

Three-dimensional geoelectric modelling with optimal work/accuracy rate using an adaptive wavelet algorithm

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SUMMARY

Despite the ever-increasing power of modern computers, realistic modelling of complex 3-D earth models is still a challenging task and requires substantial computing resources. The overwhelming majority of current geophysical modelling approaches includes either finite difference or non-adaptive finite element algorithms and variants thereof. These numerical methods usually require the subsurface to be discretized with a fine mesh to accurately capture the behaviour of the physical fields. However, this may result in excessive memory consumption and computing times. A common feature of most of these algorithms is that the modelled data discretizations are independent of the model complexity, which may be wasteful when there are only minor to moderate spatial variations in the subsurface parameters. Recent developments in the theory of adaptive numerical solvers have the potential to overcome this problem. Here, we consider an adaptive wavelet-based approach that is applicable to a large range of problems, also including nonlinear problems. In comparison with earlier applications of adaptive solvers to geophysical problems we employ here a new adaptive scheme whose core ingredients arose from a rigorous analysis of the overall asymptotically optimal computational complexity, including in particular, an optimal work/accuracy rate. Our adaptive wavelet algorithm offers several attractive features: (i) for a given subsurface model, it allows the forward modelling domain to be discretized with a quasi minimal number of degrees of freedom, (ii) sparsity of the associated system matrices is guaranteed, which makes the algorithm memory efficient and (iii) the modelling accuracy scales linearly with computing time. We have implemented the adaptive wavelet algorithm for solving 3-D geoelectric problems. To test its performance, numerical experiments were conducted with a series of conductivity models exhibiting varying degrees of structural complexity. Results were compared with a non-adaptive finite element algorithm, which incorporates an unstructured mesh to best-fitting subsurface boundaries. Such algorithms represent the current state-of-the-art in geoelectric modelling. An analysis of the numerical accuracy as a function of the number of degrees of freedom revealed that the adaptive wavelet algorithm outperforms the finite element solver for simple and moderately complex models, whereas the results become comparable for models with high spatial variability of electrical conductivities. The linear dependence of the modelling error and the computing time proved to be model-independent. This feature will allow very efficient computations using large-scale models as soon as our experimental code is optimized in terms of its implementation.

Key words: Numerical solutions; Wavelet transform; Numerical approximations and analysis; Non-linear differential equations; Electrical properties.

1 INTRODUCTION

Numerical modelling of geophysical data is an important component of tomographic inversion algorithms and many other tasks in Earth sciences. A key requirement in most applications is that the modelling algorithms are able to provide swiftly and efficiently the accurate response for a given Earth model. If only a few anomalous

bodies are embedded in a homogeneous medium, integral equation and boundary element methods may be preferable and beneficial (e.g. Beard *et al.* 1996), but for more complicated structures, as they typically arise in tomographic inversion problems, finite difference or finite element algorithms, and variants thereof, are more suitable (e.g. Morton & Mayers 2005; Brenner & Scott 2008). These numerical techniques parametrize the subsurface properties

(electrical conductivities, seismic velocities, etc.) either with structured or unstructured meshes and the unknown quantities (electrical potentials, acoustic pressure fields, etc.) are determined at the mesh vertices or edges.

Finite difference and finite element methods applied to linear problems can be formulated as

$$\mathbf{A}U = B, \quad (1)$$

where \mathbf{A} is a system matrix that depends on the governing partial differential equation (including the material properties) and the mesh geometry. U is a vector containing the unknown geophysical field and vector B specifies the source properties (location, type, etc.). It is beyond the scope of this paper to review finite difference and finite element techniques in detail, but for our purposes it is important to note that they employ small-support basis functions for approximating the unknown quantities in U . These basis functions have non-zero values only within a particular cell or block (e.g. Brenner & Scott 2008). This is advantageous in the sense that the resulting system matrix \mathbf{A} in eq. (1) becomes very sparse. The downside of these approaches is that accuracy criteria often dictate a very dense mesh, which results in sizeable system matrices \mathbf{A} .

Similar problems have been recognized for representing digital images. Storage of high-resolution images using pixel-based storage schemes (i.e. using small-support basis functions) result in excessively large data volumes. This motivated the development of the wavelet transform in the early 1980s (e.g. Mallat 1998). This mathematical technique allows the digital images to be represented using only a few small-support and large-support basis functions, which results in a substantial decrease of the data volume to be stored. The term ‘large-support’ indicates that these basis functions may extend over larger areas of the domain of interest. A key feature of such image compression schemes is the consideration of the image complexity, such that an image with only a few structural details can be stored more compactly than a more complex image.

In recent years several techniques have been proposed to take advantage of the wavelet transform technique in geophysical applications. An overview of the quite extensive literature can be found, for example, in Kumar & Fofoula-Georgiou (1994). Most of these articles focus on data compression, data filtering and multiscale data analysis. Further applications are related to inversion of geophysical data, where optimal model parametrizations are derived (e.g. Ling-Yun & Wen-Tzong 2003; Loris *et al.* 2007; Kamm *et al.* 2009), or the Jacobian matrix is compressed, such that it can be inverted with sparse matrix techniques (Li & Oldenburg 2003).

Some attempts have been made within the geophysical community to take advantage of wavelet based techniques for numerical modelling. For example, Hong & Kennett (2003) and Hustedt *et al.* (2003) employed wavelet transforms to implement finite difference algorithms suitable for simulating elastic wave propagation. They demonstrated the feasibility of the approach, but the computational savings were at best marginal.

Most of these applications of the wavelet transform including image compression follow a common philosophy: they decompose an original data structure, parametrized with small-support basis functions, using a wavelet transformation and retain only those components of the transformed quantities that are essential for representing the original data with a prescribed accuracy. This implies that the original data structure needs to be known up-front, which is a serious limitation particularly for numerical modelling applications. Conceptually, it would be preferable to approximate the original data structure using only a few large-support basis functions, and then to progressively add further details until the approxima-

tion is sufficiently accurate. That is, it would never be necessary to compute the complete original data structure.

The latter concept forms the idea of adaptive wavelet modelling. Early attempts for implementing wavelet techniques were published by Glowinski *et al.* (1990), Maday *et al.* (1991) and Jaffard (1992). Dahlke *et al.* (1997) proposed an adaptive algorithm suitable for solving elliptic differential equations, but its work/accuracy rate was not shown to be optimal. Vasilyev & Paolucci (1997) proposed an adaptive wavelet algorithm, which was improved by Kevlahan & Vasilyev (2005). Geophysical applications were presented for example in Vasilyev *et al.* (1997, 2004). They claim to solve the discrete problem at a computational expense that stays proportional to the generated number of degrees of freedom. However, they did not show the (asymptotic) optimality of the corresponding work/accuracy rate, namely that the number of adaptively generated degrees of freedom stays proportional to the smallest possible number of degrees of freedom required to achieve the desired accuracy. A landmark paper in the field of adaptive wavelet and also general numerical modelling was presented by Cohen *et al.* (2001). They describe a new algorithm for elliptic problems based on a new paradigm. This algorithm has an optimal work/accuracy rate, which could not be shown for earlier methods. In order to reach this optimality, a series of novel algorithmic concepts needed to be developed. The first numerical experiments using this algorithm in one and two dimensions are shown in Barinka *et al.* (2001). Extensions of the Cohen *et al.* (2001) algorithm to more general linear and even to non-linear problems are found in Cohen *et al.* (2002) and Cohen *et al.* (2003b). In Stevenson (2003), the work/accuracy rate of the Cohen *et al.* (2002) algorithm was improved in the sense that it is no longer limited by the compressibility of the stiffness matrix but only by the regularity of the underlying problem and the applied wavelet basis. Gantumur *et al.* (2007) describe an optimal adaptive wavelet algorithm for elliptic problems based on the Cohen *et al.* (2001) algorithm, which does not depend on a coarsening procedure. Burstedde & Kunoth (2008) implemented the Cohen *et al.* (2001) algorithm using a conjugate gradient solver. An application of the more general linear algorithm to Stokes’ equation was presented by Jiang & Liu (2008).

To our knowledge, no application of such adaptive wavelet modelling has been published so far in the geophysical literature, but we judge it to be highly beneficial for a wide range of geophysical problems. Particularly at an initial stage of a tomographic inversion, when the model structures exhibit a low degree of complexity, it is expected that geophysical data can be modelled efficiently using only a few suitable basis functions. In this paper, we present an application of adaptive wavelet modelling to the 3-D geoelectric problem. We start with a brief introduction of the governing equations, followed by a general outline of adaptive wavelet modelling. Benefits and limitations are demonstrated using a series of conductivity models that exhibit different degrees of complexity. Results are compared with a non-adaptive unstructured mesh finite element algorithm, which represents the current state-of-the-art in geoelectric modelling.

2 THEORY

2.1 The geoelectric problem

Geoelectrical data are governed by the Poisson equation, which can be written as

$$-\nabla \cdot (\sigma \nabla u^{\text{tot}}) = I \delta_s, \quad (2)$$

where σ is the electrical conductivity, u^{tot} is the resulting total electric potential, I is the injection current and δ_s is the delta functional, which is non-zero only at the current injection point x_s . At the surface of the modelling domain Neumann no-normal-flow boundary conditions need to be imposed, and the artificial ground boundaries can be either approximated with Dirichlet or mixed boundary conditions (Dey & Morrison 1979) or with infinite elements (Blome *et al.* 2009).

Note that the classical weak formulation of eq. (2) requires solutions in $H^1(\Omega)$, the space of square integrable functions whose gradients are also square integrable [or a closed subspace of $H^1(\Omega)$], see for example Brenner & Scott (2008) for more details. This requires the right-hand side to belong to the space of all continuous linear functionals mapping $H^1(\Omega)$ (or the closed subspace) into the real numbers. This is not true for the 3-D delta functional. Hence the formulation in eq. (2) leads to difficulties particularly when using adaptive methods.

To account for this problem, a singularity removal technique, as introduced by Lowry *et al.* (1989) and later refined by Zhao & Yedlin (1996) and Blome *et al.* (2009) is applied. In the flat-topography case, the total potential u^{tot} is split up into a sum of the Green's function for homogeneous conductivities $u_s = I/(2\pi\sigma_s r)$ and an unknown secondary potential u . Here, σ_s is the conductivity at the current injection point and r is the distance from the current injection point. The modified Poisson equation after singularity removal is

$$-\nabla \cdot (\sigma \nabla u) = -\nabla \cdot [(\sigma_s - \sigma) \nabla u_s]. \tag{3}$$

For a wide range of conductivities σ (e.g. piecewise constant and not varying in a neighbourhood of the source) this new right-hand side is contained in $H^{-1}(\Omega)$. A favourable side effect of singularity removal is the fact that if the structural complexity of the subsurface is low, the secondary potentials exhibit relatively simple shapes, which can be approximated with only a few basis functions.

2.2 Adaptive Galerkin methods and wavelet basis functions

Adaptive wavelet algorithms belong to the class of Galerkin methods (e.g. Brenner & Scott 2008), and are thus closely related to finite elements. The basic principle of a Galerkin method is to transform the original equation $L(u) = b$ (e.g. eq. 2 or 3) into a weak or variational formulation (e.g. Brenner & Scott 2008). Then the solution u is approximated by a finite set of basis functions $\phi_1, \phi_2, \dots, \phi_N$, such that u can be written as a linear combination of this set

$$u = \sum_{i=1}^N u_i \phi_i, \tag{4}$$

where u_i are the unknown coefficients to be determined. Additionally $\phi_1, \phi_2, \dots, \phi_N$ are employed as testing functions. This leads finally to a system of equations as written in eq. (1).

Traditional approaches such as finite differences and standard finite elements employ small-support basis functions, such that one function only influences the region in the vicinity of a single point, as shown for a 1-D domain in Fig. 1(c) for a finite element basis. All basis functions must be considered for the solution of the problem $L(u) = b$, since otherwise the solution would be zero at the omitted functions point value. This may result in a very large set of equations that needs to be solved in order to attain sufficient accuracy.

Typically, large areas of the solution do not vary too strongly and could hence be approximated with a less dense mesh. However, it is generally not known *a priori*, where these areas are. A

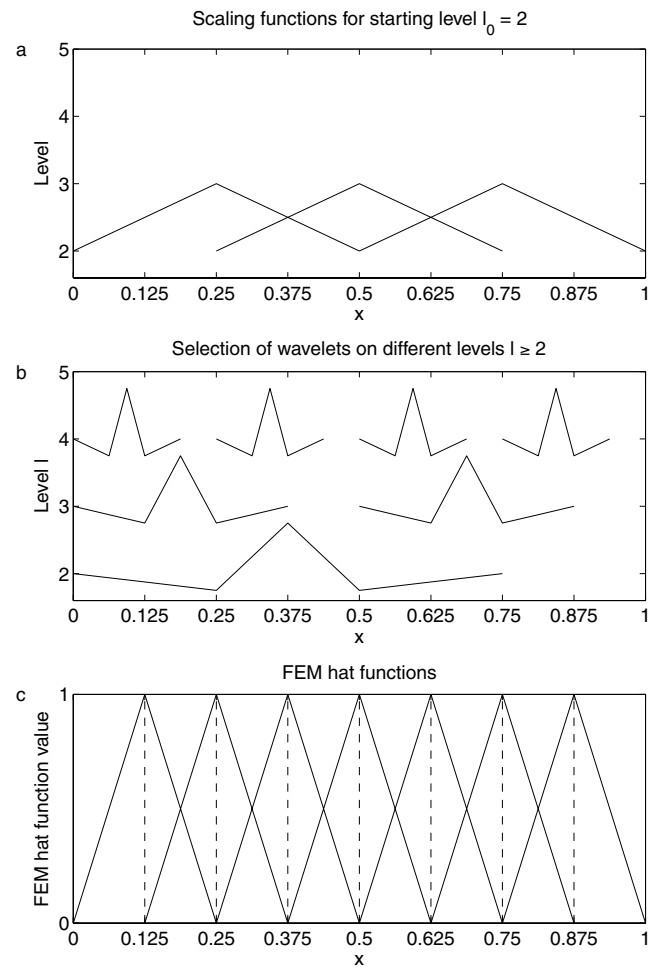


Figure 1. Examples of 1-D model parametrizations. (a) Scaling functions at level 2. (b) A selection of wavelets on different levels with different positions. (c) FEM hat functions for an equivalent resolution as the wavelet basis up to level 2. The dashed lines indicate the nodes of the hat functions. The finite elements are the intervals between the dashed lines on the x-axis.

possible option to address this problem is to employ adaptive algorithms, where the computational domain is discretized initially with a coarse mesh. Then, the mesh is locally refined until the desired accuracy is reached. During the past few years, significant improvements of such adaptive algorithms could be achieved. Among strong improvements in finite element based approaches (e.g. Binev *et al.* 2004; Cascon *et al.* 2008), also adaptive wavelet algorithms were proposed (e.g. Cohen *et al.* 2001, 2003b). In contrast to the adaptive finite element algorithms, refinements of the mesh in a particular area is achieved by simply considering more small-support functions.

Adaptive wavelet algorithms employ a hierarchically structured set of functions, a so-called wavelet basis, in which one can distinguish between scaling functions φ and wavelets ψ . There are different possibilities to implement wavelet bases (Cohen *et al.* 1992; Dahmen *et al.* 1999). We choose the shapes of the scaling functions (Fig. 1a) to be identical to those of the linear finite element basis functions (Fig. 1c)

$$\varphi_{l,k}(x) := \begin{cases} 2^{\frac{3l}{2}} [x - 2^{-l}(k-1)] & \text{if } 2^{-l}(k-1) \leq x \leq 2^{-l}k \\ 2^{\frac{3l}{2}} [2^{-l}(k+1) - x] & \text{if } 2^{-l}k < x \leq 2^{-l}(k+1) \\ 0 & \text{elsewhere,} \end{cases} \tag{5}$$

where the index l specifies the level and index k with $1 \leq k \leq 2^l - 1$ the position of the scaling function. The wavelets (Fig. 1b) are defined as

$$\psi_{l,k} = \frac{1}{\sqrt{2}} \left(-\frac{1}{8}\varphi_{l+1,2k-3} - \frac{1}{4}\varphi_{l+1,2k-2} + \frac{3}{4}\varphi_{l+1,2k-1} + \right. \\ \left. -\frac{1}{4}\varphi_{l+1,2k} - \frac{1}{8}\varphi_{l+1,2k+1} \right), \quad (6)$$

with $2 \leq k \leq 2^l - 1$. At the boundaries, suitably modified scaling functions and wavelets are applied.

A hierarchical set of basis functions starts at a prescribed level l_0 . In principle, one could start with $l_0 = 0$, but higher (or negative) levels are possible as well. For example, the simulations shown later in the paper always start at level $l_0 = 3$. Scaling functions are only considered at level l_0 , and wavelets are chosen at levels $\geq l_0$. Scaling functions at level l_0 , together with all wavelets at levels l_0 to $l > l_0$, describe exactly the same information as a corresponding finite element basis with a mesh size of $2^{-(l+1)}$ but the mesh of the wavelet basis can be refined or coarsened by simply adding or removing wavelets in a specific area (Cohen *et al.* 2001). More details on our choice of scaling functions and wavelets are given in Appendix A, where we also outline, how the concept can be extended to higher dimensions.

Wavelet bases for our purposes offer the following three principal features (see e.g. Dahmen 2003):

- (i) *Locality*: Wavelets are only nonzero in a small area. The size of this area is geometrically reduced for higher levels.
- (ii) *Cancellation property*: Integration against wavelets annihilates smooth parts.
- (iii) *Norm equivalence*: The norm of the wavelet coefficient sequence is equivalent to the norm of the function it represents.

These main features lead to the following beneficial characteristics: Wavelet parametrization allows optimal diagonal pre-conditioning of the system matrix in eq. (1). That is, a diagonal pre-conditioning matrix can be calculated, such that the condition number of the resulting system of equations does not exceed a value c_{\max} , which is independent of the detail level chosen (Cohen *et al.* 2001, 2003b). This allows eq. (1) to be solved efficiently with iterative methods such as conjugate gradient algorithms.

Here, the cancellation property is implemented by the property of vanishing moments, meaning that polynomials up to a fixed degree can be represented exactly using solely the scaling functions (Dahmen *et al.* 1999). This is advantageous for functions, which almost behave like those polynomials in certain areas of the domain, for example, functions that describe geoelectric secondary potentials in areas with only small conductivity contrasts.

Finally, adaptive wavelet algorithms have been proven to exhibit optimal work/accuracy rates for a wide scope of problems including types of non-linear problems (Cohen *et al.* 2003b). At present analogous convergence and complexity estimates for such a wide range of problems do not seem to be available for other discretization concepts.

These properties allow the unknown field contained in vector U (eq. 1) to be well approximated with a relatively small number of basis functions (i.e. a wavelet based algorithm has the potential to be computer memory efficient), and the resulting system of equations can be solved with a relatively small number of matrix vector multiplications (i.e. the algorithm has the potential to be efficient in terms of computing time). This holds for many different geophysical problems.

2.3 The adaptive wavelet algorithm

As a first step, the wavelet expansion of the right-hand side vector in eq. (1) is performed using all scaling functions and wavelets up to a specified level l_{\max} . Furthermore, all coefficients of the initial solution vector \tilde{U} are initially set to zero. In the next step, the residual vector $R_{\text{total}} = B_{\text{total}} - A_{\text{total}}\tilde{U}$ (where A_{total} and B_{total} are the operator and the right-hand side expanded in the full wavelet basis) is approximated with an accuracy of η by \tilde{R} , defined as

$$\tilde{R} = \tilde{B} - \tilde{A}\tilde{U}, \quad (7)$$

where \tilde{B} is chosen such that a minimal number of wavelet basis functions is employed (i.e. a minimal number of the associated coefficients are non-zero) and $\|B_{\text{total}} - \tilde{B}\|$ is smaller than $\eta/2$. This procedure is referred to as *coarsening*. Additionally, the matrix-vector product $A_{\text{total}}\tilde{U}$ is approximated, such that a minimum number of wavelet basis functions is employed, and the norm $\|A_{\text{total}}\tilde{U} - \tilde{A}\tilde{U}\|$ is also smaller than $\eta/2$. This procedure is referred to as *adaptive operator application*, which is the most important component of the entire algorithm. More details on coarsening and adaptive operator application are given in Appendix B.

In the next stage of the scheme, the wavelet basis functions associated with non-zero entries in \tilde{B} and $\tilde{A}\tilde{U}$ are assembled in a system of equations

$$\mathbf{A}U = B. \quad (8)$$

This system is solved with an iterative solver. The adaptive wavelet algorithm is proven to converge for certain types of iterative solvers as for example the damped Richardson iteration (see Cohen *et al.* 2003b). For practical reasons we apply the conjugate gradient (CG) algorithm. Although the scheme is not proven to converge on varying sets of basis functions, the CG algorithm shows good results in our examples. CG iterations are carried out, until the ‘CG residual’

$$R^k = B - \mathbf{A}U \quad (9)$$

is reduced by a factor α . Note that all matrix-vector multiplications within the CG algorithm are computed using the *adaptive operator*

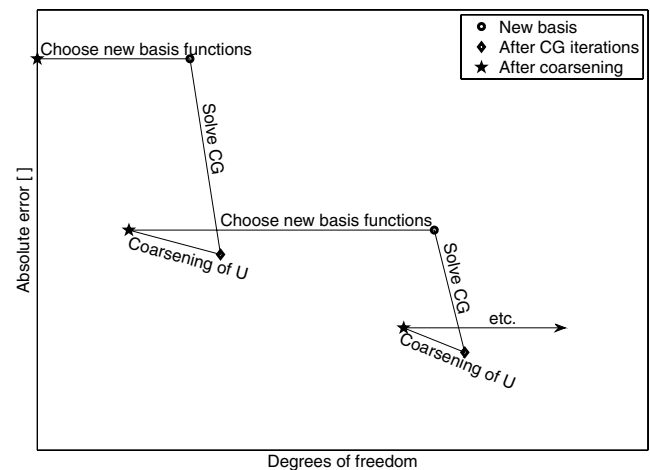


Figure 2. Sketch of two ESC cycles. When choosing new basis functions, the corresponding coefficients are set to zero. Hence, the number of DoF increases while the solution and therefore the error is not affected. During CG-iterations additional basis functions may be added. Therefore an increase in the number of DoF is possible. After coarsening the number of DoF decreases, but the error may increase.

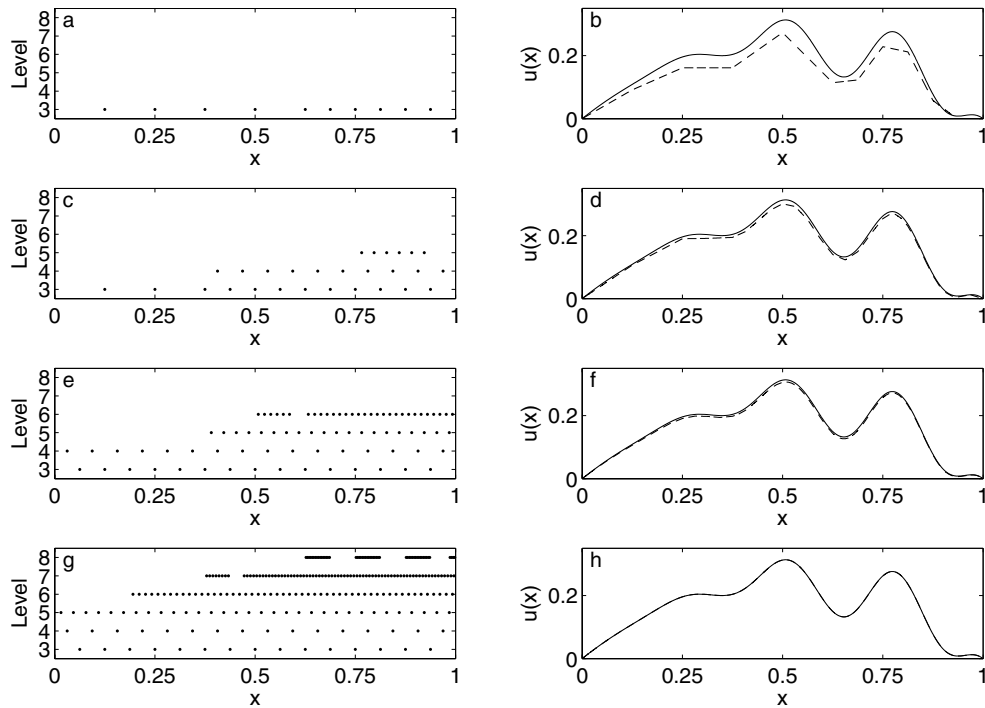


Figure 3. (a), (c), (e), (g) The positions of the wavelets used for the ESC cycles 2, 4, 6 and 8 after coarsening. The scaling functions are not displayed. (b), (d), (f), (h) show the adaptive wavelet solution after ESC cycles 2, 4, 6 and 8 (dashed line) compared to the analytic solution (solid line). Wherever rapid changes in the solution occur, high-level wavelets are needed. In areas, where the analytic solution almost shows linear behaviour, only a small number of wavelets is required.

application as introduced above. As a consequence of that, the wavelet basis may slightly grow during the CG iterations.

Since the matrix A always has a small condition number, which does not exceed a maximum value c_{max} (Cohen *et al.* 2003b), each CG iteration on a fixed set of wavelet basis functions reduces the CG residual by a fixed factor. Hence if the chosen set of wavelets only varies in the first few iteration steps only a fixed, typically small maximum number of CG iterations is required to reach the reduction by a factor of α . This maximum number of CG iterations remains constant during the execution of the entire wavelet algorithm.

Once the residual reduction by α has been achieved, some of the coefficients associated with the solution vector U may be quite small and can thus be eliminated. This is achieved by applying a coarsening on vector U resulting in a new vector \tilde{U} , as described earlier for the right-hand side vector B_{total} . Then the residual R_{total} is approximated again (eq. 7) for a new accuracy $\eta' = 0.5\eta$ and new scaling functions and wavelets are selected. The procedure is repeated until the residual \tilde{R} is acceptably low.

Fig. 2 summarizes the iterative procedure. The vertical axis indicates the true modelling error and the horizontal axis indicates the degrees of freedom (DoF, i.e. the number of scaling functions and wavelets chosen). Here, the error is defined as the average absolute deviation between the true function values (or a numerical reference solution calculated on a very fine mesh using a finite element method) and their approximations determined on a fine sampling grid. The work/accuracy results for such adaptive wavelet schemes refer to error bounds for the approximate solutions with respect to the energy norm (in the present situation to the H^1 -norm, the sum of the square norm of the function and the square norm of its gradient). In our subsequent tests we will, however, monitor averages of pointwise errors as explained above which is not covered by the existing theory and may therefore offer an interesting insight in this

regard. The first horizontal segment of the process curve represents the choice of new coefficients taken from the approximation of the residual \tilde{R} and the subsequent inclined segment indicates the accuracy improvement achieved during the CG iterations. The following coarsening of vector U reduces the number of DoF, but may also result in a small increase of the modelling error. The following segments represent the repeated cycles of

Estimate residual/choose new basis functions—Solve with CG—Coarsening (ESC).

A more extensive description of the algorithm is found in Appendix B and in Cohen *et al.* (2003b). Cohen *et al.* (2003b) also includes the proofs of the following distinctive features of the algorithm:

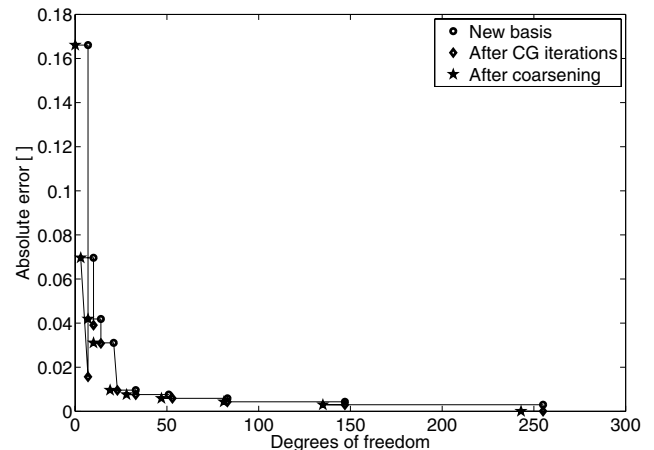


Figure 4. ESC cycles for the simple 1-D example shown in Fig. 3.

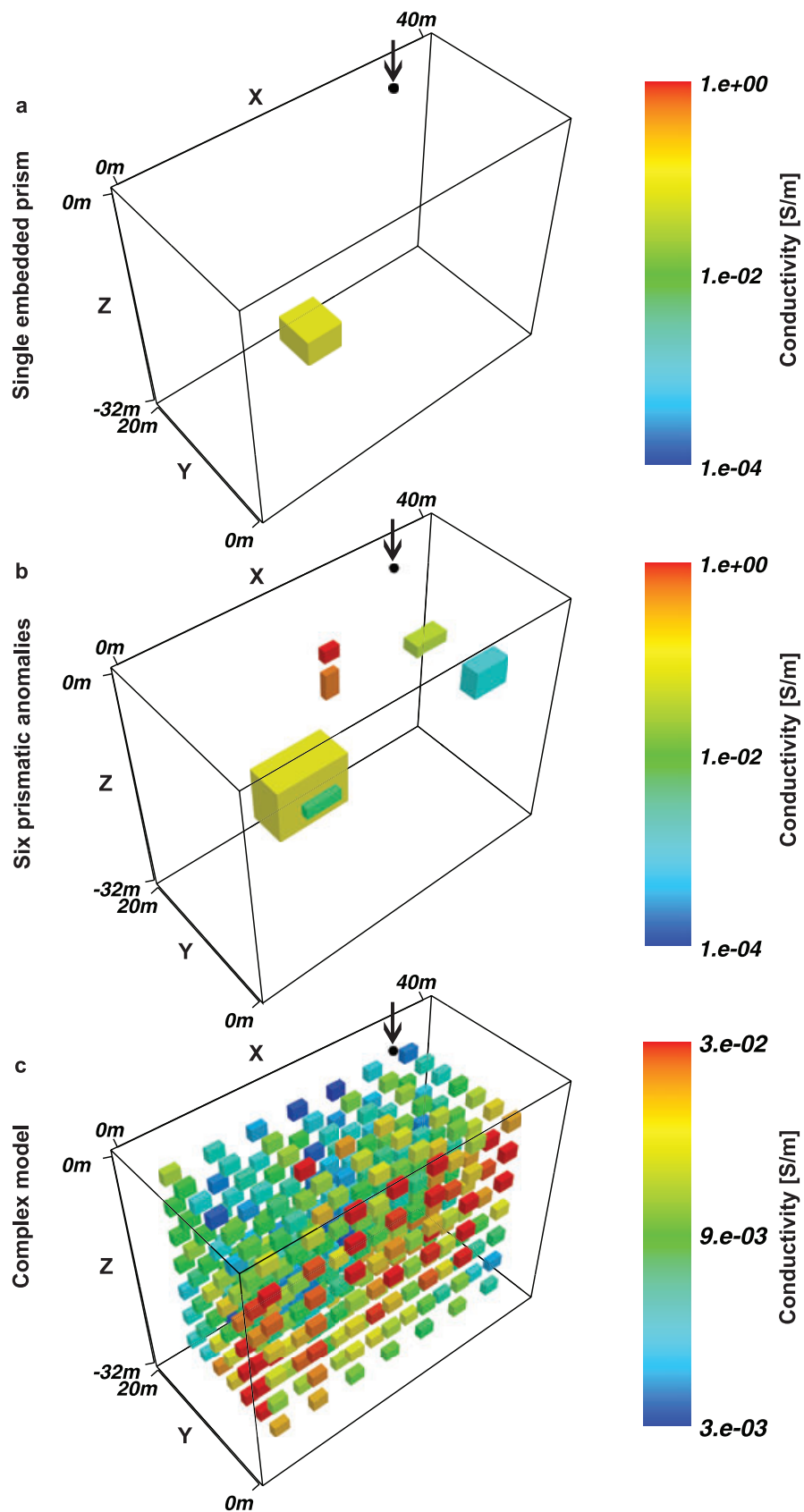


Figure 5. Conductivity models used to test the adaptive wavelet algorithm. The background conductivity is 0.01 S m^{-1} for each model. Source positions are indicated by arrows.

(i) The final number of DoF required is optimal in the sense that it scales linearly with the theoretical minimum number of DoF for a given accuracy (in the energy norm, as described above).

(ii) Memory consumption scales linearly with the final number of DoF. Hence, the sparsity of the system matrix in eq. (1) remains constant.

(iii) The number of scalar operations (i.e. scalar multiplications, including sorting) involved in the algorithm scales linearly with the final number of DoF. Hence, computation time also scales linearly with the final number of DoF.

2.4 A simple example

The functionality of the algorithm is demonstrated using a simple 1-D Laplace problem with zero boundary conditions:

$$\Delta u(x) = f(x), \quad (10)$$

where the function $f(x)$ is chosen such that the solution should be

$$u(x) = [x^2 \sin(7\pi x) - 1](x - 1)x. \quad (11)$$

The left-column panels in Fig. 3 indicate the wavelets chosen within each iteration, whereas the right-column panels show the true (solid line) and approximated (dashed line) solutions. After iteration 2, the true solution is roughly approximated and after four iterations the accuracy is already quite good. Further iterations still improve the accuracy, but the associated error plot in Fig. 4 indicates that the absolute error begins to flatten out. This is due to the reduction of the error by a constant factor: if an error of ε is reached, the error after the next iteration is at most $\beta \varepsilon$ for some fixed $\beta \in (0, 1)$, which may lead to insignificant improvements, if ε is already small.

Note that areas, where the solution shows almost linear behaviour, require a small number of wavelet basis functions, whereas highly non-linear areas lead to a larger number of wavelet basis functions (Fig. 3). This effective compression is caused by the vanishing moments of the wavelet basis.

3 NUMERICAL PERFORMANCE TESTS

We have applied our adaptive wavelet algorithm to a 3-D geoelectric problem on a rectangular prism domain with Neumann boundary conditions on the surface boundary and mixed type boundary conditions along the artificial ground boundaries. Furthermore, singularity removal was applied, that is, eq. (3) is solved.

The algorithm is expected to perform best when the structural complexity of the conductivity distribution in the modelling domain is low. With increasing subsurface complexity, the performance may degrade in terms of number of DoF. In fact, adaptivity shows the best performance when it is applied in order to capture isolated features using only a small number of DoF. Conductivities that exhibit rapid spatial variations across the domain require a fine mesh everywhere, which leads to an almost uniform refinement.

To investigate the behaviour of the algorithm, we have constructed three models of increasing complexity. The first model consists of a homogeneous background conductivity (0.01 S m^{-1}) with a single prismatic anomaly (0.1 S m^{-1} , Fig. 5a). The second model comprises six prismatic anomalies of different sizes and shapes (Fig. 5b). Conductivities lie between 0.001 and 1 S m^{-1} . The third model includes 343 equally sized blocks of stochastically distributed conductivities between 0.003 and 0.08 equally distributed in a homogeneous background medium (Fig. 5c). For all computations we considered a single current injection point located at $(30, 15, 0)$ (indicated by the arrows in Figs 5a–c).

In order to assess the performance of the adaptive wavelet algorithm and to show improvements compared to widely used algorithms in the geophysical community, we additionally computed the response of the three models in Fig. 5 using the non-adaptive finite element code B2009 as described in Blome *et al.* (2009). This finite element code is representative of the current state-of-the-art in geoelectric modelling. It employs unstructured meshes and a direct matrix solver. To make the results more comparable with the adaptive wavelet algorithm, we substituted the direct matrix solver of Blome *et al.* (2009) with a conjugate gradient solver using SSOR pre-conditioning (as is used in Spitzer 1995, for the finite difference method). For this type of problems, direct and CG solvers provide a similar accuracy, when sufficient iterations are performed. Reference solutions were computed with the B2009 algorithm using a very large number of elements (1.5 million DoF). The modelling error was determined by interpolating the adaptive wavelet algorithm solution on the fine mesh of the reference solution and computing the average absolute deviation with respect to the reference solution.

Fig. 6 depicts the ESC cycles for the computations with the 3 models shown in Fig. 5. Additionally, the absolute errors of the B2009 algorithm are plotted as a function of the number of DoF. CG iterations were carried out for the B2009 finite element algorithm until the CG residual reached 10^{-9} , which is well below the actual modelling error. As expected, the performance of the adaptive wavelet algorithm is excellent for the simple single embedded prism model (Fig. 6a). After only 3 ESC cycles the absolute

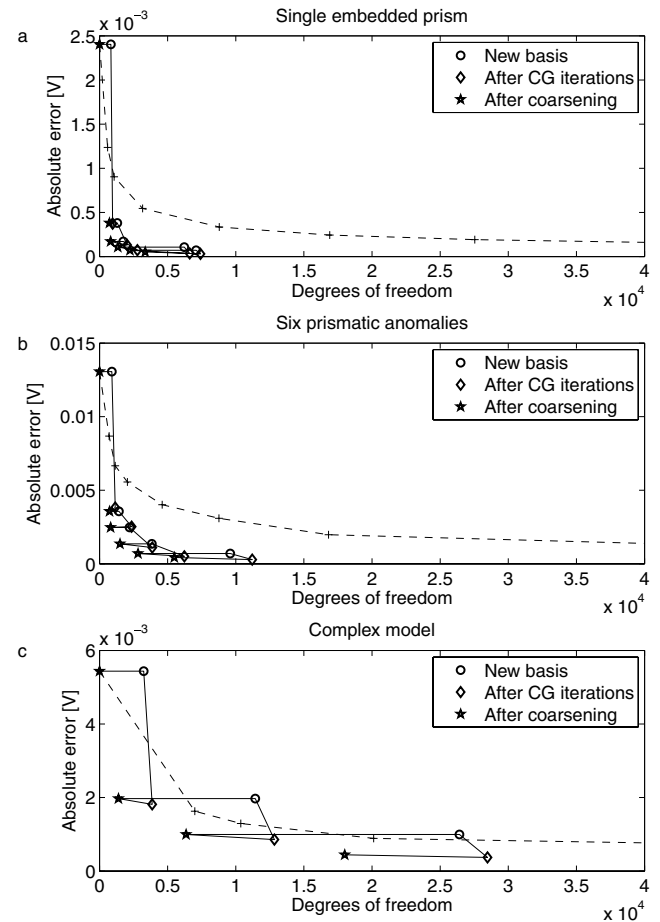


Figure 6. ESC cycles for the 3-D geoelectric models (solid line) together with solutions using the B2009 finite element algorithm (dashed line), which represents the state-of-the-art in geoelectric modelling.

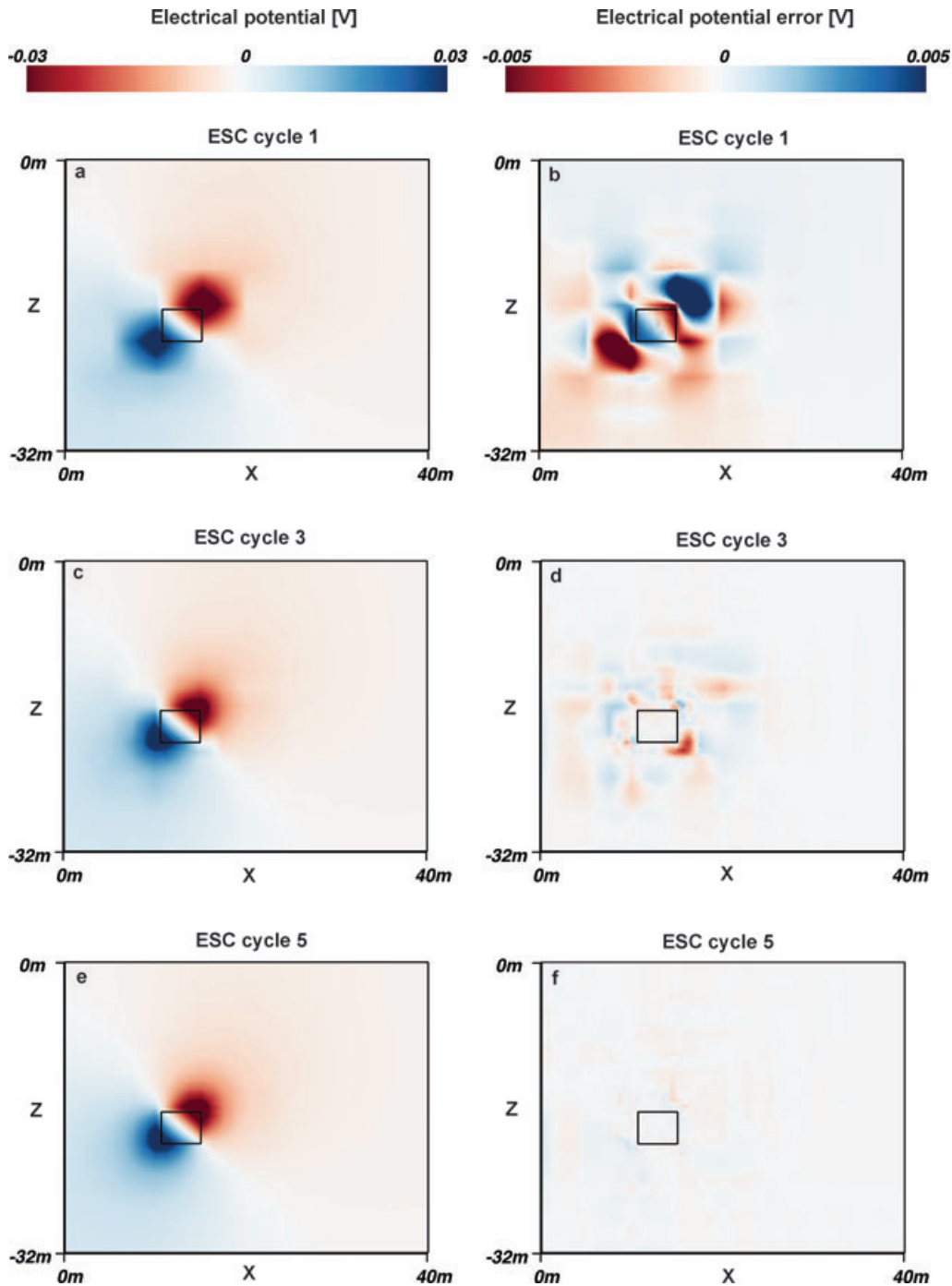


Figure 7. (a), (c), (e) Slices through the centre of the prismatic anomaly in the single embedded prism model for ESC cycles 1, 3 and 5. (b), (d), (f) Slices through the centre of the prismatic anomaly for the difference to the FEM reference solution computed with 1.5 million DoF for ESC cycles 1, 3 and 5.

error is at about 10^{-4} , which is well below the error of the B2009 solution with a comparable number of DoF. To achieve the same accuracy with the B2009 algorithm, roughly twenty times more DoF would be required. Similar results were also obtained for the model with six prismatic anomalies (Fig. 6b). For the most complex model (Fig. 6c) the performance of the adaptive wavelet algorithm in terms of number of degrees of freedom degrades (as expected) and becomes comparable to the B2009 finite element algorithm. Nevertheless, the adaptive method guarantees a desired accuracy. If even more complex models would be considered, the performance of the adaptive wavelet algorithm may further degrade during the

first ESC cycles. In such situations homogenization or other upscaling techniques may be required.

Besides this overall measure of accuracy (vertical axis in Fig. 6), it is also instructive to observe how the errors are distributed within the modelling domain. For that purpose we plotted slices through the adaptive wavelet solutions (only the secondary potentials arising from the anomalous prism are displayed) using the single prismatic anomaly model after completion of ESC cycles 1, 3 and 5 (Fig. 7). Additionally, the corresponding differences to the reference solution are displayed. After the first cycle, the solution is rather blocky, since it only considers scaling functions and low-level wavelets.

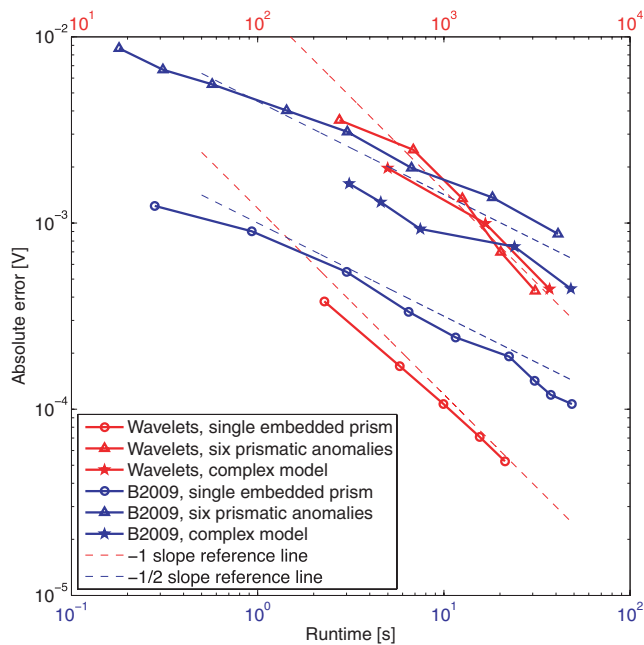


Figure 8. Error versus time slopes for the adaptive wavelet algorithm (red lines) and the B2009 finite element algorithm (blue lines) for the three models Fig. 5(a) (circles), Fig. 5(b) (triangles) and Fig. 5(c) (stars).

Nevertheless, it already captures the most important features of the bipolar secondary field created by the prismatic anomaly. After ESC cycle 3, the solution improves significantly, and after ESC cycle 5 the relative errors become negligibly small.

As seen for the simple 1-D example in Fig. 3, an excellent approximation of the solution is already achieved with a few low-level wavelet basis functions in areas where the solution shows almost linear behaviour (away from the conductivity contrasts). Close to the contrast, a number of higher-level wavelet basis functions is required in order to accurately represent the solution.

Results in Fig. 6 demonstrate the memory efficiency of the adaptive wavelet algorithm. That is, a high accuracy can be achieved with a small number of DoF. Fig. 8 illustrates the other important property of the numerical algorithm—its computing time efficiency. In Fig. 8, we plot in log-log form the modelling error as a function of the computing time. Computing time is not only a function of the inherent performance of an algorithm, but also largely depends on the efficiency of its implementation. The B2009 finite element algorithm is based on highly optimized finite element and BLAS libraries, whereas our adaptive wavelet code is still experimental and needs to be optimized in terms of its implementation. Here, we are primarily interested in the decline of the modelling error as a function of computing time and have therefore plotted the adaptive wavelet curves with a shifted time axis such that they can be compared easily with the corresponding B2009 curves. The most important observation in Fig. 8 is that all adaptive wavelet curves exhibit a slope of approximately -1 , thereby indicating that the accuracy improvements scale linearly with computing time. This behaviour was predicted theoretically in Cohen *et al.* (2003b). By contrast, the B2009 curves have a slope of approximately $-1/2$, which indicates that the modelling accuracy scales with the computing time squared.

Initially, the slopes of Fig. 8 deviate from -1 . This is caused by parametrization of the conductivity model, which has a higher spatial resolution than the initially applied large-support wavelet

basis functions (the scaling functions and the low-level wavelets). Therefore, the computation of the system matrix entries needs to be conducted with a higher resolution than required for the wavelet basis functions. However, it can be observed that as soon as the wavelet resolution reaches the conductivity model resolution, a linear decrease of the error is achieved. This does not have a strong effect on the overall computation time, since this only applies to the first few steps, where computations of the single ESC cycles are very fast.

It is also instructive to compare the relative vertical shifts of the individual curves. The adaptive wavelet curves for the six prismatic anomalies model and the complex model lie on top of each other, whereas the six prismatic anomalies curve for the B2009 algorithm lies well above the corresponding complex model curve. This is most likely the result of the optimal pre-conditioning in the wavelet basis. The computational time of the adaptive wavelet algorithm does not depend on the magnitudes of the contrasts but only on their geometrical distribution and hence the number of wavelets needed to approximate the solution. In contrast, the non-adaptive B2009 computation time does not so much depend on the geometry of the conductivity contrasts but mostly on their magnitudes, since this strongly affects the condition number of the system of equations in eq. (1). Hence the adaptive wavelet algorithm is highly efficient, when the model complexity is low. Although the adaptive wavelet algorithm shows a decrease in efficiency in terms of number of DoF when the models are more complex, its slope of -1 still leads to superior performance compared to the B2009 method for higher accuracies.

4 DISCUSSION AND CONCLUSIONS

Using the example of 3-D geoelectric forward modelling we have demonstrated the capabilities and limitations of adaptive wavelet algorithms with optimal work/accuracy rate, a novel technique that was proposed recently in the mathematical literature. To the best of our knowledge this is the first application of such techniques to a geophysical problem. From our calculations we observe the following.

- (i) The adaptive wavelet algorithm with optimal work/accuracy rate together with singularity removal is a powerful method for geoelectric modelling.
- (ii) The error convergence rate is also good in the discrete L_1 -norm, which has not yet been covered by the theory.
- (iii) The performance in terms of memory consumption and time-versus-error rate is superior to the common methods currently applied in geoelectric modelling.
- (iv) General features of adaptive methods offer scope for further developments.

Future research should focus on an optimized implementation of adaptive wavelet algorithms with optimal work/accuracy rate. During the past few decades, probably a 1000 person years or even more have been dedicated to the optimization of finite element codes, while wavelet codes are still in an experimental stage and thus far away from optimality. Fully exploiting the memory and computing time efficiency of adaptive wavelet solvers will undoubtedly lead to substantial improvements in geophysical modelling.

This could be good news for those concerned with the challenging seismic modelling problem. With the increasing popularity of seismic waveform inversions, there is an urgent need for efficient modelling algorithms. Conceptually, adaptive wavelet algorithms

are well suited for acoustic and elastic waveform modelling problems in the frequency domain, but care should be taken with the choice of the right-hand side in eq. (2) (source term) that must have an appropriate smoothness, which is dictated by the corresponding function space. This may require application of singularity removal techniques to the governing differential equations.

An important difference between potential field problems, as discussed in this paper, and wavefield problems, such as seismic waveform modelling, concerns the spatial variability of the fields. Particularly at high frequencies, seismic modelling may require a large number of degrees of freedom to be considered. In fact, our computations for the complex model (Fig. 5c) demonstrate that in such a case there are little benefits with regard to memory consumption (Fig. 6c). However, even when a large number of degrees of freedom must be considered, our algorithm is still beneficial in terms of computing time, as it is demonstrated in Fig. 8.

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APPENDIX A: WAVELETS

A1 More on 1-D wavelet basis functions

The 1-D scaling functions and wavelets considered in this appendix are confined to powers of the unit interval $[0, 1]$, but extensions to other intervals can be achieved by shifting and dilation. The wavelet basis functions on the inside of the interval are described with eqs (5) and (6) in Section 2.2. At the boundaries 0 and 1, the following functions are used

$$\varphi_{l,0}(x) = \begin{cases} 2^{\frac{3l}{2}}(2^{-l} - x) & \text{if } 0 \leq x \leq 2^{-l} \\ 0 & \text{elsewhere} \end{cases} \quad (\text{A1})$$

and

$$\varphi_{l,2^l}(x) = \begin{cases} 2^{\frac{3l}{2}}(x + 2^{-l} - 1) & \text{if } 1 - 2^{-l} \leq x \leq 1 \\ 0 & \text{elsewhere,} \end{cases} \quad (\text{A2})$$

for the scaling functions and

$$\psi_{l,1} = \frac{1}{\sqrt{2}} \left(-\frac{3}{4}\varphi_{l+1,0} + \frac{9}{16}\varphi_{l+1,1} + \frac{1}{8}\varphi_{l+1,2} - \frac{1}{16}\varphi_{l+1,3} \right) \quad (\text{A3})$$

and

$$\psi_{l,2^l} = \frac{1}{\sqrt{2}} \left(-\frac{1}{16}\varphi_{l+1,2^{l+1}-3} - \frac{1}{8}\varphi_{l+1,2^{l+1}-2} + \frac{9}{16}\varphi_{l+1,2^{l+1}-1} - \frac{3}{4}\varphi_{l+1,2^l} \right), \quad (\text{A4})$$

for the wavelets (Cohen *et al.* 1992; Dahmen *et al.* 1999).

$V_l^{1D} : \text{span}(\varphi_{l,k} \mid 0 \leq k \leq 2^l)$ is the vector space of all possible linear combinations of the scaling functions at level l and $W_l^{1D} : \text{span}(\psi_{l,k} \mid 1 \leq k \leq 2^l)$ is the vector space of all possible linear combinations of the wavelets at level l . They are related as follows:

$$\dots \subset V_2^{1D} \subset V_3^{1D} \subset V_4^{1D} \subset \dots, \quad (\text{A5})$$

$$W_l^{1D} \subset V_{l+1}^{1D} \text{ and } V_{l+1}^{1D} = V_l^{1D} \oplus W_l^{1D}. \quad (\text{A6})$$

These piecewise linear wavelets have the advantage that they are very simple to handle within integrals. Furthermore, they are not orthogonal (not required for our algorithm) but biorthogonal (Cohen *et al.* 1992).

A2 Wavelet basis functions in two and more dimensions

Tensor product constructions can be used for creating higher-dimensional wavelet basis functions (Dahmen & Schneider 1999). The tensor product of a function $f(x)$ with a function $g(y)$ is defined as

$$(f \otimes g)(x, y) := f(x)g(y). \quad (\text{A7})$$

The tensor product of two function spaces V and W is the linear span of all tensor products of functions in V with functions in W . Note that in general $f \otimes g \neq g \otimes f$. We use this definition to create wavelet basis functions in two dimensions. 2-D scaling functions are identified with three parameters: level l , shift in x -direction k_x and shift in y -direction k_y . The scaling functions $\varphi_{l,k_x,k_y}(x, y)$ are defined as

$$\begin{aligned} \varphi_{l,k_x,k_y}(x, y) &:= (\varphi_{l,k_x} \otimes \varphi_{l,k_y})(x, y) \\ &= \varphi_{l,k_x}(x)\varphi_{l,k_y}(y). \end{aligned} \quad (\text{A8})$$

We denote the 2-D scaling functions by $V_l^{2D} := \text{span}(\varphi_{l,k_x,k_y} \mid 0 \leq k_x \leq 2^l \text{ and } 0 \leq k_y \leq 2^l)$. Wavelets in two dimensions are the complement of V_l^{2D} in V_{l+1}^{2D} . Using $V_l^{2D} = V_l^{1D} \otimes V_l^{1D}$ we get

$$\begin{aligned} V_{l+1}^{2D} &= V_{l+1}^{1D} \otimes V_{l+1}^{1D} = (V_l^{1D} \oplus W_l^{1D}) \otimes (V_l^{1D} \oplus W_l^{1D}) \\ &= (V_l^{1D} \otimes V_l^{1D}) \oplus (V_l^{1D} \otimes W_l^{1D}) \oplus \\ &\quad \oplus (W_l^{1D} \otimes V_l^{1D}) \oplus (W_l^{1D} \otimes W_l^{1D}). \end{aligned} \quad (\text{A9})$$

Hence

$$\begin{aligned} W_l^{2D} &= (V_l^{1D} \otimes W_l^{1D}) \oplus (W_l^{1D} \otimes V_l^{1D}) \oplus \\ &\quad \oplus (W_l^{1D} \otimes W_l^{1D}). \end{aligned} \quad (\text{A10})$$

Therefore the wavelets in two dimensions consist of functions of the shape $\varphi_{l,k_x}(x)\psi_{l,k_y}(y)$, $\psi_{l,k_x}(x)\varphi_{l,k_y}(y)$ and $\psi_{l,k_x}(x)\psi_{l,k_y}(y)$. Wavelet bases in higher dimensions can be constructed accordingly.

APPENDIX B: THE ADAPTIVE WAVELET ALGORITHM

In this Appendix, we give an overview of the implementation of our algorithm that largely follows Cohen *et al.* (2003b). For more details, we therefore refer to the Cohen *et al.* (2003b) paper and the references contained therein. For practical reasons, we have replaced the damped Richardson iteration in Cohen *et al.* (2003b) by a CG method.

The algorithm depends on a set of parameters, which we will describe briefly. The coefficient β estimates the ratio of the absolute error between a given approximation U of the solution U_{total} and the estimated residual of U depending on the underlying problem and the chosen iterative solver (here CG). C^* controls the $\mathcal{A}_{\text{tree}}^s$ -norms of the resulting vector after the coarsening, where $\mathcal{A}_{\text{tree}}^s$ -norm is a measure for the approximability of a vector by small trees. The parameter γ , which plays an important role in the adaptive operator approximation describes the wavelet compressibility of the operator. The parameter $\bar{\rho} \in (0, 1)$ and the summable sequence of parameters $\{\omega_k\}_{k=0}^{\infty}$ can be freely chosen. They influence the computation time and the memory consumption but do not influence the linear work/accuracy rate. Note that these parameters are adapted to the damped Richardson iteration and no mathematical proof exists for the application of the CG method. In our case, we set $\beta = 100$, $C^* = 2$, $\gamma = 7$, $\bar{\rho} = 0.95$, $\omega_k = 0.9^k$.

Sets of wavelet basis functions (which in this algorithm always form a tree) are denoted with Λ . We write $\tilde{\Lambda}_n$ for sets of newly

acquired functions, Λ_n for the sets after the CG-iterations and $\tilde{\Lambda}_n$ for the coarsened sets. The associated vectors of coefficients are denoted by B for the right-hand side, U for the solution and R for the approximation of the residual, where the index set is indicated in the subscript.

Algorithm AdaptiveSolve (ε)

Input: desired accuracy

Output: Optimal set of functions Λ_{opt} , solution $U_{\Lambda_{\text{opt}}}$

(* Main algorithm *)

1. Calculate the wavelet expansion of the right-hand side

$$\sum_{\lambda \in \Lambda_{\text{full}}} b_\lambda \phi_\lambda$$
2. Set $B_{\Lambda_{\text{full}}} = (b_\lambda)_{\lambda \in \Lambda_{\text{full}}}$
3. Set $n = 0$; $\tilde{\Lambda}_0 = \emptyset$; $\tilde{U}_{\tilde{\Lambda}_0} = 0$
4. Set $\varepsilon_0 = \|B_{\Lambda_{\text{full}}}\|_2$
5. **while** $\varepsilon_n > \varepsilon$
6. **do** Set $n = n + 1$
7. $[\tilde{\Lambda}_n, \tilde{R}_{\tilde{\Lambda}_n}] = \text{EstimateResidual}$
 $(\tilde{\Lambda}_{n-1}, \tilde{U}_{\tilde{\Lambda}_{n-1}}, B_{\Lambda_{\text{full}}}, \omega_0 \varepsilon_{n-1})$
8. $[\Lambda_n, U_{\Lambda_n}] = \text{SolveCG}(\tilde{\Lambda}_n, \tilde{U}_{\tilde{\Lambda}_{n-1}}, \tilde{R}_{\tilde{\Lambda}_n}, \varepsilon_{n-1})$
9. $[\tilde{\Lambda}_n, \tilde{U}_{\tilde{\Lambda}_n}] = \text{Coarse}(U_{\Lambda_n}, \varepsilon_{n-1} C^*/(2 + 2C^*))$
10. Set $\varepsilon_n = \varepsilon_{n-1}/2$
11. **return** $\Lambda_{\text{opt}} = \tilde{\Lambda}_n$; $U_{\Lambda_{\text{opt}}} = \tilde{U}_{\tilde{\Lambda}_n}$

The three steps *EstimateResidual*, *SolveCG* and *Coarse* correspond to the ESC steps described in Section 2.3. The subroutine *EstimateResidual* is defined as

Algorithm EstimateResidual ($\tilde{\Lambda}_{n-1}, \tilde{U}_{\tilde{\Lambda}_{n-1}}, B_{\Lambda_{\text{full}}}, \varepsilon_{n-1}$)

Input: Set of functions, solution, right-hand side, desired accuracy

Output: Set of functions $\tilde{\Lambda}_n$, Approximation of the residual, $\tilde{R}_{\tilde{\Lambda}_n}$

(* Approximates the residual *)

1. $[\Lambda_1, V] = \text{ApplyOperator}(\tilde{U}_{\tilde{\Lambda}_{n-1}}, 0.5\omega_0\varepsilon_{n-1})$
2. $[\Lambda_2, W] = \text{Coarse}(B_{\Lambda_{\text{full}}}, 0.5\omega_0\varepsilon_{n-1})$
3. **return** $\tilde{R}_{\tilde{\Lambda}_n} := V - W$ and $\tilde{\Lambda}_n :=$ Those functions in $\Lambda_1 \cup \Lambda_2$, for which $V - W$ has non-zero entries

In this subroutine the function *ApplyOperator*, which approximates the application of the operator to the current solution with the given accuracy is the core ingredient of the adaptive wavelet algorithm. Since the application of the operator cannot be computed (this would result in a multiplication of a rectangular infinite matrix with a finite vector), it needs to be approximated. The approximation is conducted by first setting up a tree of wavelet basis functions for which the coefficients will approximate the application with the desired accuracy (see Cohen *et al.* 2003a, theorem 3.4 and the related construction of the tree), then calculating the coefficients using the fast top-down evaluation scheme described in Dahmen

et al. (2000). Before the approximation is calculated, a diagonal pre-conditioner $d_i = 1/\sqrt{a_{ii}}$ is applied, where a_{ii} are the diagonal entries of the system matrix A in eq. (8). This ensures an optimal condition number (Cohen & Masson 1999). Here, ‘optimality’ indicates that the condition number of the pre-conditioned system matrix is bounded for all detail levels. Hence all solutions using a CG algorithm on a fixed basis can be calculated up to a given accuracy using a fixed (small) number of CG iterations. Other possibilities of optimal pre-conditioning can be found in Cohen & Masson (1999).

The subroutine *SolveCG* is set up as

Algorithm SolveCG ($\tilde{\Lambda}_n, \tilde{U}_{\tilde{\Lambda}_{n-1}}, \tilde{R}_{\tilde{\Lambda}_n}, \varepsilon_{n-1}$)

Input: Set of functions, previous solution, approximated residual of the previous solution, desired accuracy

Output: Set of functions Λ_n , solution U_{Λ_n} ,

(* Modified conjugate gradient solver *)

1. Set $k = 0$; $\Lambda^0 = \tilde{\Lambda}_n$; $U^0 = \tilde{U}_{\tilde{\Lambda}_{n-1}}$
2. Set $P^k = \tilde{R}_{\tilde{\Lambda}_n}$; $R^k = -\tilde{R}_{\tilde{\Lambda}_n}$
3. **while** $\omega_k \bar{\rho}^k \varepsilon_{n-1} + \|R^k\|_2 > \varepsilon_{n-1}/((2 + 2C^*)\beta)$
4. **do** Set $k = k + 1$
5. $[\Lambda^k, V] = \text{ApplyOperator}(P^{k-1}, 0.5\omega_k \bar{\rho}^k \varepsilon_{n-1})$
6. $U^k = U^{k-1} + \frac{(R^{k-1}, R^{k-1})}{(P^{k-1}, V)} P^{k-1}$
7. $R^k = R^{k-1} + \frac{(R^{k-1}, R^{k-1})}{(P^{k-1}, V)} V$
8. $P^k = \frac{(R^k, R^k)}{(R^{k-1}, R^{k-1})} P^{k-1} - R^k$
9. **return** $\Lambda_n = \Lambda^k$; $U_{\Lambda_n} = U^k$

This routine is a generic conjugate gradient solver (e.g. Shewchuk 1994), except that the application of the operator restricted to $\tilde{\Lambda}_n$ is replaced by the function *ApplyOperator* described above.

In the function *Coarse* an as large as possible number of coefficients is removed from the given vector, such that the norm of the difference from the initial vector is smaller than a prescribed value $0.5\omega_0\varepsilon_{n-1}$. Additionally, the tree structure is preserved. An exact description of this procedure can be found in Binev & DeVore (2004).

Optimality is achieved by keeping the number of scalar operations linear with the number of wavelet basis functions in the routines *ApplyOperator* and *Coarse*. Since the condition number of the diagonally pre-conditioned operator in the wavelet basis is always smaller than c_{max} , the number of iterations inside the *SolveCG* routine does not exceed a maximum number K if the basis does not vary after the first few steps. Because each ESC cycle leads to an error reduction by a constant factor, only a fixed maximum number of iterations is required to reach a given target accuracy. Therefore, the number of total scalar operations scales linearly with the final number of degrees of freedom.