}^{(2)}\right)\right\| \le k\left\|\widetilde{\mathbf{E}}^{(1)} - \widetilde{\mathbf{E}}^{(2)}\right\|, \tag{20}$$

where $\|\ldots\|$ is L_2 norm, $k < 1$, and $\widetilde{\mathbf{E}}^{(1)}$ and $\widetilde{\mathbf{E}}^{(2)}$ are any two different solutions. That is why this method is called the contraction integral equation (CIE) technique, and $\mathbf{C}$ is called a contraction Green's operator.

[17] Using the original Green's operator given by the expression (2) and taking into account formula (16), one can rewrite equation (19) as follows:

$$\widetilde{\mathbf{E}} = \sqrt{Re\widetilde{\sigma}_b}\mathbf{G}_E\left(2\sqrt{Re\widetilde{\sigma}_b}ba^{-1}\widetilde{\mathbf{E}}\right) + ba^{-1}\widetilde{\mathbf{E}} + \sqrt{Re\widetilde{\sigma}_b}\mathbf{E}^b,$$

or, after some transformation

$$\left(1 - ba^{-1}\right)\widetilde{\mathbf{E}} - \sqrt{Re\widetilde{\sigma}_b}\mathbf{G}_E\left(\Delta\widetilde{\sigma}a^{-1}\widetilde{\mathbf{E}}\right) = \sqrt{Re\widetilde{\sigma}_b}\mathbf{E}^b.$$

Note that according to (15),

$$1 - ba^{-1} = (a - b)a^{-1} = \sqrt{Re\widetilde{\sigma}_b}a^{-1}.$$

Therefore, the final form of the contraction integral equation with respect to the scaled electric field $\widetilde{\mathbf{E}}$ is:

$$\sqrt{Re\widetilde{\sigma}_b}a^{-1}\widetilde{\mathbf{E}} = \sqrt{Re\widetilde{\sigma}_b}\mathbf{E}^b + \sqrt{Re\widetilde{\sigma}_b}\mathbf{G}_E\left(\Delta\widetilde{\sigma}a^{-1}\widetilde{\mathbf{E}}\right). \tag{21}$$

This is the basic equation of the CIE electromagnetic modeling method. Note that this is equivalent to (12), expanded with preconditioners:

$$\sqrt{Re\widetilde{\sigma}_b}\left(a^{-1}\widetilde{\mathbf{E}}\right) = \sqrt{Re\widetilde{\sigma}_b}\mathbf{A}^t\left(a^{-1}\widetilde{\mathbf{E}}\right). \tag{22}$$

4. Numerical Solution of the Integral Equations

[18] In this section we demonstrate that discretization of (22) leads to a preconditioned variant of the linear system arising from the original equation (8), where the preconditioners are diagonal matrices. Thus, not only we can easily construct new programs to solve the preconditioned system, but existing codes can be modified without requiring a major debugging effort.

[19] To solve the integral equation numerically we need to discretize the anomalous body by N cells (Figure 2). Assuming that in each individual cell the complex conductivity $\Delta\widetilde{\sigma}$ and the electric field are constant, we can rewrite (7) in a discrete form as

$$\mathbf{e}^a = \widehat{\mathbf{G}}_D\widehat{\mathbf{S}}^a\left(\mathbf{e}^a + \mathbf{e}^b\right), \tag{23}$$

where $\widehat{\mathbf{G}}_D$ is a $3N \times 3N$ matrix containing electric Green's tensor integrals

$$\widehat{\mathbf{G}}_D = \begin{bmatrix} \Gamma_{xx}^{11} & \cdots & \Gamma_{xx}^{1N} & \Gamma_{xy}^{11} & \cdots & \Gamma_{xy}^{1N} & \Gamma_{xz}^{11} & \cdots & \Gamma_{xz}^{1N} \\ & & & \vdots & & & & & \\ \Gamma_{xx}^{N1} & \cdots & \Gamma_{xx}^{NN} & \Gamma_{xy}^{N1} & \cdots & \Gamma_{xy}^{NN} & \Gamma_{xz}^{N1} & \cdots & \Gamma_{xz}^{NN} \\ \Gamma_{yx}^{11} & \cdots & \Gamma_{yx}^{1N} & \Gamma_{yy}^{11} & \cdots & \Gamma_{yy}^{1N} & \Gamma_{yz}^{11} & \cdots & \Gamma_{yz}^{1N} \\ & & & \vdots & & & & & \\ \Gamma_{yx}^{N1} & \cdots & \Gamma_{yx}^{NN} & \Gamma_{yy}^{N1} & \cdots & \Gamma_{yy}^{NN} & \Gamma_{yz}^{N1} & \cdots & \Gamma_{yz}^{NN} \\ \Gamma_{zx}^{11} & \cdots & \Gamma_{zx}^{1N} & \Gamma_{zy}^{11} & \cdots & \Gamma_{zy}^{1N} & \Gamma_{zz}^{11} & \cdots & \Gamma_{zz}^{1N} \\ & & & \vdots & & & & & \\ \Gamma_{zx}^{N1} & \cdots & \Gamma_{zx}^{NN} & \Gamma_{zy}^{N1} & \cdots & \Gamma_{zy}^{NN} & \Gamma_{zz}^{N1} & \cdots & \Gamma_{zz}^{NN} \end{bmatrix},$$

$$\Gamma_{\alpha\beta}^{jk} = \int\int\int_{D_k} G_{\alpha\beta}^E\left(\mathbf{r}_j \mid \mathbf{r}_k\right)dv, \quad \alpha,\beta = x,y,z, \tag{24}$$

$\mathbf{e}^b$ and $\mathbf{e}^a$ are $3N \times 1$ vector columns of the background and anomalous fields,

$$\mathbf{e}^b = \left[E_{x,1}^b, \ldots E_{x,N}^b, E_{y,1}^b, \ldots E_{y,N}^b, E_{z,1}^b, \ldots E_{z,N}^b\right]^T,$$

$$\mathbf{e}^a = \left[E_{x,1}^a, \ldots E_{x,N}^a, E_{y,1}^a, \ldots E_{y,N}^a, E_{z,1}^a, \ldots E_{z,N}^a\right]^T.$$

and $\widehat{\mathbf{S}}^a$ is a $3N \times 3N$ diagonal matrix with the anomalous conductivities.

$$\widehat{\mathbf{S}}^a = diag([\Delta\widetilde{\sigma}_1, \ldots, \Delta\widetilde{\sigma}_N, \Delta\widetilde{\sigma}_1, \ldots, \Delta\widetilde{\sigma}_N, \Delta\widetilde{\sigma}_1, \ldots, \Delta\widetilde{\sigma}_N]).$$

Note that integration in (24) requires the principle value of the Green's tensor [*Hohmann*, 1975; *Wannamaker et al.*, 1984; *Xiong*, 1992].

[20] We can also define the matrix with the background conductivity values inside each cell:

$$\widehat{\mathbf{S}}^b = diag\left([\widetilde{\sigma}_1^b, \ldots, \widetilde{\sigma}_N^b, \widetilde{\sigma}_1^b, \ldots, \widetilde{\sigma}_N^b, \widetilde{\sigma}_1^b, \ldots, \widetilde{\sigma}_N^b]\right).$$

Equation (23) can be rewritten with respect to the total electric field $\mathbf{e} = \mathbf{e}^a + \mathbf{e}^b$:

$$\mathbf{e} = \mathbf{e}^b + \widehat{\mathbf{G}}_D\widehat{\mathbf{S}}^a\mathbf{e}. \tag{25}$$

This equation is a $3N \times 3N$ linear system with respect to the total electric field,

$$\widehat{\mathbf{A}}\mathbf{e} = \mathbf{e}^b, \tag{26}$$

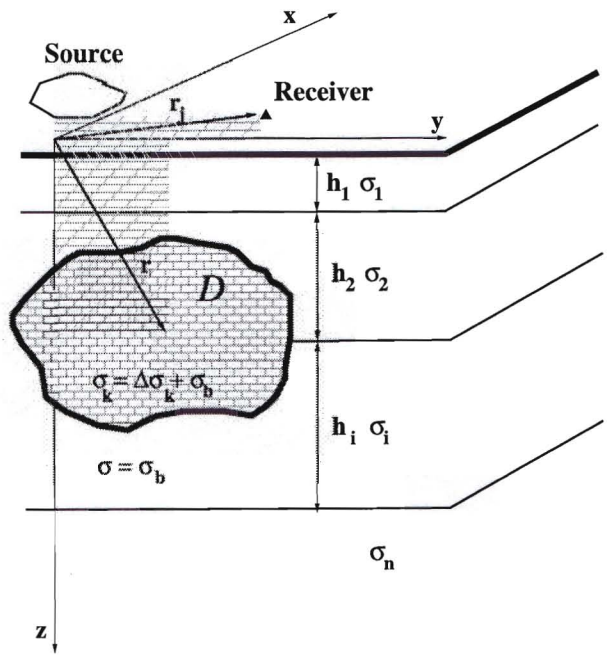

Figure 2. Model of the local body discretized by rectangular cells.

where

$$\widehat{\mathbf{A}} = \widehat{\mathbf{I}} - \widehat{\mathbf{G}}_D \widehat{\mathbf{S}}^a. \tag{27}$$

[21] Matrix $\widehat{\mathbf{A}}$ is a $3N \times 3N$ complex non-Hermitian matrix with a full structure. For a small number of unknowns the direct solvers are practical, especially in the case of multiple sources. If N is large, the storage of $\widehat{\mathbf{A}}$ is extremely memory consuming, not to mention the $O(N^3)$ complexity of direct matrix inversion. However, it has been demonstrated that we can perform multiplications with $\widehat{\mathbf{A}}$ without storing it in its full size [*Avdeev et al.*, 1997; *Ellis*, 1999; *Hursán*, 2001]. Thus, iterative techniques based on repetitive matrix multiplications are particularly adequate for finding the solution of (26).

[22] However, in general, $\widehat{\mathbf{A}}$ can be ill-conditioned, especially for large models with high conductivity contrasts. This causes slow convergence or even divergence of iterative algorithms. Below it is demonstrated that solving the discrete form of the contraction integral equation (21) instead of (25) results in a considerable speed-up with all iterative solvers, due to the stabilizing effect of the preconditioners. It can be easily shown that the discrete form of (21) is the following:

$$\sqrt{Re\widehat{\mathbf{S}}^b}\left(\widehat{\mathbf{I}} - \widehat{\mathbf{G}}_D \widehat{\mathbf{S}}^a\right)\widehat{\mathbf{a}}^{-1}\widetilde{\mathbf{e}} = \sqrt{Re\widehat{\mathbf{S}}^b}\mathbf{e}^b, \tag{28}$$

where diagonal matrix $\widehat{\mathbf{a}}$ is equal to

$$\widehat{\mathbf{a}} = \left(2\sqrt{Re\widehat{\mathbf{S}}^b}\right)^{-1}\left(2Re\widehat{\mathbf{S}}^b + \widehat{\mathbf{S}}^a\right), \tag{29}$$

and

$$\widetilde{\mathbf{e}} = \widehat{\mathbf{a}}\mathbf{e}. \tag{30}$$

[23] Considering (26) and (27), we can easily see that equation (28) is just the preconditioned variant of (26),

$$\widetilde{\mathbf{A}}\widetilde{\mathbf{e}} = \widetilde{\mathbf{e}}^b, \tag{31}$$

where

$$\widetilde{\mathbf{A}} = \widehat{\mathbf{M}}_1\widehat{\mathbf{A}}\widehat{\mathbf{M}}_2, \quad \widetilde{\mathbf{e}}^b = \widehat{\mathbf{M}}_1\mathbf{e}^b, \tag{32}$$

and

$$\mathbf{e} = \widehat{\mathbf{M}}_2\widetilde{\mathbf{e}}, \tag{33}$$

with the notations

$$\widehat{\mathbf{M}}_1 = \sqrt{Re\widehat{\mathbf{S}}^b}, \tag{34}$$

and

$$\widehat{\mathbf{M}}_2 = \widehat{\mathbf{a}}^{-1} = \left(2\sqrt{\widehat{\mathbf{S}}^b}\right)\left(2Re\widehat{\mathbf{S}}^b + \widehat{\mathbf{S}}^a\right)^{-1}. \tag{35}$$

Thus, we have transformed the original matrix equation (26) into the preconditioned equation

$$\widehat{\mathbf{M}}_1\widehat{\mathbf{A}}\widehat{\mathbf{M}}_2\left(\widehat{\mathbf{M}}_2^{-1}\mathbf{e}\right) = \widehat{\mathbf{M}}_1\mathbf{e}^b, \tag{36}$$

where $\widehat{\mathbf{M}}_1$ is the left preconditioner, and $\widehat{\mathbf{M}}_2$ is the right preconditioner.

[24] There are different mathematical methods for introducing the preconditioners for the general matrix equation [*Golub and Van Loan*, 1996]. The main goal is constructing matrix $\widehat{\mathbf{M}}_1\widehat{\mathbf{A}}\widehat{\mathbf{M}}_2$, which has a significantly lower condition number than the original matrix $\widehat{\mathbf{A}}$. This is done by using the contraction Green's operator with the norm always less or equal to one. In other words, the physical nature of our system of equations is considered and preconditioners are formed based on a fundamental physical law that the energy flow of the anomalous electromagnetic field outside the domain containing conductivity inhomogeneity is always positive.

5. Iterative Solvers

[25] In this section we discuss the basic properties of six iterative solvers including 1) the successive iteration (SI), 2) the Conjugate Gradient Normal Equation Residual (CGNR), 3) the Biconjugate Gradient (BICG), 4) the Biconjugate Gradient Stabilized (BICGSTAB), 5) a quasi-minimal residual variant of the BiCGSTAB (QMRCGSTAB), and 6) the Complex Generalized Minimum Residual (CGMRES) methods.

5.1. Successive Iteration (SI) Method

[26] This technique is the simplest iterative solver. Given a linear equation as $\mathbf{x} = \widehat{\mathbf{F}}\mathbf{x}$, starting with an initial

guess $\mathbf{x}_0$, we obtain the next iteration as $\mathbf{x}_1 = \widehat{\mathbf{F}}\mathbf{x}_0$, $\mathbf{x}_2 = \widehat{\mathbf{F}}\mathbf{x}_1$ and so on. One step of this technique consists of one matrix multiplication only. However, the necessary condition for the convergence of this technique is that the matrix $\widehat{\mathbf{F}}$ represents a contraction operator (Banach theorem about the fixed point of the contraction operator). Otherwise, it has weak convergence or it diverges. Unfortunately in electromagnetic modeling based on the conventional integral equation method, this method usually does not converge, especially for large scatterers with high anomalous conductivities.

[27] Based on the modified Born series developed by *Pankratov et al.* [1995] and *Singer and Fainberg* [1995], *Zhdanov and Fang* [1997] found a remedy for the divergence problem by modifying the original integral equation such that the modified operator is a contraction operator for any scatterer size and conductivity distribution. In other words, if we apply the SI method to the preconditioned integral equation, described above, the convergence is guaranteed for any lossy medium. Moreover, there is an analytical expression for the upper bound for the solution error [*Zhdanov and Fang*, 1997] that can be used as a straightforward termination criteria of the iterative process. In the previous section we have shown that this nice modification can be treated as a special preconditioning, making it applicable to iterative techniques more powerful than the successive iterations.

5.2. Conjugate Gradient Normal Equation Residual (CGNR) Method

[28] Assume $\widehat{\mathbf{A}}\mathbf{x} = \mathbf{b}$ is a linear system with a positive definite Hermitian coefficient matrix. Consider

$$\phi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^*\widehat{\mathbf{A}}\mathbf{x} - \mathbf{x}^*\mathbf{b}. \tag{37}$$

Since $\nabla\phi(\mathbf{x}) = \widehat{\mathbf{A}}\mathbf{x} - \mathbf{b}$, it follows that $\mathbf{x} = \widehat{\mathbf{A}}^{-1}\mathbf{b}$ is the unique minimizer of (37). One way to produce a vector sequence $\{\mathbf{x}_k\}$ that converges to $\mathbf{x}$ is to introduce the Krylov subspace

$$\mathcal{K}\left(\widehat{\mathbf{A}}, \mathbf{r}_0\right) = span\left\{\widehat{\mathbf{A}}\mathbf{r}_0, \widehat{\mathbf{A}}^2\mathbf{r}_0, \cdots, \widehat{\mathbf{A}}^k\mathbf{r}_0\right\},$$

and where $\mathbf{r}_0 = \widehat{\mathbf{A}}\mathbf{x}_0 - \mathbf{b}$ and minimize ϕ over this space [*Golub and Van Loan*, 1996].

[29] The best known iterative method performing this operation is the Conjugate Gradient (CG) method [*Hestenes and Stiefel*, 1952]. Note that it is designed for problems with a positive definite Hermitian coefficient matrix. For nonhermitian systems it exhibits erratic convergence behavior.

[30] The simplest way to overcome this problem is to precondition the original system $\widehat{\mathbf{A}}\mathbf{x} = \mathbf{b}$ with the complex conjugate of $\widehat{\mathbf{A}}$, i.e. we solve $\widehat{\mathbf{A}}^*\widehat{\mathbf{A}}\mathbf{x} = \widehat{\mathbf{A}}^*\mathbf{b}$, where * denotes the complex conjugate transposed matrix. One step of this method contains two matrix multiplications. The CGNR method was used by *Portniaguine et al.* [1999] for solving the compressed problem. Since $\widehat{\mathbf{A}}^*\widehat{\mathbf{A}}$ is a positive definite Hermitian, the CGNR method always converges. However, the squaring of the condition number results in a slowdown in the convergence.

5.3. Biconjugate Gradient (BICG) Method

[31] This method was introduced as a generalization of CG for nonhermitian systems [*Lanczos*, 1952; *Fletcher*, 1976]. It is based on simultaneous minimization over two Krylov subspaces,

$$\mathcal{K}\left(\widehat{\mathbf{A}}, \mathbf{r}_0\right) = span\left\{\widehat{\mathbf{A}}\mathbf{r}_0, \widehat{\mathbf{A}}^2\mathbf{r}_0, \cdots, \widehat{\mathbf{A}}^k\mathbf{r}_0\right\},$$

and

$$\mathcal{K}\left(\widehat{\mathbf{A}}^*, \mathbf{r}_0\right) = span\left\{\widehat{\mathbf{A}}^*\mathbf{r}_0, \widehat{\mathbf{A}}^{2*}\mathbf{r}_0, \cdots, \widehat{\mathbf{A}}^{k*}\mathbf{r}_0\right\}.$$

It converges faster than CGNR, since no squaring of the condition number occurs. However, this method also requires that matrix $\widehat{\mathbf{A}}$ is a positive definite Hermitian coefficient matrix, which is not always the case in numerical modeling. Therefore, erratic convergence has been observed in several situations [*van der Vorst*, 1992; *Freund and Nachtigal*, 1991]. Moreover, the operations of transpose matrix-vector multiplication still appear in each iteration, resulting in difficulties when $\widehat{\mathbf{A}}^*$ is not readily available.

5.4. Biconjugate Gradient Stabilized (BICGSTAB) Method

[32] Many recently proposed methods can be viewed as improvements over some of the drawbacks of BICG. One of the most notable variants is the Conjugate Gradient Squared (CGS) suggested by *Sonneveld* [1989]. In this algorithm the calculation of $\widehat{\mathbf{A}}^*$ is not required while retaining the convergence rate of BICG. However, erratic convergence behavior may still occur. Based on similar ideas which led to CGS, *van der Vorst* [1992] introduced the Biconjugate Gradient Stabilized (BICGSTAB) method, which is reported to have better convergence rates than CGS in many situations [*Driessen and van der Vorst*, 1991; *van der Vorst*, 1992].

5.5. A Quasi-Minimal Residual Variant of BICGSTAB (QMRCGSTAB)

[33] *Freund* [1993] introduced a variant of CGS, which is reported to smooth the convergence of CGS while retaining its good convergence rate. This is based on a "quasi-minimization" of the residual over the span of the vectors evaluated during the CGS algorithm. The method is called the Transpose-Free Quasi-Minimal Residual (TFQMR) method. It has been used by *Ellis* [1999] to

calculate an EM scattering problem in time domain. Following the same logic to smooth the BICGSTAB technique, the Quasi-Minimal Residual variant of BICGSTAB (QMRCGSTAB) has been developed by *Chan et al.* [1994] This method is known to be as smooth as the TFQMR; however, its convergence rate is usually higher [*Chan et al.*, 1994].

5.6. Complex Generalized Minimal Residual (CGMRES) Method

[34] The basic idea of the conventional Generalized Minimal Residual (GMRES) method [*Saad and Schultz*, 1986] is to find the solution along an orthonormal basis

$$\left\{\widehat{\mathbf{A}}\mathbf{g}_1^n, \widehat{\mathbf{A}}\mathbf{g}_2^n, \cdots, \widehat{\mathbf{A}}\mathbf{g}_s^n\right\}$$

in the Krylov subspace

$$\mathcal{K} = span\left\{\widehat{\mathbf{A}}\mathbf{r}_n, \widehat{\mathbf{A}}^2\mathbf{r}_n, \cdots, \widehat{\mathbf{A}}^k\mathbf{r}_n\right\}$$

at the n-th step of the iterative process,

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \sum_{l=1}^{s} k_{nl}\mathbf{g}_l^{(n)}, \; s \leq n,$$

where $\mathbf{r}_n = \widehat{\mathbf{A}}\mathbf{r}_n - \mathbf{b}$.

[35] The more orthonormal basis functions are calculated (the larger s is), the smoother the convergence becomes, requiring fewer iterations with smaller amplification of the roundoff errors during the iterative process. However, at each iteration the orthogonalization process has to be performed, requiring $2s$ matrix multiplications, and the number of vectors to be stored is also proportional to s. The notation GMRES(s) is often used to emphasize the number of orthogonal basis functions. One special case is the so called "brute force" GMRES, which is based on increasing s until the desired error level is reached within one outer iteration [*Kelley*, 1995]. However, if s becomes large, the number of basis vectors to be stored may be very memory demanding.

[36] The GMRES method has been extended for the case of an operator equation in a complex Hilbert space by *Samokhin* [1993] and *Zhdanov* [2002]. We call this modification the Complex Generalized Minimal Residual (CGMRES) method. The main advantage of this new technique is that it converges even if the matrix $\widehat{\mathbf{A}}$ is not a positive definite Hermitian matrix. The only requirement for the convergence of the CGMRES method is that complex matrix $\widehat{\mathbf{A}}$ is an absolutely positively determined matrix. The last property, according to *Zhdanov* [2002], means that matrix $\widehat{\mathbf{A}}$ satisfies the condition

$$\left|\mathbf{x}^*\left(\widehat{\mathbf{A}}\mathbf{x}\right)\right| \geq \gamma(\mathbf{x}^*\mathbf{x}), \gamma > 0, \tag{38}$$

for all $\mathbf{x}$.

[37] Note that due to the energy inequality [*Zhdanov and Fang*, 1997], the coefficient matrix for electromagnetic IE forward modeling is always an absolutely positively determined, ensuring the convergence of the CGMRES for any model. However, the convergence rate can be increased significantly by applying CGMRES to the preconditioned IE system (31).

5.7. Operation Complexity

[38] Table 1 summarizes the operation count per one iteration for the tested algorithms without preconditioning. Using left and right diagonal preconditioners, two extra vector-vector multiplications are added to the displayed values for each matrix multiplication. Because of the full matrix of the integral equation, the speed is determined almost entirely by the number of matrix multiplications. For sparse systems, the relative contribution of vector-vector multiplications can also be significant.

6. Choice of the Initial Guess

[39] All iterative methods may be started from any value of $\mathbf{x}_0$. If no initial guess is specified, usually one starts from zero. However, some time can be saved by picking an appropriate initial guess having relative residuals less than one. The basic idea is that it is economical to calculate the initial solution if its cost is lower than the resulting complexity reduction during the iterative process. *Zhdanov and Fang* [1997] used the quasi-linear approximation as the initial guess of the successive iterations. Consequently, they called the method quasi-linear series. Similarly, *Zhdanov et al.* [2000] applied the quasi-analytical approximation to the SI method, obtaining the quasi-analytical series. Evidently, the concept of inexpensive approximation-based starting solutions is not limited to the method of successive iterations, it can be applied to any iterative solver.

[40] If more than one frequency is modeled, and the adjacent frequencies are not extremely different (say, they are at the same magnitude), there is an even better choice for an initial guess. With the solutions at f_1, and assuming that the variation of the background and total electric fields inside the anomalous body is similar with respect to the frequency, $\mathbf{e}$ can be picked at f_2 on the basis of $\mathbf{e}^b(f_1)$ and $\mathbf{e}(f_1)$ as

$$\mathbf{e}(f_2) = \mathbf{e}^b(f_2)\frac{\mathbf{e}(f_1)}{\mathbf{e}^b(f_1)}. \tag{39}$$

This calculation is very inexpensive (two vector products) and in the presented modeling experiments it could save approximately 40–60% of the number of iterations starting from zero even if the ratio of two frequencies was 10. For time domain modeling, where

Table 1. Summary of the Operation Count per One Iteration

Method	Number of Multiplications per Iteration	
	Matrix-Vector	Vector-Vector
SI	1	0
CGNR	2	3
BICG	2	3
BICGSTAB	2	5
QMRCGSTAB	2	7
CGMRES(s)	2s	$2 + (2 + s/2)(s - 1)$

the frequency spectra are sampled more densely, the saving factor is even higher.

7. Numerical Results

[41] In this section a comparative study of the outlined iterative solvers is performed through a 3-D forward modeling experiment. The model is one of the new generation of 3-D models of the COMMEMI project, initiated by *Zhdanov et al.* [1997]. This model was introduced by *Varentsov et al.* [2000] and named Model 3D-3. It consists of seven conductive blocks (Figure 3).

[42] Five of them are adjacent in the y-direction and are elongated in the x-direction, forming a subsurface syncline-like structure. These blocks have the same size (3 km) in the x-direction, while their sizes in the y- and z-directions (from body 1 to body 5) are different and equal to 0.4, 0.6, 0.4, 0.6 and 0.4 km, and 0.4, 0.6, 0.4, 0.6 and 0.4 km respectively. The resistivities of the blocks (from 1 to 5) are 300, 30, 100, 30 and 300 Ohm-m.

[43] The sixth block forms a middle depth local 3-D body with a very low resistivity of 0.1 Ohm-m, and with a size of $1 \times 2 \times 0.8$ km^3 in the x, y and z directions. The upper edge of this body lies at a depth of 0.2 km.

[44] The seventh body describes a regional quasi-2-D crustal structure with dimensions of $1 \times 5.6 \times 2$ km^3 in x, y and z directions respectively and with a low resistivity of 0.3 Ohm-m. Its upper edge is at a depth of 1 km.

[45] The background vertical section of the model consists of three layers with resistivities of 1000, 10000 and 10 Ohm-m, and with thicknesses for the first and the second layers of 1 and 6.5 km, respectively. The observation region selected for the comparison is $[-4, 4] \times [-4, 4]$ km^2.

[46] This model combines a high conductivity contrast up to 30000 with the anomalous structure almost outcropping at the ground surface, which is quite typical for mining EM applications and for regional MT studies. It requires a large grid to approximate all the structures with the proper resolution. The inhomogeneity discretization is as follows: each body is horizontally subdivided by 0.2×0.2 km^2 cells in the x and y directions, while the vertical discretization interval increases with depth, starting from 0.05 km for the subsurface structures and ending with 0.5 km at the bottom of the deepest quasi-2-D body. The total number of cells used for this experiment is 8008. The

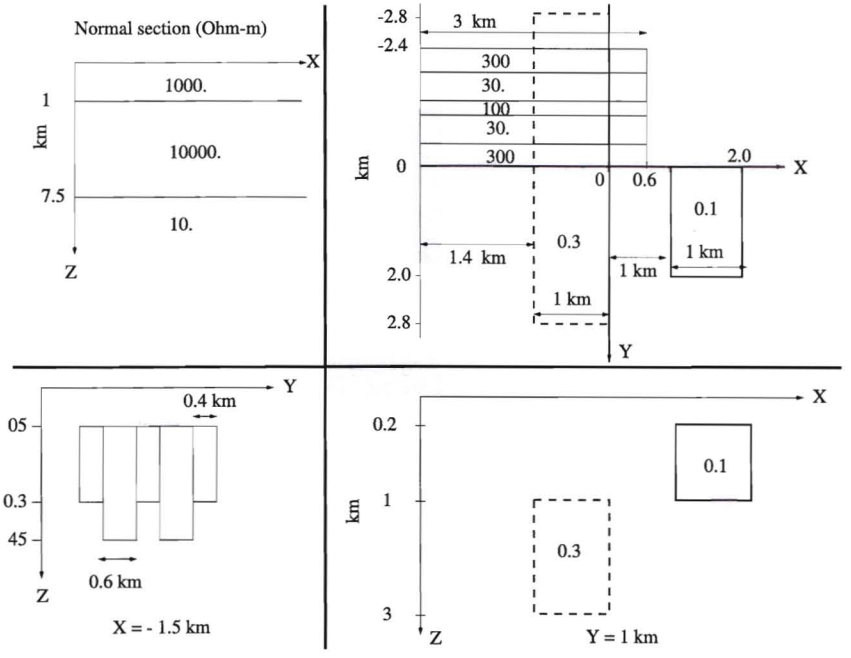

Figure 3. 3-D geoelectric model consisting of seven blocks within a layered medium excited by a plane-wave source [after *Varentsov et al.*, 2000].

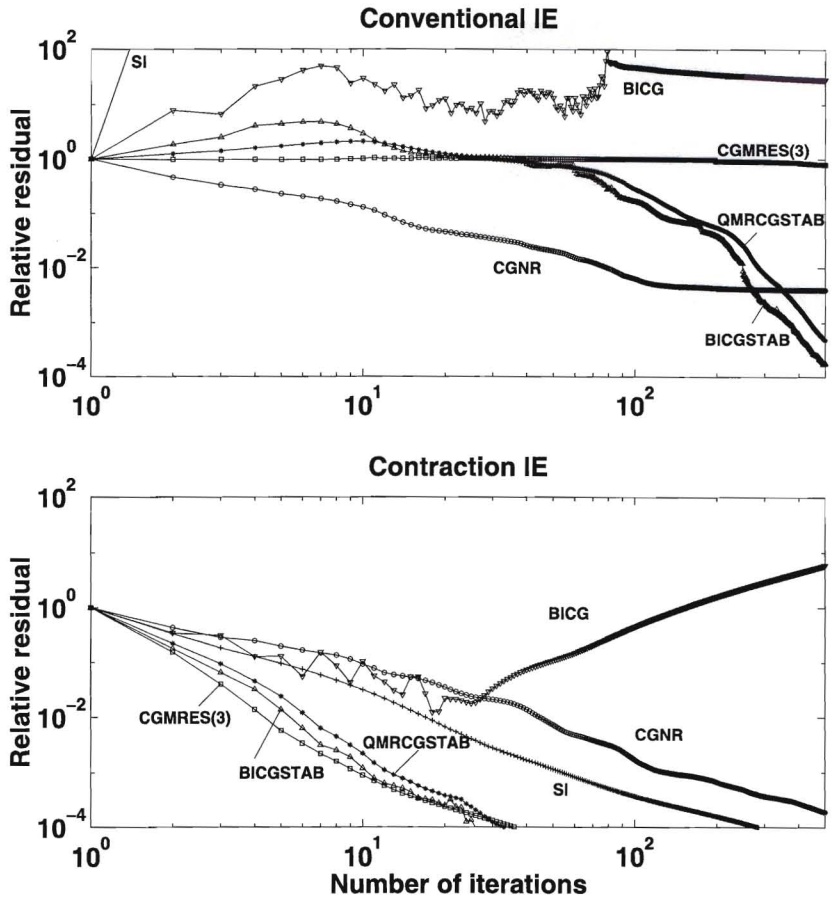

Figure 4. Behavior of the relative residual norm during the iterations without (top) and with (bottom) diagonal preconditioners in the solution of the integral equation for the 3-D modeling experiment.

model is excited by a plane-wave with an electric field oriented in the x-direction. The frequency is 1 Hz.

[47] The aim of this numerical experiment is to find the total electric field inside the anomalous body by solving the discrete conventional and contraction integral equations and to compare the convergence rates of different iterative solvers. Iterations were performed until the L_2 norm of the residual normalized to the L_2 norm of the right hand side dropped below 10^{-4}, or until the number of iterations reached 500. The choice of the stopping error level is based on information from the actual accuracy of the Green's tensor integrals of the scattering matrix [*Xiong*, 1992].

[48] The history of the relative residual during the iterations is plotted in Figure 4. The upper panel shows the behavior of the relative residual norms of the different iterative solvers applied to the discretized conventional integral equation (without preconditioning). The successive approximations clearly diverge, and the BICG method has extremely erratic behavior. The CGMRES with three orthogonal basis functions stagnates. Since the CGNR method solves the always Hermitian normal equation, monotonous convergence is provided. However, one of its typical properties is that the convergence rate decreases, so an excessively large number of iterations is required. The BICGSTAB and QMRCGSTAB techniques appear to be convergent, but neither of them could reach the desired error level within 500 iterations. Considering that one matrix multiplication requires approximately 20 seconds on a SUN Ultra Sparc-10 workstation, it is extremely expensive or impossible to obtain a solution based on the conventional IE method without preconditioning.

[49] The bottom panel of Figure 4 shows the relative residual norms after the diagonal preconditioners, based on the CIE method outlined above, have been utilized. In this case only the BICG has failed to converge, and all other methods produce decreasing errors. The convergence rates are significantly different. The CGNR method still converges very slowly due to the squaring of the

Table 2. CPU Times of Convergence to a Relative Residual of 10^{-4} Using Six Iterative Solvers Required for the Solution of the Conventional and Contraction Integral Equations for Model 1[a]

Method	CPU Times of Convergence to $\|\mathbf{r}\|/\|\mathbf{b}\| \leq 10^{-4}$	
	Conventional IE	Contraction IE
SI	No convergence	5720
CGNR	>20000	>20000
BICG	No convergence	No convergence
BICGSTAB	>20000	1052
QMRCGSTAB	>20000	1351
CGMRES(s)	>20000	3925

[a] The time units are measured in seconds.

condition number of the original equation. The successive iteration method requires almost 300 iterations, so in spite of its low cost per iteration (one matrix multiplication) the overall operation count is still large. The other transpose-free algorithms (CGMRES, QMRCGSTAB and BICGSTAB) are much faster, requiring 36, 33 and 26 iterations only.

[50] Table 2 represents the CPU time required on a SUN Ultra Sparc 1 workstation by different solvers to reach a normalized residual below 10^{-4}. The calculations were performed on a SUN Ultra Sparc 10 workstation. The cheapest techniques for this specific model are the BICGSTAB and QMRCGSTAB, since they need only two matrix multiplications per iteration, while the CGMRES(3) requires six of them.

[51] Choosing an inexpensive approximation as an initial guess, the total number of iterations decreases by two or three for each method. If results of the nearest frequency are used as an initial guess applying (39), then the saving rate can be much higher. For example, using the result calculated for $f = 0.1$ Hz results in approximately 40–60% fewer iterations than if the initial guess is zero (compare the bottom panel in Figure 4 and the top panel in Figure 5). If the result of $f = 0.5$ *Hz* is available, less than 10 iterations are needed for the CGMRES,

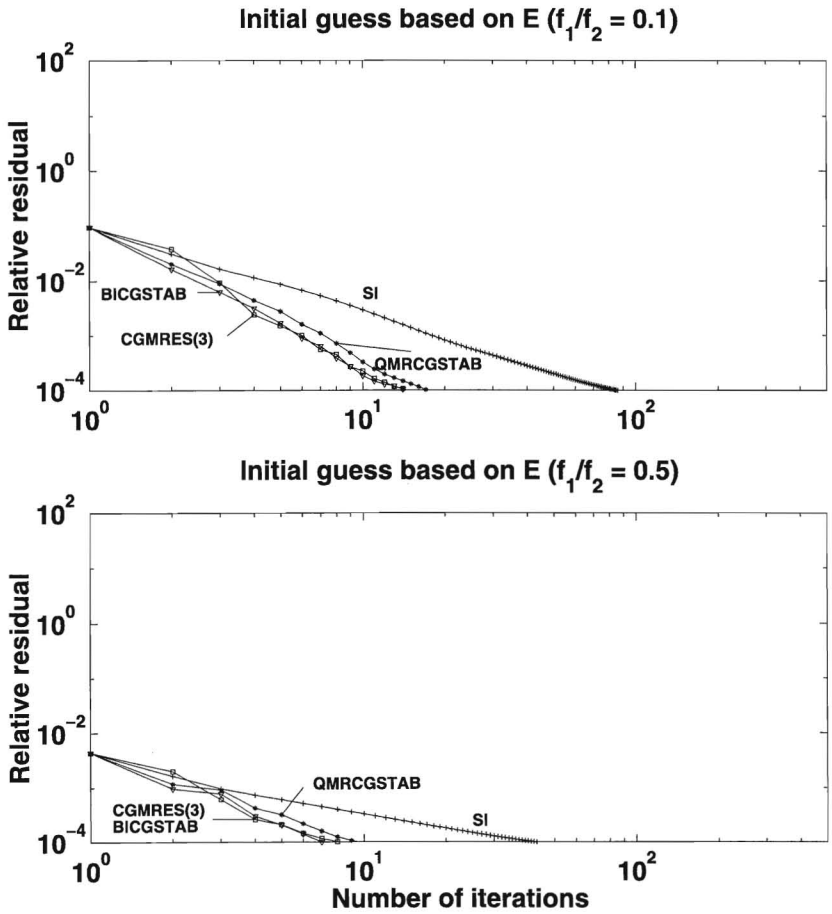

Figure 5. Behavior of the relative residual norm during the iterations using initial guesses based on the electric field calculated at $f = 0.1$ *Hz* (top) and $f = 0.5$ *Hz* (bottom) in the solution of the integral equation for the 3-D modeling experiment at $f = 1$ *Hz*.

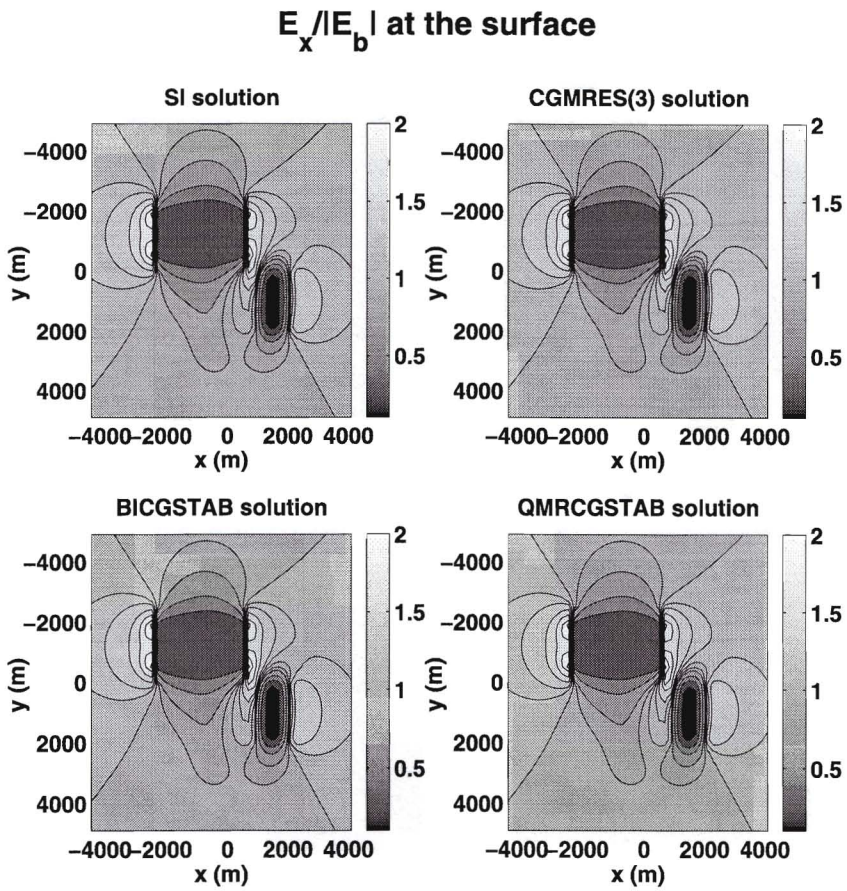

Figure 6. Amplitude of the x-component of the total electric field at the surface obtained by solving the CIE by four different solvers. The results have been normalized to the background electric field.

QMRCGSTAB and BICGSTAB methods (Figure 5, bottom panel).

[52] Figure 6 presents the comparison of the x-component of the electric field for a period of 1 s for different solution techniques. There are four solutions shown, obtained by the SI, BICGSTAB, QMRCGSTAB and CGMRES(3) solvers for the CIE system. Since the relative error is about 0.01%, there are no visible differences between the results. The SI solution has been used in the comparative experiment between different modeling techniques by *Varentsov et al.* [2000]. However, the modeling results obtained by the BICGSTAB, QMRCGSTAB and CGMRES(3) solutions applied to the CIE require much less computer resources than the SI solution.

8. Conclusions

[53] In this paper we consider the Contraction Integral Equation (CIE) method for 3-D electromagnetic modeling. The method is based on the numerical solution of the modified integral equation with the contraction Green's operator, introduced by *Pankratov et al.* [1995] and *Zhdanov and Fang* [1997]. We suggest using CG-type iterative methods to solve the contraction integral equation, which are much more powerful than the successive iterations originally used by *Pankratov et al.* [1995] and *Zhdanov and Fang* [1997]. We have examined the performance of different iterative solvers in the solution of an electromagnetic scattering problem, based on the CIE method. Also, the effect of the initial guess has been investigated. As a result, one can conclude that for this problem the CGMRES, BICGSTAB and QMRCGSTAB algorithms are fast enough to provide a practical tool to model complex geoelectric structures consisting of a large number of cells. The choice of an inexpensive initial guess for modeling several frequencies results in further reduction of operations.

[54] The high convergence rate of the iterative methods applied to the contraction integral equation is based on the fact that this new equation is the preconditioned form of the conventional integral equation with the preconditioning matrices determined by the conductivity distri-

bution within the geoelectrical model. This form of the preconditioners is based on the fundamental radiation properties of the electromagnetic field, expressed by the energy inequality, which has a clear physical interpretation: the total energy of the anomalous electromagnetic field radiated outside the domain with the anomalous conductivity is always non-negative. This physical property of the electromagnetic field provides the mathematical convergence property of the iterative methods with the new preconditioners introduced in this paper. This is probably the most important result of our research.

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