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THREE-DIMENSIONAL ELECTROMAGNETIC MODELLING AND INVERSION FROM THEORY TO APPLICATION

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Abstract. The whole subject of three-dimensional (3-D) electromagnetic (EM) modelling and inversion has experienced a tremendous progress in the last decade. Accordingly there is an increased need for reviewing the recent, and not so recent, achievements in the field. In the first part of this review paper I consider the finite-difference, finite-element and integral equation approaches that are presently applied for the rigorous numerical solution of fully 3-D EM forward problems. I mention the merits and drawbacks of these approaches, and focus on the most essential aspects of numerical implementations, such as preconditioning and solving the resulting systems of linear equations. I refer to some of the most advanced, state-of-the-art, solvers that are today available for such important geophysical applications as induction logging, airborne and controlled-source EM, magnetotellurics, and global induction studies. Then, in the second part of the paper, I review some of the methods that are commonly used to solve 3-D EM inverse problems and analyse current implementations of the methods available. In particular, I also address the important aspects of nonlinear Newton-type optimisation techniques and computation of gradients and sensitivities associated with these problems.

Keywords: three-dimensional modelling and inversion, electromagnetic fields, optimisation

Abbreviations: EM: electromagnetic; 3-D: three-dimensional; FD: finite-difference; FE: finite-element; IE: integral equation; NLCG: nonlinear conjugate gradients; QN: Quasi–Newton

1. Introduction

Over the last decade, the EM induction community had three large international meetings entirely devoted to the theory and practice of three-dimensional (3-D) electromagnetic (EM) modelling and inversion (see Oristaglio and Spies, 1999; Zhdanov and Wannamaker, 2002; Macnae and Liu, 2003). In addition, two special issues of *Inverse Problems* dedicated to the same subject have been recently published (Lesselier and Habashy, 2000; Lesselier and Chew, 2004). As a result, a multitude of various kinds of numerical solutions have been revealed to the community. An advanced reader may find it interesting to browse through the above references on his own. Here, for completeness, I must mention that several comprehensive books, for example the work of Zhdanov (2002), have also been published on the same subject.

In this paper, I will review the finite-difference (FD), finite-element (FE) and integral equation (IE) numerical solutions for fully 3-D geoelectromagnetic modelling and inverse problems. I will leave aside the variety of so-called *approximate* solutions, that impose additional constrains on the conductivity models and/or EM field behaviour, such as – thin sheet solutions (Vasseur and Weidelt, 1977; Dawson and Weaver, 1979; McKirdy et al., 1985; Singer and Fainberg, 1985; among others), artificial neural network solutions (Spichak and Popova, 2000; among others) and those that are based on every kind of approximation of the Born–Rytov type requiring a low-contrast assumption (Habashy et al., 1993; Torres-Verdin and Habashy, 1994, 2002; Zhdanov and Fang, 1996; Chew, 1999; Tseng et al., 2003; Song and Liu, 2004). I will also ignore solutions that are applicable only to direct current problems (Tamarchenko et al., 1999; Li and Oldenburg, 2000; Li and Spitzer, 2002, among many others). Nevertheless, the subject still remains so vast that it is impossible to review all material. So, in what follows I will further confine myself to only some numerical aspects of recent developments in fully 3D EM forward and inverse solutions, which I believe to be important.

2. Three-Dimensional Modelling

Three-dimensional (3-D) electromagnetic (EM) numerical modelling is used today, (1) sometimes, as an engine for 3-D EM inversion; (2) commonly, for verification of hypothetical 3-D conductivity models constructed using various approaches; and (3) as an adequate tool for various feasibility studies.

The whole field of 3-D EM modelling is now developing so fast that most of the published results on the performances, computational loads and accuracies of existing numerical solutions are out-of-date (sometimes even before they are published). This is why in this review of *current* modeling solutions I avoid addressing these topics, as these kinds of comparisons may be misleading. However, the COMMEMI project of Zhdanov et al. (1997) is entirely devoted to the comparisons of different solutions (primarily 2-D but some 3-D solutions were included).

2.1 How We Do It

During 3-D modelling we solve numerically Maxwell's equations (here presented in the frequency-domain)

$$\nabla \times \mathbf{H} = \tilde{\sigma} \cdot \mathbf{E} + \mathbf{j}^{\mathrm{ext}}, \tag{1a}$$

$$\nabla \times \mathbf{E} = i\omega\mu \cdot \mathbf{H}, \tag{1b}$$

where μ and ε are, respectively, the permeability and permittivity of the medium, $\tilde{\sigma} = \sigma - i\omega\varepsilon$ where σ is the electrical conductivity and ω is the angular frequency of the field with assumed time-dependence $\exp(-i\omega t)$, and where $\mathbf{j}^{\mathrm{ext}}$ is the impressed current source. This allows us to calculate the electric **E** and magnetic **H** fields within a volume of interest, whatever it might be. There are three commonly used approaches to obtain the numerical solution.

2.1.1 *Finite-Difference Approach*

The first, probably the most commonly employed, is the finite-difference approach (Yee 1966; Jones and Pascoe, 1972; Dey and Morrison, 1979; Judin, 1980; Spichak, 1983; Madden and Mackie, 1989; Smith and Booker, 1991; Mackie et al., 1993, 1994; Wang and Hohmann, 1993; Weaver, 1994; Newman and Alumbaugh, 1995; Alumbaugh et al., 1996; Smith, 1996a, b; Varentsov, 1999; Weaver et al., 1999; Champagne et al., 1999; Xiong et al., 2000; Fomenko and Mogi, 2002; Newman and Alumbaugh, 2002; among others). In this approach, the conductivity ($\tilde{\sigma}$), the EM fields and Maxwell's differential equations are approximated by their finite-difference counterparts within a rectangular 3-D grid of $M = N_x \times N_y \times N_z$ size. This leads to the resulting system of linear equations, $A_{\mathrm{FD}} \cdot x = b$, where the $3M$-vector x is the vector consisting of the grid nodal values of the EM field, the $3M$-vector b represents the sources and boundary conditions. The resulting $3M \times 3M$ matrix A_{FD} is complex, large, sparse and symmetric. Weidelt (1999) and Weiss and Newman (2002, 2003) have extended this approach to fully anisotropic media. In the time-domain, the FD schemes have been developed by Wang and Hohmann (1993), Wang and Tripp (1996), Haber et al. (2002), Commer and Newman (2004), among others. The main attraction of the FD approach for EM software developers is an apparent simplicity of its numerical implementation, especially when compared to other approaches.

2.1.2 *Finite-Element Approach*

In the finite-element approach, which is still not widely used, the EM field (or its potentials) are decomposed to some basic (usually, edge and nodal) functions. The coefficients of the decomposition, a vector x, are sought using the Galerkin method. This produces a nonsymmetric sparse complex system of linear equations, $A_{\mathrm{FE}} \cdot x = b$. The main attraction of the FE approach for geophysicists is that it is commonly believed to be better able than other approaches to accurately account for geometry (shapes of ore-bodies, topography, cylindrical wells, etc.). This apparent attraction is counterbalanced by a nontrivial and usually time-consuming construction of the finite elements themselves. The FE approach has been implemented by many developers (Reddy et al., 1977; Pridmore et al., 1981; Paulsen et al., 1988; Boyce et al., 1992; Livelybrooks, 1993; Lager and Mur, 1998; Sugeng et al., 1999; Zunoubi et al., 1999; Ratz, 1999; Ellis, 1999; Haber, 1999; Zyserman and Santos, 2000; Badea et al., 2001; Mitsuhata and Uchida, 2004, among others).

2.1.3 *Integral Equation Approach*

Finally, with the integral equation approach Maxwell's differential equations (1) are first reduced to a second-kind Fredholm's integral equation (Dmitriev, 1969; Raiche, 1974; Hohmann, 1975; Weidelt, 1975, Tabarovsky, 1975)

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_o(\mathbf{r}) + \int_{V^s} \underset{=o}{G}(\mathbf{r};\mathbf{r}')(\tilde{\sigma} - \tilde{\sigma}_o)\mathbf{E}(\mathbf{r}')d\mathbf{r}' \tag{2}$$

with respect to the electric field. This is known as the scattering equation (SE). To derive SE the Green's function technique is usually applied. In Equation (2), the free term $\mathbf{E}_o$ is known, $\underset{=o}{G}$ is the 3×3 dyadic for the Green's function of the 1-D reference medium, and V^s is the volume where $(\tilde{\sigma} - \tilde{\sigma}_o)$ differs from zero. A discretization of the SE yields the linear system $A_{\mathrm{IE}} \cdot x = b$, provided that both conductivity $\tilde{\sigma}$ and the unknown electric field $\mathbf{E}$ are assumed to be constant within each cell. The system matrix A_{IE} is complex and dense, with all entries filled, but more compact than the A_{FD}, or A_{FE} matrices. The main merit of the IE approach is that only the scattering volume V^s is subject to discretization. This reduces the size of system matrix A_{IE} dramatically. All other approaches require a larger volume to be discretized. However, most EM software developers refrain from implementation of the IE approach, since accurate computation of the matrix A_{IE} is indeed an extremely tedious and nontrivial problem itself. Yet this approach has been implemented in several studies (Ting and Hohmann, 1981; Wannamaker et al., 1984; Newman and Hohmann, 1988; Hohmann, 1988; Cerv, 1990; Wannamaker, 1991; Dmitriev and Nesmeyanova, 1992; Xiong, 1992; Xiong and Tripp, 1995; Kaufman and Eaton, 2001, among others).

2.1.4 *Techniques to Improve Solutions Using the Physics of the EM Problem*

The important point, regardless of what approach is employed, is that the initial EM forward problem is always reduced to the solution of a system of linear equations

$$A \cdot x = b. \tag{3}$$

Nowadays, the system is commonly solved iteratively by a preconditioned Krylov method (see Appendices A and B). The properties of the matrix A

are determined by which method (FD, FE or IE) is applied to solve the forward problem. In this respect, only two aspects are important, (1) how accurate the system $A \cdot x = b$ represents Maxwell's equations, and (2) how well-preconditioned the system matrix A is (see Appendix B). This is because condition numbers $\kappa(A)$ of the unpreconditioned system matrices A may easily be as large as 10^9–10^{12} (cf. Tamarchenko et al., 1999), and such poorly preconditioned systems slowly converge, if indeed they are convergent at all.

To address the first issue *staggered-grids* (see Figure 1) are commonly used since they produce coercive approximation – conservation laws ($\nabla \times (\nabla f) = 0$ and $\nabla \cdot (\nabla \times \mathbf{f}) = 0$) are satisfied. This approximation follows naturally from the interaction between Ampere's and Faraday's laws given in Equations (1a) and (1b), respectively.

In order to address the second issue, a variety of the *preconditioners* have been designed and applied. For instance, with the IE approach, to get a well-preconditioned matrix system A_{IE}, the *modified iterative-dissipative method* (MIDM) has been successfully developed (Singer, 1995; Pankratov et al., 1995, 1997; Singer and Fainberg, 1995, 1997) and implemented (Avdeev et al., 1997, 1998, 2000, 2002a, 2002b; Zhdanov and Fang, 1997; Hursan and Zhdanov, 2002; Singer et al., 2003). It is remarkable that the MIDM-preconditioned system matrix A_{IE} has such a small condition number, $\kappa(A_{\mathrm{IE}}) \leq \sqrt{C_{\mathrm{l}}}$, where C_{l} is the lateral contrast of conductivity. Comparisons with the finite-difference solution of Newman and Alumbaugh (2002) show similar performances for both solutions (see Table I).

Within the methodology of FD and FE approaches, the most favourable preconditioners are, Jacobi, SSOR and incomplete LU decomposition (typical example, $M = 25 \times 22 \times 21 = 11550$, $N_{\mathrm{bicgstab}} = 396$; $t_{\mathrm{cpu}} = 18$ min on a 1-GHz Pentium 3 PC; Mitsuhata and Uchida, 2004). From moderate to high frequencies these preconditioners work reasonably well, providing convergence of Krylov iterations. However, at low frequencies, or more exactly, at low induction numbers

$$\lambda = \sqrt{\omega\mu\sigma}\Delta \ll 1, \tag{4}$$

the convergence meets a certain difficulty, since Maxwell's equations (1) degenerate. In Equation (4) Δ stands for the characteristic grid size and other parameters are defined elsewhere in the text. To get around this inherent difficulty Smith (1996b) proposed a "divergence correction" that dramatically improves convergence. His ideas have been subsequently refined in (Everett and Schultz, 1996; LaBracque, 1999; Druskin et al., 1999). Presently, the low induction number (LIN; Newman and Alumbaugh, 2002; Weiss and Newman, 2003) and multigrid (Aruliah and Ascher, 2003; Haber, 2005, $M = 65^3 = 274625$; $t_{\mathrm{cpu}} = 2.5$ min per the source position) preconditioners demonstrate their superiority over more traditional ones. Figure 2 and

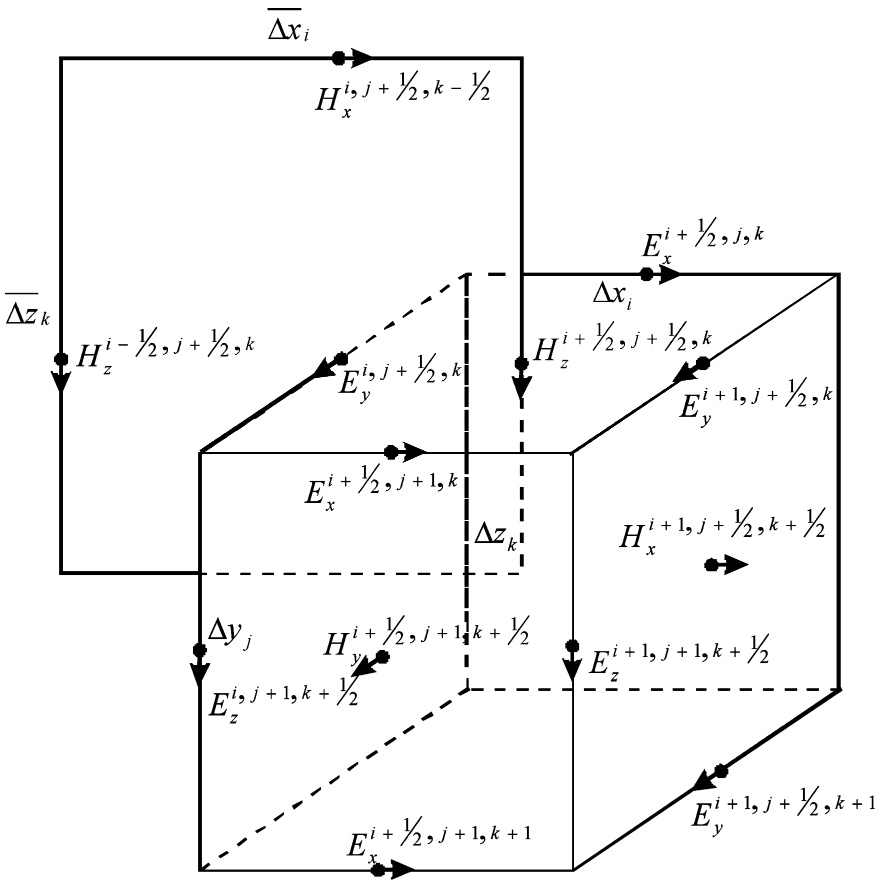

Figure 1. A fragment of a straggered grid of Yee (1966). The electric field is sampled at the centers of the prism edges, and the magnetic field is sampled at the centers of the prism faces.

Table II give such an example. Figure 3 demonstrates the grid-independency of the multigrid preconditioner, when $\lambda \leq 1$.

Usage of the EM potentials, as in the case of Helmholtz's potentials with a Coulomb gauge, instead of the EM fields also helps to greatly improve and accelerate solution convergence (Haber et al., 2000a; Mitsuhata and Ushida, 2004, among others).

The techniques presented in this section are more fundamental than mere mathematical tricks for accelerating the solution convergence. They are deeply rooted in the physics of the EM induction problem and so they allow us to more precisely describe it.

2.1.5 *Spectral Lancsoz Decomposition Method*

Another very efficient FD approach is the spectral Lancsoz decomposition method (SLDM) (Druskin and Knizhnerman, 1994; Druskin et al., 1999).

TABLE I

Computational statistics for a 3-D induction logging model (after Avdeev et al. (2002a))

Method	Grid $N_x \times N_y \times N_z = M$	Frequency (kHz)	Preconditioner	Iterates-m	Run time[a](s)
IE	$31 \times 31 \times 32 =$ 30 752	10, 1600, 5000	MIDM	7	2950
	563 328	10	LIN	17	2121
FD	435 334	160	Jacobi	6000	5686
	435 334	5000	Jacobi	1200	1101

[a] Times are presented for Pentium/350 MHz PC (IE code) and for IBM RS-6000 590 workstation (FD code).

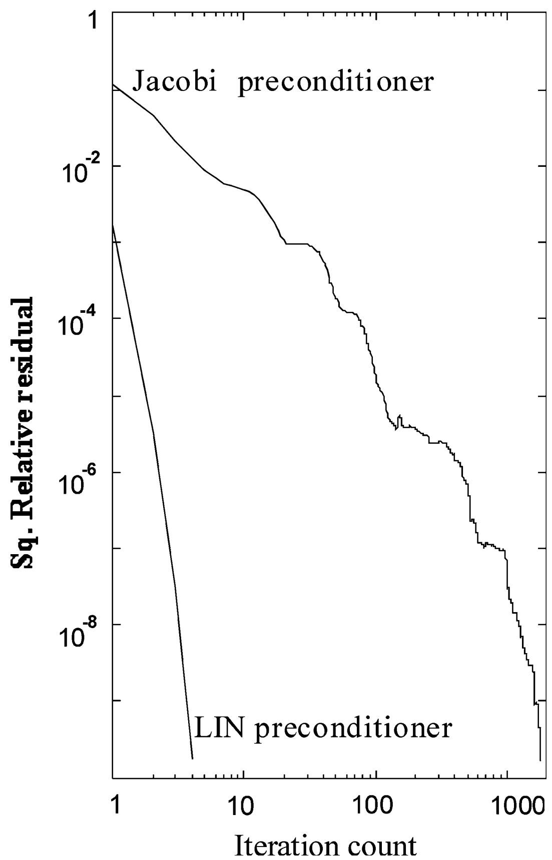

Figure 2. The convergence rate of FD solution for the Jacobi and LIN preconditioning (after Newman and Alumbaugh, 2002).

TABLE II

Number of iterations to convergence (within a tolerance of 10^{-7}) as a function of frequencies

	Number of cells	ω (Hz)					
		10^1	10^2	10^3	10^4	10^5	10^6
M_M	30^3	3	3	3	6	12	98
	40^3	3	3	3	6	13	116
	50^3	3	3	3	6	12	128
M_I	30^3	30	27	31	55	166	642
	40^3	40	40	42	76	210	1180
	50^3	46	48	51	97	273	1551

The results are presented for the multigrid (M_M) and incomplete Cholesky decomposition (M_I) preconditioners (after Aruliah and Ascher, 2003).

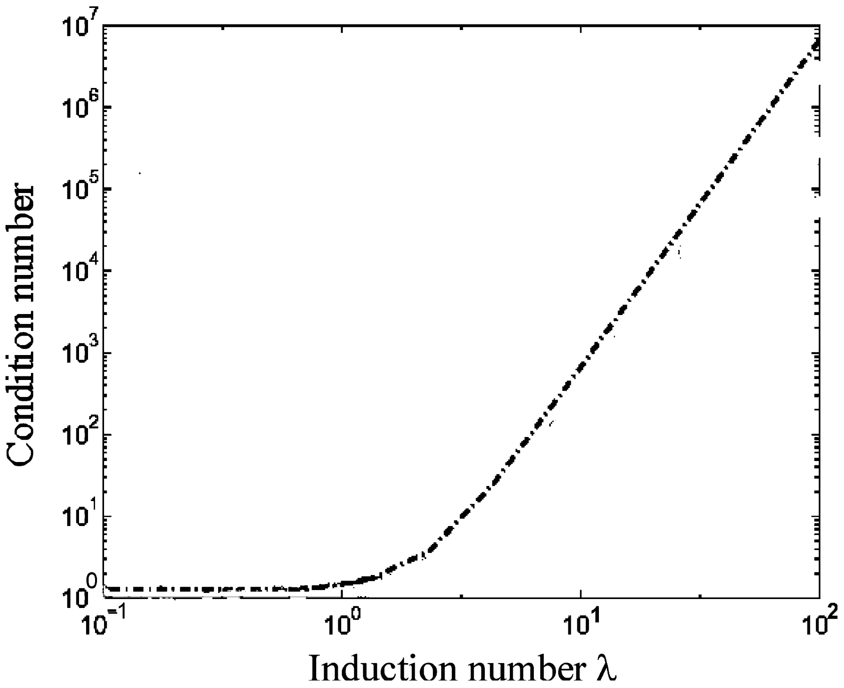

Figure 3. The condition number as a function of the induction number (after Aruliah and Ascher, 2003).

It is commonly considered as a method of choice when multi-frequency modelling of the EM field is required. The reason is that the SLDM is able to solve Maxwell's equations at many frequencies for a cost that is only slightly greater than that paid for a single frequency. But, such numerical effectiveness of the SLDM slightly sacrifices its universality. Indeed, the SLDM assumes that conductivity $\tilde{\sigma}$ and impressed current $\mathbf{j}^{\text{ext}}$ of Equation (1) are frequency-independent. However, this then means for example that the IP effects cannot be taken so easily on board. Wang and Fang (2001) extended the SLDM to anisotropic media. Recently, Davydycheva et al. (2003) proposed a special conductivity averaging and spectral optimal grid refinement procedure that reduces grid size and accelerates computation by the SLDM method. These authors claim that their new scheme outperforms other known FD schemes by an order of magnitude.

The basics of the SLDM method can be also found in Golub and Van Loan (1996).

2.1.6 *Spherical Earth Models*

Numerical implementations mentioned above use Cartesian geometry, and extensively cover such important geophysical applications, such as induction logging, airborne EM, magnetotellurics and controlled-source EM. At the same time, a number of implementations are also available to simulate the EM fields excited in 3-D spherical earth models, including those based on the spectral decomposition (Tarits, 1994; Grammatica and Tarits, 2002), finite-element (Everett and Schultz, 1996; Weiss and Everett, 1998; Yoshimura and Oshiman, 2002), spectral finite-element (Martinec, 1999), finite-difference (Uyeshima and Schultz, 2000) and integral equation (Koyama et al., 2002; Kuvshinov et al., 2002, 2005) approaches. Also, in order to deal with the complicated spatial and temporal variability of the satellite induction data, several time-domain techniques for computing 3-D EM fields of a transient external source have recently been developed (Hamano, 2002; Velimsky et al., 2003; Kuvshinov and Olsen, 2004).

2.2 Conclusion

Competition between various modelling approaches (FD, FE and IE) is today focused entirely on the two issues mentioned above. The ultimate goal of 3-D modellers is, first, to design a more accurate approximation to Maxwell's equations within a coarser grid discretization. The second important challenge is to find a faster preconditioned linear solver. Fortunately, as a result of this competition between methods, we now have several very effective codes for numerical modelling of 3-D EM fields at our disposal today.

3. Three-Dimensional Inversion

3.1 Why Is It Important?

Recent huge improvements in both instrumentation and data acquisition techniques have made electromagnetic surveys (magnetotelluric, controlled-source EM, crosshole EM tomography, etc.) a more common procedure. Accordingly there is an increased need for reliable methods of interpretation of particularly three-dimensional (3-D) datasets.

3.2 Why Is It Numerically Tough?

Even with the relatively high level of modern computing possibilities, the proper numerical solution of the 3-D inverse problem still remains a very difficult and computationally intense task for the following reasons. (1) It requires a fast, accurate and reliable forward 3-D problem solution. Approximate forward solutions (Zhdanov et al., 2000; Torres-Verdin and Habashy, 2002; Tseng et al., 2003; Zhang, 2003; among others) may deliver a rapid solution of the inverse problem (especially, for models with low conductivity contrasts), but the general reliability and accuracy of this solution are still open to question. (2) The inverse problem is large-scale; usually with thousands of data points (N) to be inverted in the tens of thousands of model parameters (M). In this case, the sensitivities are too numerous to be directly computed and stored in memory. (3) The problem is ill-posed in nature with nonlinear and extremely sensitive solutions. This means that due to the fact that data are limited and contaminated by noise there are many models that can equally fit the data within a given tolerance threshold. (4) To make the solution unique and depend stably on the data it is necessary to include a stabilizing functional (Tikhonov and Arsenin, 1977). This functional is a part of the penalty functional that trades off between the data misfit and *a priori* information given in the model or/and data. It may reflect any information on the model smoothness, sharp boundaries, a static shift in the data etc. (cf. Portniaguine and Zhdanov, 1999; Sasaki, 2004; Haber, 2005). Choice of such a stabilizator is of extreme importance since it heavily impacts on the solution obtained (cf. Farquharson and Oldenburg, 1998).

It is important to stress that the first encouraging examples of fully 3-D inversion solutions have appeared only within the last 3–5 years and the problem, in general, is currently an area of very intensive research. A typical example of computational loads inherent in, say, the 3-D MT inverse problem is as follows (Farquharson et al., 2002; inexact preconditioned Gauss–Newton method, $N = 1296$, $\mathrm{M} = 37 \times 41 \times 24 = 36408$, $N_{\mathrm{GN}} = 12$; $t_{\mathrm{cpu}} = 24$ h on three 1GHz processors.) The above example indicates why such kind of work requires very intensive numerical calculations and, hence, why it is preferable to solve it within a multi-processor framework.

3.3 How Is It Commonly Solved?

The first pioneering solution of the fully 3-D EM inverse problem was presented by Eaton (1989) more than 15 years ago. Yet in spite of this, until recently, the trial-and-error forward modelling was almost the only available tool to interpret the fully 3-D EM dataset. Today the situation has slightly improved, and the methods of unconstrained nonlinear optimisation (Nocedal and Wright, 1999) are gaining popularity to address the problem. Thus fortunately, the nonlinear optimisation methods have undergone tremendous progress, especially in their mathematical aspects.

In standard nomenclature a solution is sought as a stationary point of a penalty functional (Tikhonov and Arsenin, 1977).

$$\varphi(m,\lambda) = \varphi_d(m) + \lambda \cdot R(m) \underset{m,\lambda}{\longrightarrow} \min, \tag{5}$$

where $\varphi_d(m) = \frac{1}{2}\left\|d^{\text{obs}} - F(m)\right\|^2$ is the data misfit, $R(m)$ is the stabilizing functional, $F(m)$ is the forward problem mapping, $m = \log(\sigma)$ is the log conductivity, and $\lambda > 0$ is a regularization (Lagrange) multiplier. Traditionally, to find a solution to this optimisation problem geophysicists apply *nonlinear Newton-type iterations* (such as the classical full Newton, Gauss–Newton, quasi–Newton iterations, or some modification thereof) in the model parameter space (see Appendix C). This in turn entails, at each step of a Newton-type iteration, the computation of the sensitivity $N \times M$ matrix ($J = \frac{\partial F}{\partial m}$) and Hessian $M \times M$ matrix ($H = \frac{\partial^2 \varphi}{m^2}$), or its approximation (such as $H \approx J^{\mathrm{T}} J$). It also involves solving a large and dense system of linear equations

$$H \cdot \delta m = -g \tag{6}$$

in order to find a model update δm, where $g = \frac{\partial \varphi}{\partial m}$ is the gradient vector. Once δm is found, the new model is given by $m^{(i+1)} = m^{(i)} + \beta \cdot \delta m$, where β ($0 < \beta < 1$) is determined by a line search.

One important feature of inverse problems, is that within the straightforward Newton-type methods the sensitivity $N \times M$ matrix ($J = \frac{\partial F}{\partial m}$) must be computed and stored in memory. However, even with the use of the most efficient reciprocity techniques (McGillivray and Oldenburg, 1990; among others), the straightforward evaluation of the sensitivity matrix J still requires the solution of K forward (and adjoint) problems, where $K = \min\{N,M\}$ (see Appendix D for details). Such a numerical procedure, while tractable for 1-D and 2-D inverse problems, may become computationally prohibitive for larger and more complicated 3-D inverse problems. It is, then, not surprising that much effort has been directed towards economizing, or even bypassing, the evaluation of the sensitivity matrix (Smith and Booker, 1991; Torres-Verdin and Habashy, 1994; Farquharson and Oldenburg, 1996; Yamane et al., 2000, among others).

In order to solve a Newton system, given in Equation (6), more effectively the preconditioned conjugate gradient (CG) iterative method is commonly applied (cf. Newman and Alumbaugh, 1997; Haber et al., 2000a) since it allows solving the system without calculating J explicitly. At each step, the CG method requires calculating only matrix-vector products Jv and $J^{T}w$ and it is equivalent to the solution of two forward problems (see Appendix D). Thus, the total number of forward solutions involved in whole inversion process is proportional to $N_{GN}\times$ $(2\times$ $N_{CG})$, where N_{GN} is the number of nonlinear Gauss–Newton iterations, and N_{CG} is the number of linear CG iterations. The method may require extra forward problem solutions if a line search is invoked.

Mackie and Madden (1993) applied this approach to coarsely parameterised models (so that M remains relatively small) to invert 3-D MT data. Newman and Alumbaugh (1997) also used it to invert crosswell EM data, and Ellis (2002) used this approach to invert a fixed wing airborne TEM synthetic dataset. Ellis's solution is interesting since its engine – a forward problem solution – uses the integral equation approach. Nevertheless, the results demonstrated, in particular, that such a relatively straightforward approach is nearly useless for the numerical solution of practical 3-D EM inversion problems on a regular PC. More details on this approach can be found in (Newman and Hoversten, 2000). Significantly in this respect N_{GN} is usually small, however very occasionally N_{CG} may be relatively large. The slower convergence of the CG iterations is reflected in a large value of N_{CG}. To diminish further the number of CG iterations the inexact Gauss–Newton method (IGN; Kelly, 1999) can be applied. Haber et al. (2002) presented a 3-D frequency-domain controlled-source (CS) EM inversion based on the IGN method with the smoothness regularization.

Alternatively, Newman and Alumbaugh (2000), Rodi and Mackie (2001) and Mackie et al. (2001) proposed to solve the 3-D inverse problem using the *nonlinear conjugate gradient method* (NLCG) by Fletcher and Reeves (1964) and Polak and Ribiere (1969) that requires for computation only the gradient vectors $g = \frac{\partial \varphi}{\partial m}$, rather than sensitivities J (see Appendix C for details). The idea of applying gradient vectors to solve nonlinear geophysical inverse problems was first suggested by Tarantola (1987) and is also related to the EM migration technique of Zhdanov (2002; and the references therein). The motivation for using the NLCG method is that evaluating the gradients involves single solution of one forward and one adjoint problem at each NLCG iteration (see Appendix D and references therein). This is almost $K/2$ times faster than evaluating the full Jacobian matrix J required by Newton-type methods. Such great acceleration is slightly counterbalanced by the fact that the NLCG approach requires the solution of the 1-D minimization problem (so-called line search) at each iteration. Rodi and Mackie (2001) proposed an algorithm for the line search, equivalent in computational time to only three solutions of the forward problem. In spite of such a dramatic increase in speed, the NLCG approach still has to be implemented either within a massively parallel computing architecture (Newman and Alumbaugh, 2000; Newman et al., 2002; Newman and Boggs, 2004) or with the help of message passing interface (MPI) running on PC-clusters (Mackie et al., 2001). Newman et al. (2003) described an excellent application of this approach to the synthetic and experimental 3-D radio MT dataset (N = 25600, M = 132553; N_{NLCG} = 68; t_{cpu} = 120 h using 252 processors on the Sandia Nat. Lab. Ascii Red computer; for a fixed regularization parameter λ). Recently, Newman and Commer (2005) applied the NLCG approach to invert a transient EM dataset ($N = 99 \times 90 \times 2 = 17820$; N_{NLCG} = 87; t_{cpu} = 18 days using 336 processors on the Red computer). They advanced the original technique first introduced by Wang et al. (1994) for casual and diffusive EM fields and subsequently implemented by Zhdanov and Portniaguine (1997) in the framework of iterative migration. For synthetic examples considered in the paper of Newman and Commer (2005) they found that the migration of the initial data error into the model as presented by Zhdanov and Portniaguine (1997), without iteration or preconditioning, is not an effective imaging strategy.

Mackie et al. (2001) also implemented the NLCG approach to solve the 3-D MT inverse problem (typical example, N = 2000, $M = 39 \times 44 \times 19 = 32604$; N_{NLCG} = 20; t_{cpu} = 10–12 h on a 400 MHz desktop computer). These authors are able to invert wideband (1000–0.001 Hz) MT datasets with up to 600 MT sites and with model grids up to $70 \times 70 \times 40$. They have inverted probably 100 commercial datasets to date (Mackie, 2004, Private communication).

Dorn et al. (1999) have used a similar adjoint method to invert cross-well EM data.

Zhdanov and Golubev (2003) applied the NLCG method combined with an approximate forward modelling solution to invert the synthetic and experimental MT datasets (typical example, N = 3120, $M = 15 \times 13 \times 8 = 1560$; a model with the conductivity contrast of 10). In both synthetic examples presented in their paper, the true conductivity model is reconstructed qualitatively. Other computational loads are not referred to. They also applied such an approach to experimental MT data (N = 25 600, $M = 56 \times 50 \times 12$ = 33 600; $N_{\mathrm{NLCG}} = 30$; $t_{\mathrm{cpu}} = 14$ min). To increase the accuracy of inversion, Zhdanov and Tolstaya (2004) applied rigorous forward modelling based on the IE approach at the final stage of the inversion. Again, they considered a couple of low-contrasting models (typical example, $N = 3600$, $M = 16 \times 25 \times 8 = 3200$; $N_{\mathrm{NLCG}} = 82$, $t_{\mathrm{cpu}} = 200$ s; a model with the conductivity contrast of 33). For the last few inversion iterations a rigorous (rather than approximate) IE forward modeling code was used. This time, the type of computer used for the calculations is not referred to.

Using the Gauss–Newton iterative approach with smoothness regularization, Siripunvaraporn et al. (2004b), however, managed to reformulate the inverse problem for the data space so as to solve the $N \times N$ normal system of linear equations instead of the traditional $M \times M$ normal system. In many cases, when $N \ll M$, it may reduce the computational loads significantly.

They successfully inverted a synthetic 3-D MT dataset ($N = 1440$, $M = 28 \times 28 \times 21 = 16464$; $N_{\mathrm{GN}} = 5$; $t_{\mathrm{cpu}} = 84$ h on a Dec 666 MHz computer with 1 Gbyte of RAM). Also they applied the data space approach for inverting an experimental 3-D network-MT dataset (Siripunvaraporn et al., 2004a).

Sasaki (2001) applied the Gauss–Newton iteration with smoothness regularization in the model space to invert synthetic controlled-source 3-D EM datasets. Typical computational loads in this study are, $N = 210$, $M = 7 \times 5 \times 5 = 175$; $N_{\mathrm{GN}} = 3$; $t_{\mathrm{cpu}} = 25$ h on a Pentium II PC. As I mentioned above, with $M = 175$ the problem is severely under parameterised, and this computational approach may hardly satisfy the practical needs for inverting the huge datasets of regular airborne EM surveys. Sasaki (2004) also developed a solution of the 3-D MT inverse problem again based on the Gauss–Newton iteration with smoothness regularization in model space solving simultaneously for both conductivities and static shift parameters. The diagonal entries of the impedance are not included into inversion. Also to save computational time the sensitivity matrices are computed at only a limited number of iterations (practically only at two iterations). He tested the solution on a synthetic dataset and a real dataset for a geothermal exploration. Respective computational loads in this study are, $N = 3600$, $M = 10 \times 10 \times 11 = 1100$; $N_{\mathrm{GN}} = 7$; $t_{\mathrm{cpu}} = 7$ h and $N = 3300$, $M = 26 \times 8 \times 13 = 2704$; $N_{\mathrm{GN}} = 7$; $t_{\mathrm{cpu}} = 24$ h on a 2.53-GHz Pentium 4 PC. Another example of the application Sasaki's solution to geothermal 3-D MT exploration is given in Uchida and Sasaki (2003); ($N = 6900$, $M = 18 \times 15 \times 14 = 3780$; $N_{\mathrm{GN}} = 8$).

Varentsov (2002) applied the Gauss–Newton iteration with various regularizations in the model space to invert a synthetic 3-D MT dataset ($N = 1176$, $M = 14$ with one finite function describing a 3-D anomaly; $N_{\mathrm{GN}} = 15$; $t_{\mathrm{cpu}} = 30$ min on a 450-MHz Pentium II PC).

3.4 Constrained Optimisation

Constrained optimisation methods for the solution of 3-D EM inverse problem are now underway. With these methods the forward problem and the inverse problem are solved simultaneously in one iterative process (Haber et al., 2000b). These authors mention that the forward problem does not have to be solved exactly until the very end of the optimisation process. In other words, at the first steps of the iterative inversion procedure, it is sufficient to solve the forward problem approximately. The first promising results based on such a method (so-called all-at-once approach) were demonstrated by Haber et al. (2004). They successfully inverted a synthetic CSAMT dataset ($N = 3080$, $M = 64 \times 50 \times 30 = 96000$), as well as a synthetic time-domain dataset ($N = 4320$, $M = 40 \times 40 \times 32 = 51200$) where receivers are put in boreholes and a transmitting square loop is put on the surface. The computational loads enabled are not referred to.

The simple idea that lies behind the all-at-once approach is that it is not necessary to solve the forward problem accurately while the misfit φ_d of Equation (5) is still relatively large. Obviously, this consideration does not depend on the method selected for solution of the forward problem. The method may be equally either FD, FE or IE approach. For instance, with an IE approach, to get the accuracy of the forward problem solution that is required at the initial steps of inversion, one can terminate the solution iteration after the few first iterations. However, it is important not to be overoptimistic with this approach and to understand that at the late stage of inversion the proper inversion algorithm still must include a rigorous forward problem solution. As previously mentioned, Zhdanov and Golubev (2003) and Zhdanov and Tolstaya (2004) assert that they successfully applied such an approach for inversion of magnetotelluric data.

3.5 Global Induction Studies

3-D EM inversion for spherical earth models is still a subject for future investigations. At present, only one publication exists on the topic (Schultz and Pritchard, 1999).

3.6 Static Limit

Several promising works on the numerical solution of the fully 3-D EM problem in the static limit (so-called dc regime) have been recently published. Haber (2005) presented a comparison between various Gauss–Newton modifications and quasi–Newton (QN) solution for large-scale dc resistivity surveys (synthetic dataset, $N = 65536$, $M = 65^3 = 274625$). The QN inversion in total required only 92 solutions of the forward problem with $t_{\mathrm{cpu}} = 1$ h for each. The reason for such speed is that in his study the matrix J is approximated by a low rank matrix. Abubakar et al. (2001) presented the results based on the contrast source inversion (CSI) method for electrode logging in a deviated well with invasion (typical example, $N = 210$, $M = 1470$; $N_{\mathrm{csi}} = 1024$; $t_{\mathrm{cpu}} = 4$ h on a 200-MHz Pentium PC). Abubakar and van der Berg (2000) inverted the cross-well electrical logging synthetic dataset (loads typically are, $N = 448$, $M = 28 \times 28 \times 28 = 21952$; $N_{\mathrm{csi}} = 254$; $t_{\mathrm{cpu}} = 30$ h on a 400-MHz Pentium PC.)

3.7 Conclusion

As correctly stated by Newman et al. (2003), even with the recent advancements in 3D EM inversion, nonuniqueness and solution uncertainty issues remain a formidable problem.

I would like to conclude this review with the following general remark. The most important challenge that faces the EM community today is to convince software developers to put their 3-D EM forward and inverse solutions into the public domain, at least after some time. This would have a strong impact on the whole subject and the developers would benefit from feedback regarding the real needs of the end-users.

Time constraints have not allowed me to mention all important work on 3-D EM modelling and inversion, conducted by my colleagues. I apologize for this and hope that you all understand.

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Appendix A. Krylov Subspace Methods

Let me first recall a couple of important notions from the theory of linear operators (Greenbaum, 1997). In general, a linear operator/matrix A: $H \rightarrow H$ is called Hermitian if the equality

$$(u, Av) = (Au, v) \tag{A.1}$$

holds for any $u,v \in H$, where H is the Hilbert linear space with an inner product $(\cdot, \cdot)$. There are many ways to define this inner product. In particular, for complex-valued vectors u,v it can be defined as

$$(u, v) = \overline{u}^{\mathrm{T}} v = \sum_{l} \overline{u_l} v_l, \tag{A.2}$$

where superscript T means transpose, and $\overline{u}$ means complex conjugate of u. Note that whether the matrix A is Hermitian, or not, depends entirely on the definition of the inner product. From Equations (A.1) and (A.2) it follows that

$$A^{\mathrm{T}} = \overline{A}, \tag{A.3}$$

for any Hermitian matrix A. If $A^{\mathrm{T}} = A$ then the matrix A is called symmetric.

Since the work of Hestenes and Stiefel (1952) and Lanczos (1952) for solving linear systems $A{\cdot}x = b$, as given in Equation (3), the Krylov subspace methods such as those of Lanczos, Arnoldi, conjugate gradients, GMRES, CGS, QMR, and an alphabet soup of them are commonly applied (O'Leary, 1996). Krylov subspace methods generate successive approximations $x^{(1)}$, $x^{(2)}$,..., so that

$$x^{(m)} \in x^{(0)} + \mathrm{span}\left\{r^{(0)}, A \cdot r^{(0)}, \ldots, A^{(m-1)} \cdot r^{(0)}\right\}, \tag{A.4}$$

where $x^{(0)}$ is an initial guess, and $r^{(0)} = b - A{\cdot}x^{(0)}$ is the initial residual. The linear space span $\{r^{(0)}, A{\cdot}r^{(0)}, \ldots, A^{(m-1)}{\cdot}r^{(0)}\}$ is usually referred to as a Krylov subspace of size m, generated by A and $r^{(0)}$. As a matter of fact, the Krylov subspace methods use several, say k, previous approximations $x^{(m-1)}, x^{(m-2)}, \ldots, x^{(m-k)}$ to generate the mth approximation $x^{(m)}$ (so-called k-terms recurrence). While the methods of choice and convergence analysis for Hermitian matrices A are well known (e.g. an algorithm that generates optimal approximations is MINRES by Paige and Sounders (1974)), the methods for non-Hermitian matrices A (that is our case) are not so well developed (Greenbaum, 1997). Aforementioned optimal approximations are the approximations $x^{(m)}$ whose residuals, $r^{(m)} = b - A{\cdot}x^{(m)}$, have the smallest Euclidean norm, $\left\|r^{(m)}\right\| = \sqrt{\sum_i r_i^{(m)^2}}$. Faber and Manteuffel (1984) proved that for most of the non-Hermitian matrices A there is no short-term recurrence to generate the optimal approximations, and so work and storage must grow linearly with the iteration count, m. Indeed, the GMRES method by Saad and Schultz (1986) finds the optimal approximations, at the cost of additional work and storage, while other non-Hermitian Krylov methods (BSG, CGS, QMR, BiCGSTAB, GPBiCG, restarted GMRES, hybrid GMRES, etc.) that use short-term recurrence (and so they can be implemented with relatively low work and storage) generate non-optimal approximations. Besides, these short-term recurrence methods usually have rather irregular convergence behaviour with oscillations and peaks of the residual.

Appendix B. Preconditioning the Systems of Linear Equations

Again let me first recall some definitions (Greenbaum, 1997). Matrix A is well conditioned if its condition number

$$\kappa(A) = ||A|| \cdot ||A^{-1}|| \tag{B.1}$$

is relatively small. Here A^{-1} is the inverse matrix, and $\|A\| = \max_u \frac{\|Au\|}{\|u\|}$, where $\|u\| = \sqrt{(u,u)}$. If $\kappa(A)$ is relatively large, matrix A is poorly conditioned. In order to get a faster solution of a system of linear equations

$$A \cdot x = b \tag{B.2}$$

by a Krylov subspace method one can transform the original system given in Equation (B.2) to a preconditioned form, as

$$(AM^{-1}) \cdot y = b, \tag{B.3}$$

where $y = M \cdot x$ is the vector of modified unknowns and M^{-1} is the inverse of M. When the modified system (B.3) is eventually solved to give an approximate solution $\widetilde{y}$, the solution $\widetilde{x}$ of the original system (B.2) is resolved from the following system of linear equations $M \cdot \widetilde{x} = \widetilde{y}$. Matrix M in Equation (B.3) is called the (right-)preconditioner, and, in general, it is sought so that the matrix AM^{-1} turns out to be as close as possible to the identity matrix. In other words, it is desirable to choose preconditioner M so that the modified system (B.3) is better preconditioned than the original system (B.2). In the terms of condition numbers this requirement is expressed as

$$1 \approx \kappa(AM^{-1}) \ll \kappa(A). \tag{B.4}$$

If M is equal to the main diagonal of A, M is called the Jacobi preconditioner. If A is decomposed as $A = A_1 + A_2$, where A_1 in some way dominates over A_2, then $= A_1$ can be used as a preconditioner. In this case the preconditioned system is

$$(1 + A_2 A_1^{-1}) \cdot y = b, \tag{B.5}$$

where

$$A_1 \cdot x = y \tag{B.6}$$

The preconditioning as given in Equation (B.5) is typically applied to precondition the EM problems in the static limit.

Appendix C. Nonlinear Optimisation for EM Problems

Let me consider here an unconstrained optimization (Nocedal and Wright, 1999) of a Tikhonov-type regularized functional (Tikhonov and Arsenin, 1977) of the form

$$\varphi = \frac{1}{2} \left\| d^{\text{obs}} - F(m) \right\|^2 + \lambda \cdot R(m, m^{\text{ref}}) \underset{m,\lambda}{\longrightarrow} \min, \tag{C.1}$$

where $d^{\text{obs}} = (d_1^{\text{obs}}, \ldots, d_N^{\text{obs}})^{\mathrm{T}}$ is the complex-valued vector that comprises the observed data values, and forward problem $F(m)$ nonlinearly maps the model space of real-valued vectors $m = (m_1, \ldots, m_M)^{\mathrm{T}}$ to the space of the predicted complex-valued data d. In Equation (C.1) m^{ref} is the reference model and λ ($\lambda > 0$) is the regularization parameter that trades off between the data misfit $\varphi_d = \frac{1}{2}\left\|d^{\text{obs}} - F(m)\right\|^2$ and model smoothness $R(m,m^{\text{ref}})$. It may happen that a suitable value of λ may be chosen with the GCV and L-curve criteria (see Farquharson and Oldenburg, 2004 for details), or the Akaike's Bayesian information criterion (Mitsuhata et al., 2002). A typical choice of $R(m,m^{\text{ref}})$ is

$$R(m, m^{\text{ref}}) = \frac{1}{2}\left\| W(m - m^{\text{ref}})\right\|^2, \tag{C.2}$$

where W is a real $M\times M$ smoothing matrix (Newman and Hoversten, 2000, among others). The norm $\|u\|^2 = (u, u)_2$ given in Equations (C.1), (C.2) is induced by the L_2 inner product

$$(u, v)_2 = \int \overline{u} v dV. \tag{C.3}$$

The finite dimensional form of Equation (C.3) is $\|u\|^2 = \overline{u}^{\text{T}} u = \sum_{k=1}^{N} \overline{u_i} u_i$, where the upper bar means the complex conjugate, and superscript T stands for the transpose (cf. Equation (A.2) of Appendix A).

For what follows, it is better to rewrite Equation (C.1) as

$$\varphi = \frac{1}{2}(d^{\text{obs}} - F(m), d^{\text{obs}} - F(m))_2 + \lambda \cdot R(m, m^{\text{ref}}) \underset{m,\lambda}{\longrightarrow} \min. \tag{C.4}$$

The necessary conditions to minimize functional (C.4) is delivered by its stationary points

$$g = \frac{\partial \varphi}{\partial m} = \left(\frac{\partial \varphi}{\partial m_1}, \ldots, \frac{\partial \varphi}{\partial m_M}\right)^{\text{T}} = 0. \tag{C.5}$$

From Equation (C.4) and after some algebra, the gradient $g = \frac{\partial \varphi}{\partial m}$ can be found as

$$g = -\text{Re}\left(d^{\text{obs}} - F(m), \frac{\partial F(m)}{\partial m}\right)_2 + \lambda \cdot \frac{\partial R}{\partial m} = \text{Re}\left\{J^{\text{T}}(\overline{F} - \overline{d^{\text{obs}}})\right\} + \lambda \frac{\partial R}{\partial m}, \tag{C.6}$$

where $J^{\text{T}}(m)$ is the transpose of the sensitivity matrix

$$J(m) = \begin{pmatrix} \frac{\partial F_1}{\partial m_1} & \cdots & \frac{\partial F_1}{\partial m_M} \\ \cdots & \cdots & \cdots \\ \frac{\partial F_N}{\partial m_1} & \cdots & \frac{\partial F_N}{\partial m_M} \end{pmatrix}, \tag{C.7}$$

and where Re refers to the real part of the complex argument. Combining Equations (C.5) and (C.6) yields

$$-\mathrm{Re}\left(d^{\mathrm{obs}} - F(m), \frac{\partial F(m)}{\partial m}\right)_2 + \lambda \cdot \frac{\partial R}{\partial m} = \mathrm{Re}\left\{J^{\mathrm{T}}(\overline{F} - \overline{d^{\mathrm{obs}}})\right\} + \lambda \frac{\partial R}{\partial m} = 0. \quad (C.8)$$

C.1 Newton Method

The general technique to minimize the functional (C.1) is to use Newton's method for solving the nonlinear system of equations (C.8) (Dennis and Schnabel, 1996). Given ith Newton's approximation $m^{(i)}$, the next approximation $m^{(i+1)}$ is sought to satisfy the following

$$H^{(i)} \cdot m^{(i+1)} = H^{(i)} \cdot m^{(i)} - g^{(i)}, \quad (C.9)$$

where $g^{(i)} = \frac{\partial \varphi}{\partial m}(m^{(i)})$ and $H^{(i)} = \frac{\partial^2 \varphi}{\partial m^2}(m^{(i)})$ are the gradient and Hessian both determined at $m = m^{(i)}$, respectively. The Hessian $M \times M$ matrix

$$H = \frac{\partial^2 \varphi}{\partial m^2} = \begin{pmatrix} \frac{\partial^2 \varphi}{\partial m_1 \partial m_1} & \cdots & \frac{\partial^2 \varphi}{\partial m_1 \partial m_M} \\ \cdots & \cdots & \cdots \\ \frac{\partial^2 \varphi}{\partial m_M \partial m_1} & \cdots & \frac{\partial^2 \varphi}{\partial m_M \partial m_M} \end{pmatrix} \quad (C.10)$$

is derived from Equation (C.4) in the following form

$$\begin{aligned} H &= \mathrm{Re}\left\{\left(\frac{\partial F(m)}{\partial m}, \frac{\partial F(m)}{\partial m}\right)_2 - \left(d^{\mathrm{obs}} - F(m), \frac{\partial^2 F(m)}{\partial m^2}\right)_2\right\} + \lambda \cdot \frac{\partial^2 R}{\partial m^2} \\ &= \mathrm{Re}\left\{\overline{J}^{\mathrm{T}} J + \frac{\partial^2 F}{\partial m^2}(\overline{F} - \overline{d^{\mathrm{obs}}})\right\} + \lambda \frac{\partial^2 R}{\partial m^2} \end{aligned}, \quad (C.11)$$

where it is also assumed that $\left\{\left(\frac{\partial^2 f}{\partial m^2}\right) g\right\}_{i,j} = \sum_{k=1}^{N} \frac{\partial^2 f_k}{\partial m_i \partial m_j} g_k$. For 3-D electromagnetic problems the gradient $g^{(i)}$ and Hessian $H^{(i)}$ need not be computed explicitly (see Appendix D). Note that

$$\frac{\partial R}{\partial m} = W^{\mathrm{T}} W (m - m^{\mathrm{ref}}), \quad (C.12)$$

$$\frac{\partial^2 R}{\partial m^2} = W^{\mathrm{T}} W, \quad (C.13)$$

when $R(m, m^{\mathrm{ref}})$ is as given in Equation (C.2). Substitution of Equations (C.6), (C.11)–(C.13) into Equation (C.9) yields Newton's iteration

$$\begin{aligned} &\left[\mathrm{Re}\left\{\overline{J}^{\mathrm{T}} J + \frac{\partial^2 F}{\partial m^2}(\overline{F} - \overline{d^{\mathrm{obs}}})\right\} + \lambda W^{\mathrm{T}} W\right] \cdot \delta m^{(i)} \\ &\qquad = -\mathrm{Re}\left\{J^{\mathrm{T}}(\overline{F} - \overline{d^{\mathrm{obs}}})\right\} - \lambda W^{\mathrm{T}} W (m^{(i)} - m^{\mathrm{ref}}) \end{aligned} \quad (C.14)$$

for the model update $\delta m^{(i)} = m^{(i+1)} - m^{(i)}$.

The main advantage of Newton's method is its fast local convergence. The drawbacks are that, (1) it does not guarantee that the generated sequence $m^{(i)}$ converges to a solution of Equation (C.1), (2) it may converge locally, and (3) it does not necessarily monotonically decrease the functional of Equation (C.1). However, if the Hessian $H(m^{(i)})$ is positive definite, then the update $\delta m^{(i)}$ of Equation (C.14) is a descent direction, since $g^{(i)\mathrm{T}}\ \delta m^{(i)} = -\ g^{(i)T}\ (H^{(i)})^{-1}\ g^{(i)} < 0$. In this case, to proceed to a global minimum a linear search method may be incorporated as $m^{(i+1)} = m^{(i)} - \alpha^{(i)}\ \delta m^{(i)}$, where the stepsize $\alpha^{(i)}$ is such that $\varphi(m^{(i)} + \alpha^{(i)}\delta m^{(i)}) = \min\limits_{\alpha} \varphi(m^{(i)} + \alpha\delta m^{(i)})$.

There are several modifications of Newton's method.

C.2 Gauss–Newton Method

If the second-derivatives are discarded in Equation (C.14), one gets the Gauss–Newton iterative method

$$\left[\mathrm{Re}\left\{\overline{J}^{\mathrm{T}} J\right\} + \lambda W^{\mathrm{T}} W\right] \cdot \delta m^{(i)} = -\mathrm{Re}\left\{J^{\mathrm{T}}(\overline{F} - \overline{d^{\mathrm{obs}}})\right\} - \lambda W^{\mathrm{T}} W(m^{(i)} - m^{\mathrm{ref}}). \tag{C.15}$$

As was correctly mentioned by Haber et al. (2000a), the Gauss–Newton approximation (C.15) is widely used because calculation of the second-derivatives $\frac{\partial^2 F}{\partial m^2}$ is commonly considered prohibitively expensive. For 3D EM problems the first attempt to quantitatively compare the convergence rates of the full Newton and Gauss–Newton iterations has been undertaken by Haber et al. (2000a). Those authors demonstrated that a full Newton step does not cost much more than a Gauss–Newton step.

For 3-D large-scale problems (which is our case) forming the Hessian matrix and directly resolving the model update $\delta m^{(i)}$ via Equation (C.9) (given in whatever form of (C.14) or (C.15)) is computationally prohibitive. For this reason the system of linear equations (C.9) is usually solved by a Krylov subspace method that requires only a sequence of relatively inexpensive matrix-vector products involving that Hessian (see Appendix A). Besides, since the Hessian matrix $H^{(i)}$ of Equation (C.9) is real symmetric and positive definite, the method of choice for solving the system (C.9) is clearly the conjugate gradient (CG) method, which is commonly used for such problems. This combination of Newton's and CG methods is usually referred as the Newton–Krylov/CG method for solving nonlinear inverse problems (Newman and Hoversten, 2000).

However, sometimes the CG-solution of the linear system (C.9) may still be computationally expensive. In order to avoid such an expensive procedure it is advantageous to solve the system (C.9) by a quasi–Newton method.

C.3 Quasi–Newton Method

In Newton's method, the system (C.9) is CG-solved at each step to generate a model update $\delta m^{(i)} = -(H^{(i)})^{-1} g^{(i)}$. However, as mentioned above, for large-scale problems it may be prohibitively expensive. The quasi–Newton method allows us to circumvent this difficulty by iteratively generating matrices $G^{(i)}$ that replace the inverses of the Hessian $(H^{(i)})^{-1}$ so that

$$\delta m^{(i)} = -G^{(i)} g^{(i)}. \tag{C.16}$$

Matrices $G^{(i)}$ are updated recursively as (Broyden, 1969)

$$G^{(i)} = G^{(i-1)} + a^{(i-1)} u^{(i-1)} (u^{(i-1)})^{\mathrm{T}}, \tag{C.17}$$

where $u^{(i-1)} = \delta m^{(i-1)} - G^{(i-1)} \delta g^{(i-1)}$, $a^{(i-1)} = (u^{(i-1)})^{\mathrm{T}} \delta g^{(i-1)}$, $\delta g^{(i-1)} = g^{(i)} - g^{(i-1)}$, and $G^{(0)} = 1$. Matrices $G^{(i)}$ satisfy quasi–Newton condition

$$\delta m^{(i-1)} = G^{(i)} \delta g^{(i-1)}. \tag{C.18}$$

Thus, this quasi–Newton method requires us to calculate, and possibly to store, the gradients $g^{(i)}$ and update vectors $u^{(i)}$ only.

Alternative ways to recursively calculate matrices $G^{(i)}$ are delivered by the DFP, BFGS or L-BFGS methods (Nocedal and Wright, 1999). All these quasi–Newton methods retain the fast local convergence of Newton's method, although they are slower.

As it was advocated by Haber (2005), in the quasi–Newton approach it is sometimes more effective to approximate the Hessian only in the part that relates directly to the data misfit, rather than the full Hessian.

C.4 Nonlinear Conjugate Gradient Method (NLCG)

This is another method for minimization of the functional (C.1) that also avoids calculation of the Hessian matrices. Originally, it was proposed by Fletcher and Reeves (1964) for nonlinear optimization, and later improved by Polak and Ribiere (1969). At each NLCG step, updating the approximate solution $m^{(i)} \rightarrow m^{(i+1)}$ requires (1) calculation and storage of gradients $g^{(i)}$ and $g^{(i-1)}$ for updating the search direction $d^{(i-1)} \rightarrow d^{(i)}$, and (2) a linear search along the search direction $d^{(i)}$. Due to its apparent simplicity this method has gained popularity in the EM community as the method of choice for solving large-scale inverse problems (Rodi and Mackie, 2000; Newman and Alumbaugh, 2000; Newman and Boggs, 2004).

Still the merits of the NLCG method over the Newton's methods are questionable.

Appendix D. Calculation of the Gradient and Sensitivities

Let me demonstrate how the gradient $g = \frac{\partial}{\partial m}\varphi$ given in Equation (C.6) can be directly calculated for the price of two forward modellings only (Romanov and Kabanikhin, 1994; Dorn et al., 1999; among others).

Rewrite Maxwell's equations (1) in operator form as

$$\mathcal{B}(m)\mathbf{E}^{s} = \mathbf{j}^{s}(m), \tag{D.1}$$

where $m = \log(\sigma)$ is the log conductivity and the partial differential equation (PDE) $\mathcal{B}(m)$ operator is

$$\mathcal{B}(m) = -10^{m} + \nabla \times \frac{\mu^{-1}}{i\omega}\nabla \times . \tag{D.2}$$

For what follows, I also need to consider the adjoint Maxwell's PDE

$$\mathcal{B}^{*}(m)\mathbf{u} = \mathbf{v}, \tag{D.3}$$

where $\mathcal{B}^{*}(m)$ is an adjoint operator, which, by definition, must satisfy the following

$$(\mathcal{B}(m)\mathbf{u}, \mathbf{v})_2 = (\mathbf{u}, \mathcal{B}^{*}(m)\mathbf{v})_2 \tag{D.4}$$

for any complex-valued vectors $\mathbf{u}$,$\mathbf{v}$. Brackets in Equation (D.4) represent the L_2 inner product $(\mathbf{u}, \mathbf{v})_2 = \int \overline{\mathbf{u}}^{\mathrm{T}}\mathbf{v}dV$ where the volume integration is over the entire Cartesian space. From Equations (D.2), (D.4) it is easy to show that

$$\mathcal{B}^{*}(m) = -10^{\overline{m}} - \nabla \times \frac{\overline{\mu}^{-1}}{i\omega}\nabla \times, \tag{D.5}$$

where, as usual, the upper bar means the complex conjugate and superscript T stands for the transpose. Comparing Equations (D.2) and (D.5), one can conclude that $\overline{\mathcal{B}^{*}} = \mathcal{B}$. This means that Equation (D.3) can be solved using the same solver as used for solving Equation (D.1).

Further, from Equation (C.6) it follows that

$$g = \frac{\partial}{\partial m}\varphi = \mathrm{Re}\left\{\left(F - d^{\mathrm{obs}}, \frac{\partial}{\partial m}F\right)_2\right\} + \lambda\frac{\partial}{\partial m}R, \tag{D.6}$$

where

$$F(m) = \mathcal{Q} \cdot \mathbf{E}(\sigma), \tag{D.7}$$

is the predicted data and where $\mathcal{Q}$ is an integral, differential or interpolation linear operator, which maps the electric field $\mathbf{E}$ to $F(m)$. An explicit form of $\mathcal{Q}$ depends on the type of inverse problem under consideration. What is important for us now is that $\mathcal{Q}$ does not depend on m, and so

$$\frac{\partial}{\partial m}F = \mathcal{Q}\cdot\frac{\partial \mathbf{E}^s}{\partial m} \tag{D.8}$$

From Equation (D.1) it follows that

$$\frac{\partial \mathbf{E}^{\mathrm{s}}}{\partial m} = \mathcal{B}^{-1}\left(\frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m} - \frac{\partial \mathcal{B}}{\partial m}\mathbf{E}^{\mathrm{s}}\right). \tag{D.9}$$

Substituting Equation (D.9) into Equation (D.8) yields

$$\frac{\partial}{\partial m}F = \mathcal{Q}\cdot\mathcal{B}^{-1}\left(-\frac{\partial \mathcal{B}}{\partial m}\mathbf{E}^{\mathrm{s}} + \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m}\right). \tag{D.10}$$

D.1 Sensitivities

To calculate sensitivities $J = \frac{\partial}{\partial m}F$ one can first solve M forward problems of the form

$$\mathcal{B}\frac{\partial \mathbf{E}^{\mathrm{s}}}{\partial m_j} = \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m_j} - \frac{\partial \mathcal{B}}{\partial m_j}\mathbf{E}^{\mathrm{s}} \quad (j = 1, \ldots, M) \tag{D.11}$$

(with respect to $\frac{\partial \mathbf{E}^{\mathrm{s}}}{\partial m_j}$) and substitute the result into Equation (D.8). Alternatively, letting $\mathcal{B}$ now represent the matrix of the operator, one can solve N adjoint problems of the form

$$\mathcal{B}^{\mathrm{T}}\cdot\mathcal{V} = \mathcal{Q}^{\mathrm{T}}, \tag{D.12}$$

(with respect to columns of the $M \times N$ matrix $\mathcal{V}$) and then obtain the sensitivities as (cf. Rodi and Mackie, 2000)

$$J = \mathcal{V}^{\mathrm{T}}\left(-\frac{\partial \mathcal{B}}{\partial m}\mathbf{E}^{\mathrm{s}} + \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m}\right). \tag{D.13}$$

D.2 Gradient

Substituting Equation (D.10) in Equation (D.6) one can obtain

$$\begin{aligned} g = \frac{\partial}{\partial m}\varphi &= \mathrm{Re}\left\{\left(F - d^{\mathrm{obs}}, \mathcal{Q}\cdot\mathcal{B}^{-1}\left(-\frac{\partial \mathcal{B}}{\partial m}\mathbf{E}^{\mathrm{s}} + \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m}\right)\right)_2\right\} + \lambda\frac{\partial}{\partial m}R \\ &= \mathrm{Re}\left\{\left(\mathcal{B}^{*^{-1}}\mathcal{Q}^*(F - d^{\mathrm{obs}}), -\frac{\partial \mathcal{B}}{\partial m}\mathbf{E}^{\mathrm{s}} + \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m}\right)_2\right\} + \lambda\frac{\partial}{\partial m}R \end{aligned} \tag{D.14}$$

Here Equation (D.4) and the well-known property of adjoint operators, $\mathcal{B}^{*^{-1}} = \mathcal{B}^{-1^{*}}$, were used. From Equation (D.14) it is seen that

$$g = \mathrm{Re}\left\{ \left(\mathbf{U}, \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m} - \frac{\partial \mathcal{B}}{\partial m} \mathbf{E}^{\mathrm{s}} \right)_2 \right\} + \lambda \frac{\partial}{\partial m} R, \tag{D.15}$$

where vector $\mathbf{U}$ is a solution of the adjoint equation

$$\mathcal{B}^{*}\mathbf{U} = \mathcal{Q}^{*}(F - d^{\mathrm{obs}}). \tag{D.16}$$

It is clear, however, that the most cumbersome calculations that are presented in Equation (D.15) are those of $\mathbf{U}$ and $\mathbf{E}^{\mathrm{s}}$, since $\frac{\partial \mathcal{B}}{\partial m}, \frac{\partial \mathbf{j}^{\mathrm{s}}}{\partial m}$ and $\frac{\partial}{\partial m} R$ can be calculated analytically. Thus, computational loads to calculate the full gradient $g = \frac{\partial}{\partial m}\varphi$ are nearly the same as those for one solution of the original forward problem (to get $\mathbf{E}^{\mathrm{s}}$) and one solution of the adjoint forward problem (to get $\mathbf{U}$).

References

Abubakar, A., and Berg, P.van der: 2000. 'Non-Linear Three-Dimensional Inversion of Cross-Well Electrical Measurements', *Geophys. Prosp.* **48**, 109–134.

Abubakar, A., and Berg, P.van der: 2001. 'Nonlinear Inversion of the Electrode Logging Measurements in a Deviated Well', *Geophysics* **66**, 110–124.

Alumbaugh, D. L., Newman, G. A., Prevost, L., and Shadid, J. N.: 1996. 'Three-Dimensional Wide Band Electromagnetic Modeling on Massively Parallel Computers', *Radio Sci.* **31**, 1–23.

Aruliah, D. A., and Ascher, U. M.: 2003. 'Multigrid Preconditioning for Krylov Methods for Time-Harmonic Maxwell's Equations in 3D', *SIAM J. Scient. Comput.* **24**, 702–718.

Avdeev, D. B., Kuvshinov, A. V., Pankratov, O. V., and Newman, G.A.: 1997. 'High-Performance Three-Dimensional Electromagnetic Modeling Using Modified Neumann Series. Wide-band Numerical Solution and Examples', *J. Geomagn. Geoelectr.* **49**, 1519–1539.

Avdeev, D. B., Kuvshinov, A. V., Pankratov, O. V., and Newman, G. A.: 1998. 'Three-Dimensional Frequency-Domain Modelling of Airborne Electromagnetic Responses', *Explor. Geophy.* **29**, 111–119.

Avdeev, D. B., Kuvshinov, A. V., Pankratov, O. V., and Newman, G. A.: 2000, '3D EM Modelling Using Fast Integral Equation Approach with Krylov Subspace Accelerator, in *Expanded abstracts of the 62nd EAGE Conference*, Glasgow, Scotland, pp. 195–198.

Avdeev, D. B., Kuvshinov, A. V., Pankratov, O. V., and Newman, G. A.: 2002a. 'Three-Dimensional Induction Logging Problems. Part I. An Integral Equation Solution and Model Comparisons', *Geophysics* **67**, 413–426.

Avdeev, D. B., Kuvshinov, A. V., and Epova, X. A.: 2002b. 'Three-Dimensional Modeling of Electromagnetic Logs From Inclined-Horizontal Wells, Izvestiya', *Phys. Solid Earth* **38**, 975–980.

Badea, E. A., Everett, M. E., Newman, G. A., and Biro, O.: 2001. 'Finite-Element Analysis of Controlled-Source Electromagnetic Induction Using Coulomb-Gauged Potentials', *Geophysics* **66**, 786–799.

Boyce, W., Lynch, D., Paulsen, K., and Minerbot, G.: 1992. 'Nodal Based Finite Element Modeling Maxwell's Equations', *IEEE Trans. Antennas Propagat.* **40**, 642–651.

Broyden, C. G.: 1969. 'A New Double-Rank Minimization Algorithm', *Notices Am. Math. Soc.* **16**, 670.

Cerv, V.: 1990. 'Modelling and Analysis of Electromagnetic Fields in 3D Inhomogeneous Media', *Surv. Geophys.* **11**, 205–230.

Champagne, N. J., Berryman, J. G., Buettner, H. M., Grant, J. B., and Sharpe, R. M.: 1999, 'A Finite-Difference Frequency-Domain Code for Electromagnetic Induction Tomography', in *Proc. SAGEEP*, Oakland, CA, pp. 931–940.

Chew, W. C.: 1999, *Waves and Fields in Inhomogeneous Media*, Wiley-IEEE Press, Piscataway, NJ.

Commer, M., and Newman, G.: 2004. 'A Parallel Finite-Difference Approach for 3D Transient Electromagnetic Modeling with Galvanic Sources', *Geophysics* **69**, 1192–1202.

Davydycheva, S., Druskin, V., and Habashy, T.: 2003. 'An Efficient Finite Difference Scheme for Electromagnetic Logging in 3D Anisotropic Inhomogeneous Media', *Geophysics* **68**, 1525–1536.

Dawson, T. W., and Weaver, J. T.: 1979. 'Three-Dimensional Electromagnetic Induction in a Non-Uniform Thin Sheet at the Surface of Uniformly Conducting Earth', *Geophys. J. Roy. Astr. Soc.* **59**, 445–462.

Dennis, J. E., and Schnabel, R. B.: 1996, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, SIAM, Philadelphia.

Dey, A., and Morrison, H. F.: 1979. 'Resistivity Modelling for Arbitrary Shaped Three-Dimensional Structures', *Geophysics* **44**, 753–780.

Dmitriev, V. I.: 1969, *Electromagnetic Fields in Inhomogeneous Media*, Moscow State University, Moscow (in Russian).

Dmitriev, V. I., and Nesmeyanova, N. I.: 1992. 'Integral Equation Method in Three-Dimensional Problems of Low-Frequency Electrodynamics', *Comput. Math. Model.* **3**, 313–317.

Dorn, O., Bertete-Aguirre, H., Berryman, J. G., and Papanicolaou, G. C.: 1999. 'A Nonlinear Inversion Method for 3D Electromagnetic Imaging Using Adjoint Fields', *Inv. Prob.* **15**, 1523–1558.

Druskin, V., and Knizhnerman, L.: 1994. 'Spectral Approach to Solving Three-Dimensional Maxwell's Equations in the Time and Frequency Domains', *Radio Sci.* **29**, 937–953.

Druskin, V., Knizhnerman, L., and Lee, P.: 1999. 'A New Spectral Lanczos Decomposition Method for Induction Modeling in Arbitrary 3D Geometry', *Geophysics* **64**, 701–706.

Eaton, P. A.: 1989. '3D Electromagnetic Inversion Using Integral Equations', *Geophys. Prosp.* **37**, 407–426.

Ellis, R. G.: 1999, 'Joint 3-D Electromagnetic Inversion', in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 179–192.

Ellis, R. G.: 2002, Electromagnetic Inversion Using the QMR-FFT Fast Integral Equation Method, in *72st Ann. Internat. Mtg., Soc. Expl. Geophys.*, pp. 21–25.

Everett, M., and Schultz, A.: 1996. 'Geomagnetic Induction in a Heterogeneous Sphere, Azimuthally Symmetric Test Computations and the Response of an Undulating 660-km Discontinuity', *J. Geophys. Res.* **101**, 2765–2783.

Jones, F. W., and Pascoe, L. J.: 1972. 'The Perturbation of Alternating Geomagnetic Fields by Three-Dimensional Conductivity Inhomogeneities', *Geophys. J. Roy. Astr. Soc.* **27**, 479–484.

Judin, M. N.: 1980, *Magnetotelluric Field Calculation in Three-Dimensional Media Using a Grid Method, in Problems of the Sea Electromagnetic Investigations*, IZMIRAN, Moscow 96–101(in Russian).

Faber, V., and Manteuffel, T.: 1984. 'Necessary and Sufficient Conditions for the Existence of a Conjugate Gradient Method', *SIAM J. Numer. Anal.* **24**, 352–362.

Farquharson, C. G., and Oldenburg, D. W.: 1996. 'Approximate Sensitivities for the Electromagnetic Inverse Problem', *Geophys. J. Int.* **126**, 235–252.

Farquharson, C. G., and Oldenburg, D. W.: 1998. 'Non-Linear Inversion Using General Measures of Data Misfit and Model Structure', *Geophys. J. Int.* **134**, 213–233.

Farquharson, C. G., Oldenburg, D. W., Haber, E., and Shekhtman, R.: 2002, 'An Algotithm for The Three-Dimensional Inversion of Magnetotelluric Data,' in *72st Ann. Internat. Mtg., Soc. Expl. Geophys.*, pp.649–652.

Farquharson, C. G., and Oldenburg, D. W.: 2004. 'A Comparison of Automatic Techniques for Estimating the Regularization Parameter in Non-Linear Inverse Problems', *Geophys. J. Int.* **156**, 411–425.

Fletcher, R., and Reeves, C. M.: 1964. 'Function Minimization by Conjugate Gradients', *Comput. J.* **7**, 149–154.

Fomenko, E. Y., and Mogi, T.: 2002. 'A New Computation Method for a Staggered Grid of 3D EM Field Conservative Modeling', *Earth Planets Space* **54**, 499–509.

Golub, G. H., and Van Loan, C. F.: 1996, *Matrix Computations*, (Third ed.). The Johns Hopkins University Press, Baltimore and London.

Grammatica, N., and Tarits, P.: 2002. 'Contribution at Satellite Altitude of Electromagnetically Induced Anomalies Arising from a Three-Dimensional Heterogeneously Conducting Earth, using Sq as an Inducing Source Field', *Geophys. J. Int.* **151**, 913–923.

Greenbaum, A.: 1997, *Iterative Methods for Solving Linear Systems*, SIAM, Philadelphia.

Habashy, T. M., Groom, R. W., and Spies, B. R.: 1993. 'Beyond the Born and Rytov Approximations: A Nonlinear Approach to Electromagnetic Scattering', *J. Geophys. Res.* **98**, 1759–1775.

Haber, E.: 1999, 'Modeling 3D EM Using Potentials and Mixed Finite Elements,' in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 12–15.

Haber, E., Ascher, U. M., Aruliah, D. A., and Oldenburg, D. W.: 2000a. 'Fast Simulation of 3D Electromagnetic Problems Using Potentials', *J. Comp. Phys.* **163**, 150–171.

Haber, E., Ascher, U. M., Aruliah, D. A., and Oldenburg, D. W.: 2000b. 'On Optimisation Techniques for Solving Nonlinear Inverse Problems', *Inv. Prob.* **16**, 1263–1280.

Haber, E., Ascher, U. M., Oldenburg, D. W., Shekhtman R. and Chen J.: 2002a, '3-D Frequency Domain CSEM Inversion Using Unconstrained Optimization,' in *72st Ann. Internat. Mtg., Soc. Expl. Geophys.*, pp.653–656.

Haber, E., Ascher, U. M., and Oldenburg, D. W.: 2004. 'Inversion of 3D Electromagnetic Data in Frequency and Time Domain Using an Inexact All-at-Once Approach', *Geophysics* **69**, 1216–1228.

Haber, E.: 2005. 'Quasi–Newton Methods for Large-Scale Electromagnetic Inverse Problems', *Inv. Prob.* **21**, 305–323.

Hamano, Y.: 2002. 'A New Time-Domain Approach for the Electromagnetic Induction Problem in a Three-Dimensional Heterogeneous Earth', *Geophys. J. Int.* **150**, 753–169.

Hestenes, M. R., and Stiefel, E.: 1952. 'Methods of Conjugate Gradients for Solving Linear Systems', *J. Res. Nat. Bur. Stand.* **49**, 409–436.

Hohmann, G. W.: 1975. 'Three-Dimensional Induced-Polarization and Electromagnetic Modeling', *Geophysics* **40**, 309–324.

Hohmann G. W.: 1988, 'Numerical Modelling of Electromagnetic Methods of Geophysics', in M. N. Nabighian (ed.), *Electromagnetic methods in applied geophysics*, Vol. 1, S.E.G. Investigations in geophysics 3, pp. 314–364.

Hursan, G., and Zhdanov, M. S.: 2002. 'Contraction Integral Equation Method in Three-Dimensional Modeling', *Radio Sci.* **37**, 1089doi, 10.1029/2001RS002513.

Kaufman, A. A., and Eaton, P. A.: 2001, *The Theory of Inductive Prospectings*, Methods in Geochemistry and Geophysics 35, Elsevier, Amsterdam–NewYork–Tokyo.

Kelly, C. T.: 1999, *Iterative Methods for Optimization*, SIAM, Philadelphia.

Koyama, T., Shimizu, H., and Utada, H.: 2002. 'Possible Effects of Lateral Heterogeneity in the D' Layer on Electromagnetic Variations of Core Origin', *Phys. Earth Planet. Interiors* **129**, 99–116.

Kuvshinov, A. V., Avdeev, D. B., Pankratov, O. V., Golyshev, S. A., and Olsen, N.: 2002, 'Modelling Electromagnetic Fields in 3-D Spherical Earth Using Fast Integral Equation Approach', in M. S. Zhdanov and P. E. Wannamaker (eds.), *Three Dimensional Electromagnetics*, Methods in Geochemistry and Geophysics 35: Elsevier, pp. 43–54.

Kuvshinov, A. V., Utada, H., Avdeev, D. B., and Koyama, T.: 2005. '3-D Modelling and Analysis of Dst C-Responses in the North Pacific Ocean Region, Revisited', *Geophys. J. Int.* **160**, 505–526.

Kuvshinov, A. V., and Olsen, N..: 2004. 'Modelling the Coast Effect of Geomagnetic Storms at Ground and Satellite Altitude', in C.. Reigber, H.. Luhr, P.. Schwintzer, and J.. Wickert (eds.), *Earth Observation with CHAMP. Results from Three Years in Orbit*, Springer-Verlag, Berlin, pp. 353–359.

LaBrecque, D.: 1999, 'Finite Difference Modeling of 3-D EM Fields with Scalar and Vector Potentials', in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 148–160.

Lager, I. E., and Mur, G.: 1998. 'Generalized Cartesian finite elements', *IEEE Trans. Magn.* **34**, 2220–2227.

Lanczos, C.: 1952. 'Solution of Systems of Linear Equations by Minimized Iterations', *J. Res. Nat. Bur. Stand.* **49**, 33–53.

Lesselier, D. and Habashy, T. (eds.) 2000, 'Special Section on Electromagnetic Imaging and Inversion of the Earth's subsurface', *Inv. Prob.* **16**(5) 1083–1376.

Lesselier, D. and Chew, W. C. (eds.): 2004, 'Special Section on Electromagnetic Characterization of Buried Obstacles', *Inv. Prob.* **20**(6), S1–S256.

Li, Y., and Oldenburg, D. W.: 2000. '3-D Inversion of Induced Polarization Data', *Geophysics* **65**, 1931–1945.

Li, Y., and Spitzer, K.: 2002. 'Three-Dimensional DC Resistivity Forward Modeling Using Finite Elements in Comparison With Finite-Difference Solutions', *Geophys. J. Int.* **151**, 924–934.

Livelybrooks, D.: 1993. 'Program 3Dfeem, A Multidimensional Electromagnetic Finite Element Model', *Geophys. J. Int.* **114**, 443–458.

Mackie, R. L., and Madden, T. R.: 1993. 'Three-Dimensional Magnetotelluric Inversion Using Conjugate Gradients', *Geophys. J. Int.* **115**, 215–229.

Mackie, R. L., Madden, T. R., and Wannamaker, P.: 1993. '3-D Magnetotelluric Modeling Using Difference Equations – Theory and Comparisons to Integral Equation Solutions', *Geophysics* **58**, 215–226.

Mackie, R. L., Smith, T. J., and Madden, T. R.: 1994. '3-D Electromagnetic Modeling Using Difference Equations, The Magnetotelluric Example', *Radio Sci.* **29**, 923–935.

Mackie, R.L., Rodi, W., and Watts, M.D.: 2001, '3-D Magnetotelluric Inversion for Resource Exploration, in *71st Ann. Internat. Mtg., Soc. Expl. Geophys.*, pp. 1501–1504.

Mackie, R.L.: 2004, Private communication.

Macnae, J. and Liu, G. (eds.): 2003, *Three Dimensional Electromagnetics III*, Austr. Soc. Expl. Geophys.

Madden, T. R., and Mackie, R. L.: 1989. 'Three-Dimensional Magnetotelluric Modeling and Inversion', *Proc. IEEE* **77**, 318–333.

Martinec, Z.: 1999. 'Spectral-Finite Element Approach to Three-Dimensional Electromagnetic Induction in a Spherical Earth', *Geophys. J. Int.* **136**, 229–250.

McGillivray, P. R., and Oldenburg, D. W.: 1990. 'Methods for Calculating Frechet Derivatives and Sensitivities for the Non-Linear Inverse Problems', *Geophysics* **60**, 899–911.

McKirdy, D. McA., Weaver, J. T., and Dawson, T. W.: 1985. 'Induction in a Thin Sheet of Variable Conductance at the Surface of a Stratified Earth- II. Three-dimensional theory', *Geophys. Roy. Astr. Soc.* **80**, 177–194.

Mitsuhata, Y., Uchida, T., and Amano, H.: 2002. '2.5-D Inversion of Frequency-Domain Electromagnetic Data Generated by a Grounded-Wire Source', *Geophysics* **67**, 1753–1768.

Mitsuhata, Y., and Uchida, T.: 2004. '3D Magnetotelluric Modeling Using the T-Ω Document Finite-Element Method', *Geophysics* **69**, 108–119.

Newman, G. A., and Hohmann, G. W.: 1988. 'Transient Electromagnetic Response of High-Contrast Prisms in a Layered Earth', *Geophysics* **53**, 691–706.

Newman, G. A., and Alumbaugh, D. L.: 1995. 'Frequency-Domain Modeling of Airborne Electromagnetic Responses Using Staggered Finite Differences', *Geophys. Prosp.* **43**, 1021–1042.

Newman, G. A., and Alumbaugh, D. L.: 1997. 'Three-Dimensional Massively Parallel Electromagnetic Inversion- I.', Theory*, Geophys. J. Int.* **128**, 345–354.

Newman, G. A., and Alumbaugh, D. L.: 2000. 'Three-Dimensional Magnetotelluric Inversion Using Non-Linear Conjugate Gradients', *Geophys. J. Int.* **140**, 410–424.

Newman, G. A., and Hoversten, G. M.: 2000. 'Solution Strategies for 2D and 3D EM Inverse Problem', *Inv. Prob.* **16**, 1357–1375.

Newman, G. A., Hoversten, G. M., and Alumbaugh, D. L.: 2002, '3D Magnetotelluric Modeling and Inversion, Applications to Sub-Salt Imaging', in M.S. Zhdanov and P.E. Wannamaker (eds.), *Three Dimensional Electromagnetics*, Methods in Geochemistry and Geophysics 35, Elsevier, pp. 127–152.

Newman, G. A., and Alumbaugh, D. L.: 2002. 'Three-Dimensional Induction Logging Problems. Part I. An Integral Equation Solution and Model Comparisons', *Geophysics* **67**, 484–491.

Newman, G. A., Recher, S., Tezkan, B., and Neubauer, F. M.: 2003. '3D Inversion of a Scalar Radio Magnetotelluric Field Data Set', *Geophysics* **68**, 791–802.

Newman, G. A., and Boggs, P. T.: 2004. 'Solution Accelerators for Large-Scale Three-Dimensional Electromagnetic Inverse Problem', *Inv. Prob.* **20**, s151–s170.

Newman, G. A., and Commer, M.: 2005. 'New Advances in Three-Dimensional Transient Electromagnetic Inversion', *Geophys. J. Int.* **160**, 5–32.

Nocedal, J., and Wright, S.: 1999, *Numerical Optimization*, Springer-Verlag, New York.

O'Leary, D. P.: 1996, 'Conjugate Gradients and Related KMP Algorithms, the Beginnings', in L. Adams and J.L. Nazareth (eds.), *Linear and Nonlinear Conjugate Gradient-Related Methods*, SIAM, pp. 1–9.

Oristaglio, M. J. and Spies, B.R.: 1999, 'Three Dimensional Electromagnetics', in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7.

Paige, C. C., and Sounders, M. A.: 1974. 'Solution of Sparse Indefinite Systems of Linear Equations', *SIAM J. Numer. Anal.* **11**, 197–209.

Pankratov, O. V., Avdeev, D. B., and Kuvshinov, A. V.: 1995. 'Electromagnetic Field Scattering in a Heterogeneous Earth, A Solution to the Forward Problem', *Phys. Solid Earth* **31**, 201–209.

Pankratov, O. V., Kuvshinov, A. V., and Avdeev, D. B.: 1997. 'High-Performance Three-Dimensional Electromagnetic Modeling Using Modified Neumann series. Anisotropic case', *J. Geomagn. Geoelectr.* **49**, 1541–1547.

Paulsen, K. D., Linch, D. R., and Strohbehn, J. W.: 1988. 'Three-dimensional finite, boundary, and hybrid element solutions of the Maxwell equations for lossy dielectric media', *IEEE Trans. Microwave Theory Tech.* **36**, 682–693.

Polak, E., and Ribiere, G.: 1969. 'Note sur la convergence de methode de directions conjuguees', *Revue Francaise d'Informatique et de Recherche Operationnelle* **16**, 35–43.

Portniaguine, O., and Zhdanov, M. S.: 1999. 'Focusing Geophysical Inversion Images', *Geophysics* **64**, 874–887.

Pridmore, D. F., Hohmann, G. W., Ward, S. H., and Still, W. R.: 1981. 'An Investigation of Finite-Element Modeling For Electrical and Electromagnetic Data in Three Dimensions', *Geophysics* **46**, 1009–1024.

Raiche, A.: 1974. 'An Integral Equation Approach to Three-Dimensional Modeling', *Geophys. J.* **36**, 363–376.

Ratz, S.: 1999, 'A 3D Finite Element Code for Modeling of Electromagnetic Responses, in *Expanded abstracts of the 2nd International Symposium on 3D Electromagnetics*, Salt Lake City, Utah, pp.33–36.

Reddy, I. K., Rankin, D., and Phillips, R. J.: 1977. 'Three-dimensional modelling in magnetotelluric and magnetic variational sounding', *Geophys. J. Roy. Astr. Soc.* **51**, 313–325.

Rodi, W., and Mackie, R. L.: 2000. 'Nonlinear conjugate gradients algorithm for 2-D magnetotelluric inversion', *Geophysics* **66**, 174–187.

Romanov, V. G, and Kabanikhin, S. I.: 1994, *Inverse Problems for Maxwell's Equations*, VSP, Utrecht.

Saad, Y., and Schultz, M. H.: 1986. 'GMRES, A Generalized Minimal Residual Algorithm for Nonsymmetric Linear Systems', *SIAM J. Sci. Stat. Comput.* **7**, 856–869.

Sasaki, Y.: 2001. 'Full 3-D Inversion of Electromagnetic Data on PC', *J. Appl. Geophys.* **46**, 45–54.

Sasaki, Y.: 2004. 'Three-Dimensional Inversion of Static-Shifted Magnetotelluric Data', *Earth Planets Space* **56**, 239–248.

Schultz, A. and Pritchard, G.: 1999, Three-Dimensional Inversion for Large-Scale Structure in a Spherical Domain', in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 451–476.

Singer, B. Sh., and Fainberg, E. B.: 1985, *Electromagnetic Induction in Non-uniform Thin Layers*, IZMIRAN, Moscow (in Russian).

Singer, B. Sh.: 1995. 'Method for Solution of Maxwell's Equations in Non-Uniform Media', *Geophys. J. Int.* **120**, 590–598.

Singer, B. Sh., and Fainberg, E. B.: 1995. 'Generalization of the Iterative-Dissipative Method for Modeling Electromagnetic Fields in Nonuniform Media with Displacement Currents', *J. Appl. Geophys.* **34**, 41–46.

Singer, Sh. B., and Fainberg, E. B.: 1997. 'Fast and Stable Method for 3-D Modelling of Electromagnetic Field', *Explor. Geophys.* **28**, 130–135.

Singer, B. Sh., Mezzatesta, A., and Wang, T.: 2003, Integral equation approach based on contraction operators and Krylov subspace optimisation, in J. Macnae and G. Liu (eds.), *Three Dimensional Electromagnetics III*, Austr. Soc. Expl. Geophys.

Siripunvaraporn, W., Uyeshima, M., and Egbert, G.: 2004a. 'Three-Dimensional Inversion for Network-Magnetotelluric Data', *Earth Planets Space* **56**, 893–902.

Siripunvaraporn, W., Egbert, G., Lenbury, Y., and Uyeshima, M.: 2004b. 'Three-Dimensional Magnetotelluric Inversion: Data Space Method', *Phys. Earth Planet. Inter.* **150**, 3–14.

Smith, J. T., and Booker, J. R.: 1991. 'Rapid Inversion of Two- and Three-Dimensional Magnetotelluric Data', *J. Geophys. Res.* **96**(B3), 3905–3922.

Smith, J. T.: 1996a. 'Conservative Modeling of 3-D Electromagnetic Fields, Part I, Properties and Error Analysis', *Geophysics* **61**, 1308–1318.

Smith, J. T.: 1996b. 'Conservative Modeling of 3-D Electromagnetic Fields, Part II, Biconjugate Gradient Solution and an Accelertor', *Geophysics* **61**, 1319–1324.

Song, L.-P., and Liu, Q. H.: 2004. 'Fast Three-Dimensional Electromagnetic Nonlinear Inversion in Layered Media with a Novel Scattering Approximation', *Inv. Prob.* **20**, S171–S194.

Spichak, V. V.: 1983, *Numerically modeling the electromagnetic fields in three-dimensional media*, Ph. D. thesis, Moscow, 215 p. (in Russian).

Spichak, V., and Popova, I.: 2000. 'Artificial Neural Network Inversion of Magnetotelluric Data in Terms of Three-Dimensional Earth Macroparameters', *Geophys. J. Int.* **142**, 15–26.

Sugeng, F., Raiche, A. and Xiong, Z.: 1999, 'An Edge-Element Approach to Model the 3D EM Response of Complex Structures with High Contrasts', in *Expanded abstracts of the 2nd International Symposium on 3D Electromagnetics*, Salt Lake City, Utah, pp. 25–28.

Tabarovsky, L. A.: 1975, *Application of Integral Equation Method to Geoelectrical Problems*, Novosibirsk, Nauka (in Russian).

Tamarchenko, T., Frenkel, M., and Mezzatesta, A.: 1999, Three-dimensional modeling of microresistivity devices, in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 77–83.

Tarantola, A.: 1987, *Inverse Problem Theory*, Elsevier, Amsterdam–Oxford–New York–Tokyo.

Tarits, P.: 1994. 'Electromagnetic Studies of Global Geodynamic Processes', *Surv. Geophys.* **15**, 209–238.

Tikhonov, A. N., and Arsenin, V. Y.: 1977, *Solutions of Ill-posed Problems*, Wiley, New York..

Ting, S. C., and Hohmann, G. W.: 1981. 'Integral Equation Modeling of Three-Dimensional Magnetotelluric Response', *Geophysics* **46**, 182–197.

Torres-Verdin, C., and Habashy, T. M.: 1994. 'Rapid 2.5-D Forward Modeling and Inversion Via a New Nonlinear Scattering Approximation', *Radio Sci.* **29**, 1051–1079.

Torres-Verdin, C., and Habashy, T. M.: 2002. 'Rapid Numerical Simulations of Axisymmetric Single-well Induction Data Using the Extended Born Approximation', *Radio Sci.* **36**, 1287–1306.

Tseng, H. -W., Lee, K. H., and Becker, A.: 2003. '3-D Interpretation of Electromagnetic Data Using a Modified Extended Born Approximation', *Geophysics* **68**, 127–137.

Uyeshima, M., and Schultz, A.: 2000. 'Geoelectromagnetic Induction in a Heterogeneous Sphere, A New 3-D Forward Solver Using a Staggered-Grid Integral Formulation', *Geophys. J. Int.* **140**, 636–650.

Uchida, T. and Sasaki, Y.: 2003, Stable 3-D Inversion of MT Data and Its Application for Geothermal Exploration, in J. Macnae and G. Liu (eds.), *Three Dimensional Electromagnetics III*, Austr. Soc. Expl. Geophys.

Varentsov, Iv. M.: 1999, 'The Selection of Effective Finite Difference Solvers in 3D Electromagnetic Modeling', in *Expanded Abstracts of 2nd International Symposium on 3D Electromagnetics*, Salt Lake City, Utah.

Varentsov, Iv. M.: 2002, 'A General Approach to the Magnetotelluric Data Inversion in a Piece-Continuous Medium' *Fizika Zemli* 11 (in Russian).

Vasseur, G., and Weidelt, P.: 1977. 'Bimodal Electromagnetic Induction in Non-Uniform Thin Sheets with Application to the Northern Pyrenean Induction Anomaly', *Geophys. J. R. Astr. Soc.* **51**, 669–690.

Velimsky, J., Everett, M. E., and Martinec, Z.: 2003, 'The Transient Dst Electromagnetic Induction Signal at Satellite Altitudes for a Realistic 3-D Electrical Conductivity in the Crust and Mantle, *Geophys. Res. Letts.* **30**(7), doi,10.1029/2002GL016671.

Wang, T., and Hohmann, G. W.: 1993. 'A Finite-Difference Time-Domain Solution for Three-Dimensional Electromagnetic Modeling', *Geophysics* **58**, 797–809.

Wang, T., Oristaglio, M., Tripp, A., and Hohmann, G. W.: 1994. 'Inversion of Diffusive Transient Electromagnetic Data by a Conjugate Gradient Method', *Radio Sci.* **29**, 1143–1156.

Wang, T., and Tripp, A.: 1996. 'FDTD Simulation of EM Wave Propagation in 3-D Media', *Geophysics* **61**, 110–120.

Wang, T., and Fang, S.: 2001. '3D Electromagnetic Anisotropy Modeling Using Finite Differences', *Geophysics* **66**, 1386–1398.

Wannamaker, P. E., Hohmann, G. W., and San Filipo, W. A.: 1984. 'Electromagnetic Modeling of Three-Dimensional Bodies in Layered Earth Using Integral Equations', *Geophysics* **49**, 60–74.

Wannamaker, P. E.: 1991. 'Advances in Three-Dimensional Magnetotelluric Modeling Using Integral Equations', *Geophysics* **56**, 1716–1728.

Weaver, J. T.: 1994, *Mathematical Methods for Geo-electromagnetic Induction*, John Wiley and Sons, Taunton, UK.

Weaver, J. T., Agarwal, A. K. and Pu, X. H.: 1999, 'Three-Dimensional Finite-Difference Modeling of the Magnetic Field in Geo-Electromagnetic Induction', in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 426–443.

Weidelt, P.: 1975. 'Electromagnetic Induction in 3D Structures', *J. Geophys.* **41**, 85–109.

Weidelt, P.: 1999, 3D conductivity models, Implications of electrical anisotropy, in M. J. Oristaglio and B. R. Spies (eds.), *Three Dimensional Electromagnetics*, S.E.G. Geophysical Developments Series 7, pp. 119–137.

Weiss, Ch. J., and Everett, M. E.: 1998. 'Geomagnetic Induction in a Heterogeneous Sphere, Fully Three-Dimensional Test Computation and the Response of a Realistic Distribution of Oceans and Continents', *Geophys. J. Int.* **135**, 650–662.

Weiss, Ch. J., and Newman, G. A.: 2002. 'Electromagnetic Induction in a Fully 3-D Anisotropic Earth', *Geophysics* **67**, 1104–1114.

Weiss, Ch. J., and Newman, G. A.: 2003. 'Electromagnetic Induction in a Fully 3-D Anisotropic Earth, Part 2, The LIN Preconditioner', *Geophysics* **68**, 922–930.

Xiong, Z.: 1992. 'EM Modeling Three-Dimensional Structures by the Method of System Iteration Using Integral Equations', *Geophysics* **57**, 1556–1561.

Xiong, Z., and Tripp, A. C.: 1995. 'Electromagnetic Scattering of Large Structures in Layered Earth Using Integral Equations', *Radio Sci.* **30**, 921–929.

Xiong, Z., Raiche, A., and Sugeng, F.: 2000. 'Efficient Solution of Full Domain 3D Electromagnetic Modeling Problems', *Explor. Geophys.* **31**, 158–161.

Yamane, K., Kim, H. J., and Ashida, Y.: 2000. 'Three-Dimensional Magnetotelluric Inversion Using a Generalized RRI Method and Its Applications', *Butsuri-Tansa (Geophys. Explor.)* **53**, 1501–1513.

Yee, K. S.: 1966. 'Numerical Solution of Initial Boundary Value Problems Involving Maxwell's Equations in Isotropic Media', *IEEE Trans. Ant. Prop.* **AP-14**, 302–307.

Yoshimura, R. and Oshiman, N.: 2002, Edge-based Finite Element Approach to the Simulation of Geoelectromagnetic Induction in a 3-D sphere, *Geophys. Res. Letts.* **29**(3), doi,10.1029/2001GL014121.

Zhang, Z.: 2003. '3D Resistivity Mapping of Airborne EM Data', *Geophysics* **68**, 1896–1905.

Zhdanov, M. S., and Fang, S.: 1996. 'Quasi-Linear Approximation in 3-D EM Modeling', *Geophysics* **61**, 646–665.

Zhdanov, M. S., and Fang, S.: 1997. 'Quasi-Linear Series in Three-Dimensional Electromagnetic Modeling', *Radio Sci.* **32**, 2167–2188.

Zhdanov, M. S., and Portniaguine, O.: 1997. 'Time-Domain Electromagnetic Migration in the Solution of Inverse Problems', *Geophys. J. Int.* **131**, 293–309.

Zhdanov, M. S., Varentsov, I. M., Weaver, J. T., Golubev, N. G., and Krylov, V. A.: 1997, 'Methods for Modelling Electromagnetic Fields; Results from COMMEMI – the International Project On the Comparison of Modelling Methods for Electromagnetic Induction', in J. T. Weaver (ed.), *J. Appl. Geophys.* **37**, 133–271.

Zhdanov, M. S., Fang, S., and Hursan, G.: 2000. 'Electromagnetic Inversion using Quasi-Linear Approximation', *Geophysics* **65**, 1501–1513.

Zhdanov, M. S.: 2002, *Geophysical Inverse Theory and Regularization problems*, Elsevier, Amsterdam-New York-Tokyo.

Zhdanov, M. S. and Wannamaker, P. E.: 2002, 'Three Dimensional Electromagnetics', in M. S. Zhdanov and P. E. Wannamaker (eds.), *Three Dimensional Electromagnetics*, Methods in Geochemistry and Geophysics 35, Elsevier.

Zhdanov, M. S. and Golubev, N. G.: 2003, 'Three-Dimensional Inversion of Magnetotelluric Data in Complex Geological Structures', in J. Macnae and G. Liu (eds.), *Three Dimensional Electromagnetics III*, Austr. Soc. Expl. Geophys.

Zhdanov, M. S., and Tolstaya, E.: 2004. 'Minimum Support Nonlinear Parametrization in the Solution of a 3D Magnetotelluric Inverse Problem', *Inv. Prob.* **20**, 937–952.

Zunoubi, M. R., Jin, J. -M., Donepudi, K. C., and Chew, W. C.: 1999. 'A Spectral Lanczos Decomposition Method for Solving 3-D Low-Frequency Electromagnetic Diffusion by the Finite-Element Method', *IEEE Trans. Antennas Propogat.* **47**, 242–248.

Zyserman, F. I., and Santos, J. E.: 2000. 'Parallel Finite Element Algorithm with Domain Decomposition for Three-Dimensional Magnetotelluric Modeling', *J. Appl. Geophys.* **44**, 337–351.