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Areas for exploration in electromagnetic modelling and inversion

Adrianus T de Hoop

Delft University of Technology, Laboratory of Electromagnetic Research, Faculty of Information Technology and Systems, Mekelweg 4, 2628 CD Delft, the Netherlands

E-mail: a.t.dehoop@its.tudelft.nl

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Abstract. In this contribution some ‘*areas for exploration in electromagnetic modelling and inversion*’ are discussed, the focus being on applications in the evaluation and monitoring of subsurface fossil energy reservoirs in the Earth. Three topics receive attention: (1) the modelling of electromagnetic wavefields in strongly heterogeneous media (such as rock), for which the domain-integrated field equations method is presented as a tool, (2) the feasibility of carrying out inversion in the time Laplace-transformed domain at a set of real, positive, values of the transform parameter to which Lerch’s uniqueness theorem of the one-sided, causal Laplace transformation applies, and (3) a general operator formalism that is based on the iterative decrease in the norm of the mismatch in data equation and object equation as they occur in the contrast source formulation of the inversion problem.

1. Introduction

In this contribution three topics receive attention: (1) the computational modelling of electromagnetic wavefields in strongly heterogeneous media (such as subsurface rock in the Earth), (2) an investigation into the properties of the one-sided, causal time Laplace transformation at a set of real, positive, values of the transform parameter to which Lerch’s uniqueness theorem applies, with a view to using this transformation in electromagnetic forward modelling as well as in imaging and inversion, and (3) a short discussion, from a certain perspective (putting the *improvement condition* at the central position), of the solution procedure applying to a linear operator equation that is based on the iterative decrease in the norm of the mismatch in the equation, with a view to its application to the data equation and the object equation as they occur in the contrast source formulation of the electromagnetic inversion problem. These issues can be considered as ‘*areas for exploration in electromagnetic modelling, imaging and inversion*’ and are considered to be of importance to the evaluation and monitoring of fossil energy reservoirs in the subsurface of the Earth.

The *modelling problem* addresses the case where *electromagnetic fields* are to be evaluated in *strongly heterogeneous media* (such as subsurface rock in the Earth), i.e. media where a discontinuous constitutive behaviour persists up to the mesh size of the spatial discretization, a scale that we refer to as the *mesoscopic scale*. The concept of mesoscopic scale applies to both the physical resolving power of the sensing field involved as well as to the geometrical discretization employed in a computational algorithm. Standard computational techniques for evaluating electromagnetic fields in configurations with a degree of complexity that puts

them outside the realm of analytical methods involve the finite-element and finite-difference techniques. Both techniques are based on a description of the field behaviour in terms of partial differential equations and, hence, can only be expected to yield approximations of a controlled accuracy in subdomains of the configuration where the field quantities are continuously differentiable. The latter property holds whenever the constitutive material parameters vary continuously in space. As soon as discontinuities in material properties occur, additional computational measures have to be taken to circumvent a deterioration of the accuracy of the results in the neighbourhood of interfaces. In particular, field values exactly at interfaces (or their limiting values upon approaching either side of an interface) are often inaccurate. Especially for those applications where the latter are to be accurately modelled (such as, for example, in the geophysical interpretation of measurements carried out at a borehole wall in a fossil energy reservoir), this is a serious inadequacy. An observation of this nature applies the more so whenever fields are to be evaluated in strongly heterogeneous media where a discontinuous constitutive behaviour persists up to the mesh size of the spatial discretization (the mesoscopic scale). Under these circumstances, the standard methods fail to yield a result of uniform accuracy and other methods, not based on the property of differentiability, but still describing the physics of the problem, have to be called upon. The *domain-integrated field equations method* provides such an alternative.

Here, the domain-integrated forms of the standard partial differential equations (Maxwell's equations and compatibility relations, in our case) are taken as points of departure and, through an application of Gauss' integral theorem, the spatial differentiations are eliminated, replacing the relevant domain integral terms by surface integrals. Due to the structure of the basic equations of the field's physics, in the latter only components of the field quantities occur that are continuous upon crossing a jump discontinuity in material properties. As a consequence, these field components have a unique, bounded value. For the case of electromagnetic fields, these are: the tangential components of the electric field strength \mathbf{E} and the magnetic field strength \mathbf{H} and the normal components of the electric flux density \mathbf{D} and the magnetic flux density \mathbf{B} . Along an interface and in between interfaces intersecting the one under consideration, the field quantities still vary continuously with position and can, hence, be approximated on a polynomial basis. Using expansions of this type, the domain-integrated field equations are now, to their full extent, enforced. Out of this procedure a first system of algebraic equations in the relevant expansion coefficients results.

The next point is the incorporation of the constitutive behaviour. Due to the persistence of heterogeneity on the mesoscopic scale, it makes no sense to attribute a local value to any of the constitutive coefficients (or local constitutive convolution operators in the case of lossy media) at any interior point of an element of the geometrical discretization. Here, we adopt the procedure that an 'averaged' or 'effective' constitutive coefficient (or constitutive operator) is incorporated in the field evaluation by minimizing the discrepancy that corresponds to integrating the norm of the mismatch in the constitutive relations, the latter containing the analytical continuations of the field values into the interior of each geometrical element away from their expanded values on the boundary of it. In this way, a second system of algebraic equations in the chosen expansion coefficients results.

The total system of equations is overdetermined and has, hence, no solution. This, we stipulate, is indicative for the fact that we are truly modelling the physics of the problem: any finite-degree polynomial expansion is incapable of exactly representing the field quantities (even in a homogeneous domain). Subsequently solving our total system of equations via a minimum-norm procedure yields the best possible solution under the given circumstances (i.e. given the chosen mismatch criteria and the discretization employed).

Algebraic topology learns us that consistently linear *edge expansions* for \mathbf{E} and \mathbf{H} and

consistently linear *face expansions* for D and B do the job. With them, a further intrinsic advantage of the method is that very high contrasts in material properties are automatically dealt with, without any loss of accuracy and with a coarse geometrical discretization.

As far as the *time behaviour* of the wavefields under consideration is concerned, two approaches are standardly approached. One takes the coupled first-order system of hyperbolic spacetime partial differential equations (in our case: Maxwell's equations) as point of departure. Based on this system, finite-difference time-domain algorithms are developed to perform the computations. The other starts from the corresponding spatial differential equations from which the time coordinate has been eliminated by considering a harmonically in time-varying field constituent with fixed angular frequency. To recover the time behaviour, if needed, the computations are carried out for a number of different angular frequencies, the results pertaining to which are subsequently combined in, for example, a fast Fourier transform algorithm. A procedure of this kind has the computational advantage of decomposing the total spacetime problem into a succession of spatial problems of less computational complexity that are recombined at a later stage. In addition, some physical properties of the fields in the configuration, such as resonance behaviour in the constitutive material properties, may show up more clearly in the frequency domain than in the relevant pulse shapes in the time domain.

A disadvantage in the frequency-domain procedures is, however, that the property of *causality* in the time response of the system, a property that is at the heart of the physics as well as the mathematics of the problem, is lost. Now, from the theory of the one-sided Laplace transformation of a causal time function it is known that for such functions the relation between the relevant time function and its Laplace transform taken at a sequence of equidistant, real, positive values of the transform parameter, is unique (Lerch's theorem (Widder 1946)). This property can be considered as to be representative for the property of causality. As a consequence, it is conjectured that all computational advantages of the frequency-domain analysis can be carried over to the Laplace-transform domain at the (discrete) sequence of values that occurs in Lerch's theorem, provided that a transformation back to the time domain is feasible. For the latter, a certain algorithm is proposed. In fact, since in a procedure of this kind only real-valued functions occur, one saves by a factor of four in computation time in any multiplication, as compared with the standard frequency-domain analysis in which complex-valued functions occur.

As far as *inversion procedures* are concerned, a conceptual point of view is developed where three elements are distinguished, namely (a) the *contrast source formulation* of the scattering problem (i.e. the decomposition of the total wavefield into a known incident wavefield propagating in a known, or assumed, background medium and a scattered wavefield originating from the contrast sources in this background medium, the contrast sources having a chosen *target region* as their support), (b) the *data equation* that relates the observed wavefield values to the contrast source distributions, and (c) the *object equation* that interrelates the total wavefield in the target region and the contrast source distribution to the distribution of constitutive parameters to be reconstructed. When lined up in a particular order, the relations take the form of *linear operator equations*. To solve the latter, an iterative scheme is discussed in which the *improvement condition* is taken to play a central role. This condition enforces, at each step of the iterative procedure, a decrease in the norm of the mismatch in the relevant equation. The procedure can be considered as a *steepest descent method* and is proved to be convergent.

In section 2 the domain-integrated field equations method for time-domain electromagnetic wavefields is outlined. Section 3 deals with a number of aspects of the time Laplace transformation that are relevant to electromagnetic modelling and inversion. Section 4 discusses the formulation of the inversion problem as a succession of two linear operator equations that are amenable to the iterative solution procedure of the appendix.

The fields occur in three-dimensional Euclidean space \mathbb{R}^3 . Position in \mathbb{R}^3 is indicated by the position vector \boldsymbol{x} with respect to a given orthogonal Cartesian reference frame. The time coordinate is t . Partial differentiation with respect to t is denoted by ∂_t ; ∇ is the spatial vectorial differential operator.

2. The domain-integrated field equations method for computing time-domain electromagnetic wavefields

The domain-integrated field equations method for computing time-domain electromagnetic wavefields in strongly heterogeneous media presented in this section starts from the *domain-integrated electromagnetic field equations*

$$\int_{\partial\mathcal{D}} \boldsymbol{\nu} \times \boldsymbol{H} \, dA - \int_{\mathcal{D}} \partial_t \boldsymbol{D} \, dV = \mathbf{0}, \quad (2.1)$$

$$\int_{\partial\mathcal{D}} \boldsymbol{\nu} \times \boldsymbol{E} \, dA + \int_{\mathcal{D}} \partial_t \boldsymbol{B} \, dV = \mathbf{0}, \quad (2.2)$$

and the *domain-integrated electromagnetic compatibility relations*

$$\int_S \boldsymbol{\nu} \cdot \boldsymbol{D} \, dA = 0, \quad (2.3)$$

$$\int_S \boldsymbol{\nu} \cdot \boldsymbol{B} \, dA = 0. \quad (2.4)$$

In equations (2.1) and (2.2), $\mathcal{D} \subset \mathbb{R}^3$ is any bounded subdomain of \mathbb{R}^3 and $\partial\mathcal{D}$ is its closed boundary surface ($\boldsymbol{\nu}$ = unit vector along the outward normal to $\partial\mathcal{D}$). In equations (2.3) and (2.4), S is any closed surface in \mathbb{R}^3 ($\boldsymbol{\nu}$ = unit vector along the outward normal to S). The quantities occurring in them are: the two *electromagnetic field strengths* (\boldsymbol{E} = electric field strength, \boldsymbol{H} = magnetic field strength) that can be considered as the electromagnetic ‘intensive quantities’, and the two *electromagnetic flux densities* (\boldsymbol{D} = electric flux density, \boldsymbol{B} = magnetic flux density) that can be considered as the electromagnetic ‘extensive quantities’. The quantity $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$ represents the area density of power flow in the field; the quantity $\boldsymbol{G} = \boldsymbol{D} \times \boldsymbol{B}$ is the volume density of electromagnetic momentum carried by the field.

In any subdomain of the configuration where the field quantities are continuously differentiable, equations (2.1) and (2.2) lead to the standard electromagnetic field equations in differential form

$$\nabla \times \boldsymbol{H} - \partial_t \boldsymbol{D} = \mathbf{0}, \quad (2.5)$$

$$\nabla \times \boldsymbol{E} + \partial_t \boldsymbol{B} = \mathbf{0}, \quad (2.6)$$

and equations (2.3) and (2.4) to the electromagnetic compatibility relations in standard form

$$\nabla \cdot \boldsymbol{D} = 0, \quad (2.7)$$

$$\nabla \cdot \boldsymbol{B} = 0. \quad (2.8)$$

These results follow from our basic equations by rewriting them, through an application of a proper version of Gauss’ integral theorem to the first term on the left-hand sides, as a domain integral over \mathcal{D} and using the argument that the resulting equations are to hold for any domain \mathcal{D} . Such a procedure requires, however, continuous differentiability throughout \mathcal{D} , whereas our basic equations are valid under the weaker condition of piecewise continuity on $\partial\mathcal{D}$ for the tangential components of \boldsymbol{H} and \boldsymbol{E} and piecewise continuity throughout \mathcal{D} for \boldsymbol{D} and

B. When applied to a ‘pillbox’ at an interface between two media with different constitutive parameters, equations (2.1) and (2.2) lead to the interface boundary conditions

$$\boldsymbol{\nu} \times \mathbf{H} = \text{continuous across interface}, \quad (2.9)$$

$$\boldsymbol{\nu} \times \mathbf{E} = \text{continuous across interface}, \quad (2.10)$$

while equations (2.3) and (2.4) lead to the interface boundary conditions

$$\boldsymbol{\nu} \cdot \mathbf{D} = \text{continuous across interface}, \quad (2.11)$$

$$\boldsymbol{\nu} \cdot \mathbf{B} = \text{continuous across interface}. \quad (2.12)$$

In the *constitutive relations* we take the extensive quantities as partly homogeneously related to the intensive quantities and partly due to direct excitation by external sources. Accordingly, we write, taking the passive response of the medium to be linear, time-invariant, locally reacting and without magneto-electric or chiral properties,

$$\partial_t \mathbf{D}(\mathbf{x}, t) = \partial_t [\epsilon(\mathbf{x}, t) *^{(t)} \mathbf{E}(\mathbf{x}, t)] + \mathbf{J}(\mathbf{x}, t), \quad (2.13)$$

$$\partial_t \mathbf{B}(\mathbf{x}, t) = \partial_t [\mu(\mathbf{x}, t) *^{(t)} \mathbf{H}(\mathbf{x}, t)] + \mathbf{K}(\mathbf{x}, t), \quad (2.14)$$

where ϵ = permittivity relaxation function, μ = permeability relaxation function, $*^{(t)}$ denotes time convolution, \mathbf{J} = volume source density of external electric current and \mathbf{K} = volume source density of external magnetic current. (Note that by introducing the external volume source densities as in equations (2.13) and (2.14), we deviate from the procedure followed in de Hoop (1995). The change, however, only affects the values of \mathbf{D} and \mathbf{B} in the interior of the sources.) Although, by assumption, on the submesoscopic scale constitutive relations of this kind still hold, they cannot, for strongly heterogeneous media, be implemented as such on the mesoscopic computational scale. For any domain \mathcal{D} on the latter scale, we replace the relations by

$$\int_{\mathcal{D}} \|\partial_t \mathbf{D} - \partial_t [\bar{\epsilon} *^{(t)} \mathbf{E}] - \mathbf{J}\|_{\mathbf{D}} dV = \text{minimum}, \quad (2.15)$$

$$\int_{\mathcal{D}} \|\partial_t \mathbf{B} - \partial_t [\bar{\mu} *^{(t)} \mathbf{H}] - \mathbf{K}\|_{\mathbf{B}} dV = \text{minimum}, \quad (2.16)$$

where $\bar{\epsilon}$ is some effective value of ϵ and $\bar{\mu}$ is some effective value of μ , both on the mesoscopic scale, $\|\cdot\|_{\mathbf{D}}$ is some norm in the function space of electric flux densities and $\|\cdot\|_{\mathbf{B}}$ is some norm in the function space of magnetic flux densities. Note that even if on the submesoscopic scale the medium is isotropic (and hence ϵ and μ are scalar functions of position), $\bar{\epsilon}$ and/or $\bar{\mu}$ may be tensors of rank two due to the influence of structural anisotropy caused by different shapes of the different material constituents. In equation (2.15) the minimization is carried out by varying the expansion coefficients of \mathbf{E} and keeping those of \mathbf{D} fixed; in equation (2.16) the minimization is carried out by varying the expansion coefficients of \mathbf{H} and keeping those of \mathbf{B} fixed.

Finally, the *causality condition* requires the field quantities to vanish throughout space prior to the onset of the action of the source distributions.

The computational implementation can most consistently be carried out on a *simplicial mesh* (tetrahedra in \mathbb{R}^3 , triangles in \mathbb{R}^2). Let \mathcal{T} denote any of the tetrahedra and consider any of its vertices. Then, the edges leaving the vertex and the faces meeting at it form a system of (non-orthogonal) *reciprocal base vectors*. Let $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$ denote the three vectorial *edges* leaving a particular vertex and let $\{\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3\}$ denote the outwardly oriented vectorial *areas* of the *faces* meeting at that vertex, then with the standard numbering (edges joining remaining vertices, faces opposite to vertices) they satisfy the relations

$$\mathbf{b}_i \cdot \mathbf{A}_j = -3V_{\mathcal{T}} \delta_{i,j}, \quad (2.17)$$

where V_T is the volume of T and $\delta_{i,j} = \{1, 0\}$ for $\{i = j, i \neq j\}$. Equation (2.17) implies that the edges and faces indeed form a set of reciprocal base vectors, with $-3V_T$ as their interrelational coefficient. In principle, we can, for any of the field vectors F , employ either an *edge expansion*

$$F = (-3V_T)^{-1} \sum_{i=1}^3 \alpha_i^F A_i \quad (\text{edge expansion}) \quad (2.18)$$

with expansion coefficients

$$\alpha_i^F = F \cdot b_i \quad \text{for } i = 1, 2, 3, \quad (2.19)$$

or a *face expansion*

$$F = (-3V_T)^{-1} \sum_{i=1}^3 \beta_i^F b_i \quad (\text{face expansion}) \quad (2.20)$$

with expansion coefficients

$$\beta_i^F = F \cdot A_i \quad \text{for } i = 1, 2, 3. \quad (2.21)$$

Once, at each vertex, the type of expansion has been chosen, the field representation along edges, across faces and throughout the interior of the tetrahedron is constructed out of the vertex values by spatial linear interpolation. Note that the simplex is the only geometrical object where such a linear interpolation can be carried out in a consistent manner (Naber 1980).

Returning to our electromagnetic modelling procedure, we adopt the principle that numerical discontinuity across an interface of jump discontinuity in constitutive properties showing up in those field components that are to be continuous across this interface is to be avoided. Such a discontinuity would, in the physical picture, introduce spurious surface currents that would spoil the accuracy of the computed field values on and (at least) near that interface. In accordance with this principle and to meet the boundary conditions (2.9) and (2.10), we employ *edge expansions* for E and H , while in order to meet the boundary conditions (2.11) and (2.12) we employ *face expansions* for D and B , and in the computational scheme enforce equality, in machine precision, of the expansion coefficients applying to the simplicial star of an edge or both sides of an interface. Next, the field expansions are substituted in the domain-integrated field equations (2.1) and (2.2) and in the domain-integrated compatibility relations (2.3) and (2.4). This leads to a system of linear algebraic equations in the expansion coefficients. Finally, the field expansions are substituted in the effective constitutive relations (2.15) and (2.16) and, for given excitation, the minimization procedure is carried out. Again, a system of linear algebraic equations in the expansion coefficients results. As can be verified, the total system of equations is overdetermined. A ‘best’ solution is constructed via the minimization of the mismatch between ‘known’ and ‘unknown’ quantities in accordance with a chosen mismatch criterion.

Areas for exploration. Preliminary results of the domain-integrated field equations approach to the computation of quasi-static magnetic fields have shown that the method can handle configurations with high contrasts in magnetic properties (up to one thousand in permeability), with excellent accuracy up to the interfaces of discontinuity in constitutive parameters, on a coarse mesh and in perfectly acceptable computation times (de Hoop and Lager 1998, 1999, 2000). Especially notable is that the method needs no mesh refinement at all near interfaces, edges or corners. Experience with electromagnetic wavefields in three-dimensional configurations has to be built up. An open question still is how to handle the time coordinate.

An integration with respect to time in equations (2.1) and (2.2) gets rid of the time derivative and in the minimization procedure associated with the effective constitutive relations the norm should include the time window of computation (in the case of forward modelling) or the time window of observation (in the case of inversion). Furthermore, in order to meet the practical necessity to restrict the domain of computation to one of bounded support, some *absorbing boundary condition* at the latter's outer boundary surface has to be devised and incorporated in the scheme presented. Such a boundary condition should simulate the outward radiation of the fields into the embedding. Another possibility would be to carry out the spatial computations at a Lerch sequence of time Laplace transform parameters and reconstruct from those the time behaviour (see section 3). In the time Laplace transform domain the field quantities do show an exponential decay with increasing distance from sources and heterogeneities and hence the embedding can, perhaps, to a sufficient degree be included in the domain of computation with zero values at its outer boundary surface.

3. The time Laplace transformation, causality and Lerch's theorem

This section deals with the handling of the time coordinate in electromagnetic field problems, both in forward modelling and in (constitutive) parameter inversion. To avoid an abundance in symbols, the dependence of the quantities on position in space will, in this section, not be indicated explicitly. Let $f = f(t)$ denote any real-valued function for $t \in \mathbb{R}$, with support $\mathbb{R}^+ = \{t \in \mathbb{R}; 0 < t < \infty\}$, whose integral $\int_{t'=0}^t f(t') dt'$ exists and let

$$\hat{f}(s) = \int_{t=0}^{\infty} \exp(-st) f(t) dt \tag{3.1}$$

be its Laplace transform. As can be verified, $\hat{f}(s)$ exists for $s \in \mathbb{C}$ and $\text{Re}(s) > 0$. For our purpose, we specifically consider the real-valued sequence of Laplace transforms

$$\{\hat{f}(s_n); n = 0, 1, 2, \dots\}, \tag{3.2}$$

in which

$$s_n = s_0 + nh \quad \text{with } s_0 > 0, \quad h > 0, \quad n = 0, 1, 2, \dots \tag{3.3}$$

Whenever appropriate, we shall denote a sequence of the kind $\{s_n; n = 0, 1, 2, \dots\}$ as a *Lerch sequence*. Now, *Lerch's theorem* (Widder 1946) states that the mapping from $\{\hat{f}(s_n); n = 0, 1, 2, \dots\}$ to $\{f(t); t \in \mathbb{R}^+\}$ is one-to-one. As a consequence, the real-valued sequence $\{\hat{f}(s_n); n = 0, 1, 2, \dots\}$ should suffice to reconstruct the real-valued time function $f = f(t)$ on its (causal) support \mathbb{R}^+ . One advantage of an algorithm of this kind would be that only real-valued arithmetic is involved rather than the complex-valued arithmetic that is needed in the standard fast Fourier transform technique that applies to functions whose Fourier transform exists (for which the transform parameter s takes imaginary values). In line with the approach to the iterative solution of the linear operator equations to be discussed in section 4 in connection with the electromagnetic inversion problem and in the appendix in general terms, we propose an algorithm that proceeds as follows.

Consider, for a given sequence $\{\hat{f}(s_n); n = 0, 1, 2, \dots\}$, the relation

$$\hat{f}(s_n) = \int_{t=0}^{\infty} \exp(-s_n t) f(t) dt \quad \text{for } n = 0, 1, 2, \dots \tag{3.4}$$

as a linear operator equation of the type discussed in the appendix. Introduce an inner product on the Lerch sequence of the type

$$\langle \hat{f}, \hat{g} \rangle_s = \sum_{m,n} w_{m,n} \hat{f}(s_m) \hat{g}(s_n), \tag{3.5}$$

where $\{w_{m,n}; m = 0, 1, 2, \dots, n = 0, 1, 2, \dots\}$, with $w_{m,n} = w_{n,m}$, is a sequence of *weighting coefficients* that makes $\langle \hat{f}, \hat{f} \rangle_s$ to have the properties of a norm. Furthermore, introduce as inner product on \mathbb{R}^+

$$\langle f, g \rangle_t = \int_{t=0}^{\infty} f(t)g(t) dt. \tag{3.6}$$

Clearly, $\langle f, f \rangle_t$ is the L^2 -norm of f on \mathbb{R}^+ . Then, writing equation (3.4) as

$$\hat{f}(s_n) = \mathbf{Le}[f(t)] \quad \text{for } n = 0, 1, 2, \dots, \tag{3.7}$$

the operator \mathbf{Le}^* *adjoint to* \mathbf{Le} is found to be expressible through

$$\mathbf{Le}^*[\hat{f}(s_n)] = \sum_{m,n} w_{m,n} \exp(-s_m t) \hat{f}(s_n) \quad \text{for } t \in \mathbb{R}^+. \tag{3.8}$$

With the aid of the definitions of $\langle \cdot, \cdot \rangle_s$, $\langle \cdot, \cdot \rangle_t$, \mathbf{Le} and \mathbf{Le}^* , the iterative procedure outlined in appendix can be implemented. Since in view of Lerch's theorem the inverse \mathbf{Le}^{-1} of \mathbf{Le} exists, the algorithm converges to the exact $f(t)$.

Area for exploration. The type of algorithm presented contains the values of s_0 and h in the Lerch sequence, as well as the set of weighting coefficients $\{w_{m,n}\}$ in the inner product $\langle \cdot, \cdot \rangle_s$ as parameters. These parameters will influence the rate of convergence of the iterative procedure involved. Research in this direction seems of interest. Note that the use of the Lerch sequence applies to both forward modelling as well as to parameter inversion and that only the truncation of the sequence leads to numerical errors (apart from round-off errors).

4. Inversion of electromagnetic data: contrast source formulation, operator formalism and iterative decrease in mismatch approach

This section addresses some aspects of the electromagnetic inversion problem. It presents an operator formalism pertaining to the contrast source formulation of the problem and disusses the optimization based iterative decrease in mismatch approach to reconstruct the desired model from the observed data. We focus on the type of situation encountered in the practice of geophysical exploration and reservoir monitoring where the aim is to reconstruct, in a prescribed *target region* of bounded support $\mathcal{D}^s \in \mathbb{R}^3$, the electromagnetic constitutive parameters by irradiating the target region with a finite number $N^T \geq 1$ of *sources* or *transmitters* that generate an interrogating electromagnetic wavefield in \mathbb{R}^3 , and recording certain field related values with a finite number $N^R \geq 1$ of *receivers*. The transmitters have the disjoint bounded supports $\{\mathcal{D}_n^T; n = 1, \dots, N^T\}$ and are excited by the *source signals* $\{d_n^T = d_n^T(t); n = 1, \dots, N^T\}$ with known signature. The receivers have the disjoint bounded supports $\{\mathcal{D}_m^R; m = 1, \dots, N^R\}$; the set of *receiver signals* recorded by them is $\{d_{m,n}^R = d_{m,n}^R(t); m = 1, \dots, N^R, n = 1, \dots, N^T\}$. The supports of, several or all, receivers may coincide with the supports of, some or all, transmitters. The physical action of converting the source signals to electromagnetic wavefields is symbolized by the *transmitting operators* $\{\mathbf{T}_n; n = 1, \dots, N^T\}$ that may differ for the different sources; \mathbf{T}_n has the support \mathcal{D}_n^T . The physical action of extracting out of the electromagnetic wavefields the recorded receiver signals is symbolized by the *receiving operators* $\{\mathbf{R}_m; m = 1, \dots, N^R\}$ that may differ for the different receivers; \mathbf{R}_m has the support \mathcal{D}_m^R . Finally, the propagation of the electromagnetic wavefield from the source domains to the receiver domains is symbolized by the *propagation operator* \mathbf{P} . It is assumed that all operators just introduced are homogeneously linear. Through the relevant formalism we can write

$$d_{m,n}^R(t) = \mathbf{R}_m \mathbf{P} \mathbf{T}_n [d_n^T(t)] \quad \text{for } m = 1, \dots, N^R; \quad n = 1, \dots, N^T. \tag{4.1}$$

The target region is now considered as a *scattering region* with unknown constitutive parameters, embedded in a *background medium* with known propagation operator \mathbf{P}^b . The electromagnetic wavefield that the irradiating source with label n would generate in the embedding is denoted as the *incident wavefield* \mathbf{F}_n^i . The difference between the actual wavefield \mathbf{F}_n generated by this source and the corresponding incident wavefield is denoted as the *scattered wavefield* \mathbf{F}_n^s . Using

$$\mathbf{F}_n = \mathbf{F}_n^i + \mathbf{F}_n^s \quad \text{for } n = 1, \dots, N^T, \quad (4.2)$$

in the pertaining field equations and constitutive relations, we can write

$$\mathbf{M}^b[\mathbf{F}_n^s] = -\mathbf{Q}_n^s \quad \text{for } n = 1, \dots, N^T, \quad (4.3)$$

where \mathbf{M}^b is the Maxwell field operator pertaining to the background medium and \mathbf{Q}_n^s is the contrast volume source density associated with the irradiating source with label n . It is given by

$$\mathbf{Q}_n^s = \partial_t(\mathbf{X} \overset{(t)}{*} \mathbf{F}_n) \quad \text{for } n = 1, \dots, N^T \quad \text{and} \quad \mathbf{x} \in \mathcal{D}^s, \quad (4.4)$$

with \mathbf{X} as the contrast in constitutive parameters between the actual medium and the background medium. Evidently, \mathbf{Q}_n^s has \mathcal{D}^s as its support. (For details of the derivation, see de Hoop and de Hoop 2000.) Denoting the response of the receivers to the incident wavefield by

$$d_{m,n}^{R;i}(t) = \mathbf{R}_m \mathbf{P}^b \mathbf{T}_n[d_n^T(t)] \quad \text{for } m = 1, \dots, N^R; \quad n = 1, \dots, N^T, \quad (4.5)$$

and introducing their scattered wavefield responses as

$$d_{m,n}^{R;s}(t) = d_{m,n}^R(t) - d_{m,n}^{R;i}(t) \quad \text{for } m = 1, \dots, N^R; \quad n = 1, \dots, N^T, \quad (4.6)$$

the latter can be written as

$$d_{m,n}^{R;s}(t) = \mathbf{R}_m \mathbf{P}^b[\mathbf{Q}_n^s] \quad \text{for } m = 1, \dots, N^R; \quad n = 1, \dots, N^T. \quad (4.7)$$

As is well known, the mapping, via equations (4.4) and (4.7), from the contrast in constitutive parameters to the scattered wavefield responses is a *nonlinear* one because of the fact that also \mathbf{F}_n in equation (4.4) depends on this contrast.

Equation (4.7), which is denoted as the *data equation*, is now regarded as a linear operator equation with known data in the left-hand side and unknown contrast volume source densities in the right-hand side. Introducing a proper inner product in the data function space, the ‘optimum’ value of the contrast volume source densities can then be determined via the procedure of iterative decrease in mismatch between the left- and right-hand sides in accordance with the norm induced by the relevant inner product (for such a procedure, see the appendix). Once this optimum value of the contrast volume source densities has been determined, the scattered wavefield in \mathcal{D}^s is evaluated by using the relation

$$\mathbf{F}_n^s = \mathbf{P}^b[\mathbf{Q}_n^s] \quad \text{for } n = 1, \dots, N^T. \quad (4.8)$$

Upon substituting equation (4.8) and equation (4.2) in equation (4.4), we arrive at

$$\mathbf{Q}_n^s = \partial_t[\mathbf{X} \overset{(t)}{*} (\mathbf{F}_n^i + \mathbf{P}^b[\mathbf{Q}_n^s])] \quad \text{for } n = 1, \dots, N^T \quad \text{and} \quad \mathbf{x} \in \mathcal{D}^s. \quad (4.9)$$

This equation is denoted as the *object equation*. It is, for each n , considered as a linear operator equation with known contrast volume source densities in the left-hand side and unknown contrast in constitutive parameters in the right-hand sides. However, the contrast in constitutive properties to be reconstructed should be independent of n . Here, one can handle the situation in the ‘best’ way by introducing a proper inner product in the function space of contrast volume source densities, and determining the contrast in constitutive parameters in

\mathcal{D}^s via the procedure of iterative decrease in mismatch between the N^T left- and right-hand sides in accordance with the norm induced by the relevant inner product. Along this line of thought, the ‘best solution’ to the problem, given the acquisition geometry of sources and receivers and subject to the chosen weighting coefficients in the relevant inner products in the pertaining function spaces, has been obtained. Observe in this respect that the iterative procedures involved are convergent.

Areas for exploration. The foregoing analysis decomposes the nonlinear and (for all practical purposes) non-unique constitutive parameter inversion problem into a succession of two linear problems where a given acquisition setup of sources and receivers and an optimization approach with given mismatch criteria lead to a ‘best’ solution. Since different acquisition setups and/or different mismatch criteria will lead to different ‘best’ solutions, the non-uniqueness of the problem is still manifest. As to the nonlinearity, it is believed that it is, in each particular case, circumvented in a manner that reflects the basic physics of the problem. Numerical model experiments, where each time one of the basic ingredients is modified, can hopefully reveal some guidelines that are of interest to a range of situations met in practice.

In any case, fundamental difficulties of a methodological nature remain. The first in this category are the ‘non-radiating sources’ with support \mathcal{D}^s that have no influence on the recorded data, but that affect equation (4.9) and, hence, the reconstructed contrast in constitutive parameters. Another point of concern is that the (mathematically) reconstructed contrast in constitutive parameters can in no way be expected to satisfy a number of physical constraints, such as causality, stability or positive definiteness in energy considerations. In a time-domain analysis these aspects are difficult to keep track of; here, too, an analysis in the time Laplace transform domain (carried out at some Lerch sequence) might make things in this respect easier. Kleinman and Van den Berg (1997) proved in a numerical study that joint minimization techniques applied to equations (4.7) and (4.9) led to superior results over the successive procedure of our present approach. In their iterative procedure, however, the guaranteed convergence escapes a simple proof.

5. Conclusion

Three different, but related, areas for exploration in electromagnetic modelling and inversion have been discussed. They all have the flavour of methodological aspects, rather than focusing on a particular application. The ideas about modelling electromagnetic wavefields in strongly heterogeneous media (section 2) and the one about using a Lerch sequence in the time Laplace domain to parametrize the time behaviour (section 3) strongly deviate—as far as the author is aware—from the current trends in research in the field under consideration. Partly, this can also be said about the approach to inversion discussed in section 4. As far as the latter subject is concerned, much emphasis is usually laid on the non-uniqueness and nonlinearity of the parameter inversion problem. The non-uniqueness (for practical situations) persists, but the nonlinearity has been circumvented by a well-defined succession of two linear inversion problems, each of which has, once a mismatch criterion in the satisfaction of the equality sign in the relevant operator equations has been decided upon, a unique solution, where at least the reconstructed contrast volume source density exactly matches the observed data. Different mismatch criteria will in general lead to different reconstructed models and there seems, at present, no way to decide upon whether one of them is ‘better’ than the other.

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Appendix. Iterative solution to a linear operator equation

In this appendix we discuss an iterative solution procedure that applies to a linear operator equation of the type that occurs in inverse source and inverse scattering problems. The solution procedure is induced by an appropriate error or mismatch criterion and focuses on the construction of an iterative scheme with a guaranteed decrease in mismatch at each step ('*improvement condition*'). A rather general notation is used that suffices for the main aspects of the method. Let the operator equation under consideration be given by

$$\mathbf{d} = \Omega[\mathbf{m}], \quad (\text{A.1})$$

where the *operator* Ω that maps the '*model*' \mathbf{m} onto the '*data*' \mathbf{d} is assumed to be homogeneous and linear. For our applications, \mathbf{d} and \mathbf{m} are arrays with discrete or continuous 'subscripts' whose ranges may be different. The data are elements of the *data space*, i.e. a linear space in which an inner product, to be denoted by $\langle \cdot, \cdot \rangle_d$, is defined that has the symmetry property

$$\langle \mathbf{d}_1, \mathbf{d}_2 \rangle_d = \langle \mathbf{d}_2, \mathbf{d}_1 \rangle_d. \quad (\text{A.2})$$

Further, we write

$$\|\mathbf{d}\|_d^2 = \langle \mathbf{d}, \mathbf{d} \rangle_d, \quad (\text{A.3})$$

where $\|\cdot\|_d$ has the standard properties of a norm. The admissible models are elements of a *model space*, i.e. a linear space in which an inner product, to be denoted by $\langle \cdot, \cdot \rangle_m$, is defined that has the symmetry property

$$\langle \mathbf{m}_1, \mathbf{m}_2 \rangle_m = \langle \mathbf{m}_2, \mathbf{m}_1 \rangle_m. \quad (\text{A.4})$$

Further, we write

$$\|\mathbf{m}\|_m^2 = \langle \mathbf{m}, \mathbf{m} \rangle_m, \quad (\text{A.5})$$

where $\|\cdot\|_m$ has the standard properties of a norm.

The iterative procedure to 'solve' equation (A.1) goes as follows. Let $\mathbf{m}^{[i]}$ be an 'approximation' to \mathbf{m} and define the corresponding *residual* in the operator equation (A.1) as

$$\mathbf{r}^{[i]} = \mathbf{d} - \Omega[\mathbf{m}^{[i]}]. \quad (\text{A.6})$$

As the *mismatch* or *error* in the satisfaction of the equality sign in equation (A.1) we introduce the quantity

$$err^{[i]} = \|\mathbf{r}^{[i]}\|_d^2. \quad (\text{A.7})$$

The aim is now to construct an *update* $\mathbf{m}^{[i+1]}$ to $\mathbf{m}^{[i]}$ such that $err^{[i+1]} < err^{[i]}$ ('*improvement condition*'). To construct such an update, let

$$\mathbf{m}^{[i+1]} = \mathbf{m}^{[i]} + \delta\mathbf{m}^{[i]}. \quad (\text{A.8})$$

Then,

$$\mathbf{r}^{[i+1]} = \mathbf{r}^{[i]} - \Omega[\delta\mathbf{m}^{[i]}]. \quad (\text{A.9})$$

Substitution of this relation in the expression for $err^{[i+1]} - err^{[i]}$ leads to

$$err^{[i+1]} - err^{[i]} = -2\langle \Omega[\delta m^{[i]}], r^{[i]} \rangle_d + \|\Omega[\delta m^{[i]}\|_d^2. \tag{A.10}$$

A necessary and sufficient condition for improvement is therefore

$$-2\langle \Omega[\delta m^{[i]}], r^{[i]} \rangle_d + \|\Omega[\delta m^{[i]}\|_d^2 < 0. \tag{A.11}$$

Now, the last term on the right-hand side is positive for any $\Omega[\delta m^{[i]}] \neq \mathbf{0}$. In order to meet the condition for improvement, the inner product in the first term on the left-hand side must be sufficiently large positive for the chosen value of $\delta m^{[i]}$. Assume now that a homogeneous, linear operator Ω^* *adjoint* to Ω exists such that, for all $\delta m^{[i]}$ and $r^{[i]}$, the relation

$$\langle \Omega[\delta m^{[i]}], r^{[i]} \rangle_d = \langle \delta m^{[i]}, \Omega^*[r^{[i]}\rangle_m \tag{A.12}$$

holds. Then, a sufficient condition for the requirement expressed by equation (A.11) to be met is

$$\delta m^{[i]} = \alpha^{[i]} \Omega^*[r^{[i]}], \tag{A.13}$$

with $\alpha^{[i]} > 0$ suitably chosen. Substitution of equation (A.13) into equation (A.10) yields

$$err^{[i+1]} - err^{[i]} = -2\alpha^{[i]} B^{[i]} + \alpha^{[i]2} A^{[i]}, \tag{A.14}$$

where

$$B^{[i]} = \|\Omega^*[r^{[i]}\|_m^2 \tag{A.15}$$

and

$$A^{[i]} = \|\Omega\Omega^*[r^{[i]}\|_d^2. \tag{A.16}$$

The maximum decrease in the error is, from equation (A.14), attained for

$$\alpha^{[i]} = \frac{B^{[i]}}{A^{[i]}}. \tag{A.17}$$

(Note that, indeed, $\alpha^{[i]} > 0$.) This choice leads to the *steepest descent* update

$$\delta m^{[i]} = \frac{B^{[i]}}{A^{[i]}} \Omega^*[r^{[i]}] \tag{A.18}$$

and the steepest descent in error

$$err^{[i+1]} - err^{[i]} = -\frac{[B^{[i]}]^2}{A^{[i]}}. \tag{A.19}$$

In practice, the computations are carried out with the *normalized error*

$$\overline{err}^{[i]} = \frac{err^{[i]}}{\|\mathbf{d}\|_d^2}. \tag{A.20}$$

This normalized error has the properties $\overline{err}^{[i]} = 1$ for $r^{[i]} = \mathbf{d}$ (which corresponds to $m^{[i]} = \mathbf{0}$) and $\overline{err}^{[i]} = 0$ for $r^{[i]} = \mathbf{0}$ (i.e. for perfect data fit). The steepest descent in the normalized error is

$$\overline{err}^{[i+1]} - \overline{err}^{[i]} = -\frac{[B^{[i]}]^2}{A^{[i]}\|\mathbf{d}\|_d^2}. \tag{A.21}$$

These results form the basis for an iterative procedure where successive updates of the model lead to successive decreases in the mismatch between the given data and the ones generated by the updates of the model.

As the starting value we take $\mathbf{m}^{[0]} = \mathbf{0}$, which entails $\overline{err}^{[0]} = 1$. With

$$\overline{err}^{[i+1]} = \overline{err}^{[i]} - \frac{[B^{[i]}]^2}{A^{[i]}\|\mathbf{d}\|_d^2} \quad \text{for } i = 0, 1, 2, \dots, \quad (\text{A.22})$$

we generate the sequence $\{\overline{err}^{[i]}; i = 0, 1, 2, \dots\}$. This sequence is positive and decreasing and, hence, converges to a limit as $i \rightarrow \infty$. Denoting this limit by $\overline{err}^{[\infty]}$, we have

$$\overline{err}^{[\infty]} = 1 - \sum_{i=0}^{\infty} \frac{[B^{[i]}]^2}{A^{[i]}\|\mathbf{d}\|_d^2}. \quad (\text{A.23})$$

Note that, in general, $\overline{err}^{[\infty]} > 0$.

Another consequence of the convergence of the series on the right-hand side of equation (A.23) is that $B^{[\infty]} = 0$. On account of equation (A.15) therefore $\Omega^*[\mathbf{r}^{[\infty]}] = \mathbf{0}$. Use of equation (A.6) for $i \rightarrow \infty$ then leads to

$$\mathbf{0} = \Omega^*[\mathbf{d}] - \Omega^*\Omega[\mathbf{m}^{[\infty]}]. \quad (\text{A.24})$$

Since $\mathbf{m}^{[\infty]}$ exists and is unique, $(\Omega^*\Omega)^{-1}$ exists and is unique, and the model reconstructed by the iterative procedure is

$$\mathbf{m}^{[\infty]} = (\Omega^*\Omega)^{-1}\Omega^*[\mathbf{d}]. \quad (\text{A.25})$$

Since, in general, Ω in equation (A.1) does not have a unique inverse, $\mathbf{m}^{[\infty]}$ will, in general, differ from the model \mathbf{m} that has generated the data \mathbf{d} . The reconstructed model $\mathbf{m}^{[\infty]}$ is the *minimum-norm solution* to equation (A.1) and $(\Omega^*\Omega)^{-1}\Omega^*$ is the *pseudo-inverse* of Ω .

Operating with Ω on equation (A.24), we obtain

$$\Omega(\Omega^*\Omega)[\mathbf{m}^{[\infty]}] = \Omega\Omega^*[\mathbf{d}], \quad (\text{A.26})$$

which can be rewritten as

$$(\Omega\Omega^*)\Omega[\mathbf{m}^{[\infty]}] = \Omega\Omega^*[\mathbf{d}]. \quad (\text{A.27})$$

Since $\Omega\Omega^*$ is positive definite, it has a unique inverse. Operating on equation (A.27) with this inverse, we obtain

$$\Omega[\mathbf{m}^{[\infty]}] = [\mathbf{d}], \quad (\text{A.28})$$

i.e. the reconstructed model fits the data exactly.

The quantities $\{\mathbf{m}^{[i]}; i = 0, 1, 2, \dots\}$ are denoted as the (successive) *images* of \mathbf{m} .

Finally, it is observed that the expression given by equation (A.25) for the reconstructed model also directly follows by considering the expression

$$\begin{aligned} err &= \|\mathbf{d} - \Omega[\mathbf{m}]\|_d^2 \\ &= \langle \mathbf{d} - \Omega[\mathbf{m}], \mathbf{d} - \Omega[\mathbf{m}] \rangle_d \end{aligned} \quad (\text{A.29})$$

and defining the *optimum model* \mathbf{m}^{opt} as the one that minimizes err . Upon substituting

$$\mathbf{m} = \mathbf{m}^{\text{opt}} + \delta\mathbf{m}, \quad (\text{A.30})$$

we obtain

$$\begin{aligned} err &= err^{\text{opt}} - 2\langle \Omega[\delta\mathbf{m}], \mathbf{d} - \Omega[\mathbf{m}^{\text{opt}}] \rangle_d + \|\Omega[\delta\mathbf{m}]\|_d^2 \\ &= err^{\text{opt}} - 2\langle \delta\mathbf{m}, \Omega^*[\mathbf{d}] - \Omega^*\Omega[\mathbf{m}^{\text{opt}}] \rangle_d + \|\Omega[\delta\mathbf{m}]\|_d^2, \end{aligned} \quad (\text{A.31})$$

with

$$err^{\text{opt}} = \|\mathbf{d} - \Omega[\mathbf{m}^{\text{opt}}]\|_d^2. \quad (\text{A.32})$$

From this, it follows that $err > err^{\text{opt}}$ for any $\delta\mathbf{m} \neq \mathbf{0}$, provided that

$$\Omega^*[\mathbf{d}] = \Omega^*\Omega[\mathbf{m}^{\text{opt}}], \quad (\text{A.33})$$

which is equation (A.24), with $\mathbf{m}^{[\infty]} = \mathbf{m}^{\text{opt}}$.

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