Integral equation solver based on high-order polynomial basis

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Summary

The first-ever "high-order" solver for the volumetric integral equations (IE) of electrodynamics is presented. In contrast to previous IE solvers based on a piece-wise constant approximation of the fields inside an anomaly, the novel solver is based on a piece-wise polynomial representation. Further the utilization of Galerkin method for constructing the system of linear equations not only provides the guaranteed convergence of the iterative numerical solution, but also ensures that the system matrix is well-conditioned irrespective of the polynomials order. Computational experiments demonstrate that the new approach allows to decrease the number of unknowns by more than one order of magnitude, with corresponding speed up and memory saving.

Keywords: Integral equations, Forward modeling, Galerkin method, High-order basis

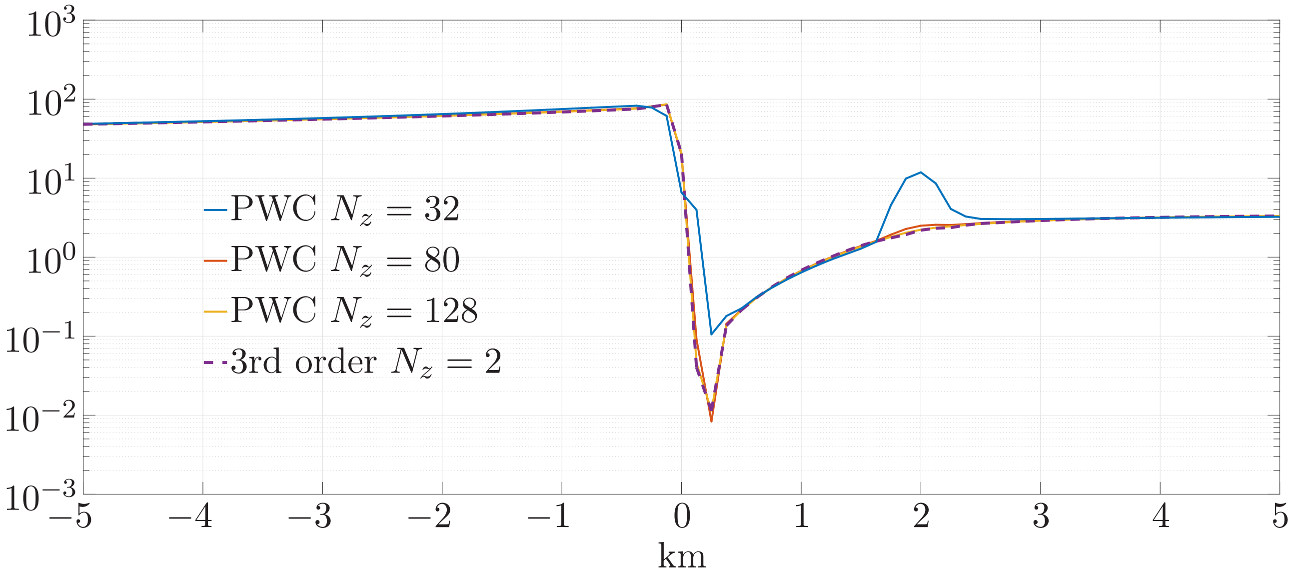

Figure 1: Apparent resistivity ρ_{xy} (at frequency 10^{-3} Hz) along profile shown in Fig 2a. Solid (blue, red and yellow curves) are the results obtained with the use of piece-wise constant (PWC) IE solver. The colors distinguish between the results of modelings with different number of cells in vertical direction N_z. Dashed curve stands for the results obtained with the use of the presented high-order IE solver. See details in the text.

Introduction

Three-dimensional (3-D) electromagnetic (EM) studies of the Earth, from the near surface to regional and global, have significantly advanced over the past decade. However still 3-D EM simulations — which are a core part of any 3-D interpretation — with realistic levels of complexity, accuracy and spatial detail remain challenging from the computational point of view. Note, that in this work we discuss a frequency domain problem set up. There exist two main approaches for simulating 3-D EM field: solving the boundary problem for Maxwell's equations, and solving the corresponding volumetric integral equations (IE). These problems are equivalent in terms of solution existence and uniqueness, but the numerical methods used for respective problems are rather different. In particular, for the boundary problem one uses finite-differences (FD) or finite-elements (FE) methods.

The main differences between FD (Egbert & Kelbert, 2012; Jaysaval et al., 2015; Mackie et al., 1994, among others) or FE (Börner, 2010; Grayver & Kolev, 2015; Ren et al., 2013, among others), and IE (Avdeev et al., 2002; Kruglyakov et al., 2016, among others) methods is that in the IE methods one works with compact system matrices. The reason for compactness is that boundary conditions are exactly accounted for via Green's functions, and thus the modeling region is confined only to 3-D conductivity structures (anomalies) under investigations. Note that typical 3-D models consist of a number of 3-D anomalies embedded in a 1-D background media. By contrast, in the FD/FE methods one has to discretize a much larger volume both laterally and vertically in order to enable the decay (or stabilization) of the EM field at the boundaries of the modeling domain. However, this advantage is counterbalanced by the fact that IE matrices are dense whereas the FD or FE matrices are sparse. Another distinction between methods is that the condition number (which controls stability of the solution) of the resulting matrices in the FD or FE approaches depends on discretization and frequency, whereas in the IE approach — practically does not. On the other hand, the FE methods much easier treat models with topography or/and bathymetry. All aforementioned merits and disadvantages of the methods in some sense compensate each other and until recently both approaches demonstrated comparable efficiency in terms of accuracy and required computational resources. Note also, that until recently all methods have been based on the piece-wise constant approximation to describe the EM field behavior, however it was well understood that the usage of piece-wise polynomial approximation is an attractive alternative.

The idea to use high-order polynomials in the FE methods was proposed more than 30 years ago, but the challenges of actual implementation have been overcome only in the last years thanks to advent of elegant and surprisingly efficient preconditioning schemes. It was shown recently (Grayver & Kolev, 2015) that the usage of second or third order polynomials in FE-based software allows to decrease the number of unknowns by 10-100 times compared with the FE formulation based on piece-wise constant approximation, and thus dramatically speeds up the simulations.

In the mean time the developers of IE-based solvers were focused on overcoming the challenges of IE modeling such as relaxing the memory requirements (Kruglyakov & Bloshanskaya, 2017), implementation of effective parallelization schemes, and more accurate calculation of matrix coefficients (Kruglyakov et al., 2016), among others. These challenges have been successfully resolved and allowed to achieve very good agreement between the results obtained with high-order FE modeling and novel IE solvers even for high-contrast models (Kruglyakov & Bloshanskaya, 2017). However it should be mentioned that the difference in the computational resources needed for FE and IE modelings was dramatic, and not in favor of IE technique. Those results clearly showed the necessity to move from piece-wise constant to high-order approximation in IE modeling.

A concept

Let us consider an integral equation formulation of EM problem in following operator form

$$\mathbf{E} - \mathrm{G_E}\,\Delta_\sigma \mathbf{E} = \mathbf{E}^b, \tag{1}$$

where $\mathbf{E}$ is the unknown total electric field in the anomalous domain Ω, i.e. in the domain with 3-D distribution of conductivity $\sigma_a(x,y,z)$, $\mathbf{E}^b$ is the background field, i.e. the field from the same source but in the 1-D background media, $\sigma_b(z)$ is the conductivity of this background media, $\Delta_\sigma = \sigma_a - \sigma_b$, and $\mathrm{G_E}$ is the "electric" Green operator., i.e "electric" fundamental solution of Maxwell's equation in 1-D background media. Let us further suppose that domain Ω is split into $N = N_x N_y N_z$ non-overlappping rectangular cells $\bigcup_{n=1}^{N} \Omega_n = \Omega$; $N_{x,y,z}$ is the number of cells in X, Y, Z direction respectively. For every cell Ω_n the local basis functions $\Psi_n^{n_x,n_y,n_z}(x,y,z)$ are introduced as follows

$$\begin{aligned}\Psi_n^{n_x,n_y,n_z}(x,y,z) =& P_{n_x}\left(2\frac{x-x^n}{h_x^n}-1\right)\times \\ & P_{n_y}\left(2\frac{y-y^n}{h_y^n}-1\right)\times \\ & P_{n_z}\left(2\frac{z-z^n}{h_z^n}-1\right)\end{aligned} \tag{2}$$

where, P_m is the normalized Legendre polynomial of the m-th order, h_x^n, h_y^n, and h_z^n are the sizes of Ω_n in x,y,z dimensions correspondingly, and x^n, y^n, z^n are the coordinates of the corner of Ω_n, $n_x, n_y, n_z = 0 \dots N_p$, and N_p is maximum polynomial order. It is trivial to show that functions $\Psi_n^{n_z,n_y,n_z}$ are orthogonal in terms of $\mathrm{L}_2[\Omega_n]$ dot product, because of orthogonality of Legendre polynomials.

Let vector functional space W be a span of vectors $\mathbf{\Psi} = (\Psi_x, \Psi_y, \Psi_z)$, where $\Psi_{x,y,z}$ are the ones of $\Psi_n^{n_x,n_y,n_z}$. Then for the fixed discretization $\{\Omega_n\}$ and polynomial order N_p we define a projection operator

$\mathrm{P_{N,N_p}}$ from $\mathrm{L}_2[\Omega]$ to W as follows

$$(\mathrm{P_{N,Np}}\,\mathbf{V})_\alpha = \sum_{n=1}^{N}\sum_{n_x,n_y,n_z=1}^{N_p} V_\alpha^{n,n_x,n_y,n_z}\Psi_n^{n_x,n_y,n_z},$$
$$V_\alpha^{n,n_x,n_y,n_z} = \int_{\Omega_n} V_\alpha(x,y,z)\Psi_n^{n_x,n_y,n_z}(x,y,z)dxdydz,$$
$$\mathbf{V} = (V_x, V_y, V_z) \quad \alpha \in x,y,z \tag{3}$$

Following the Galerkin approach, we apply operator $\mathrm{P_{N,N_p}}$ to (1) and obtain integral equation with respect to $\mathbf{U}$ in space W

$$\begin{aligned}&\mathbf{U} - \mathrm{P_{N,N_p}}\,\mathrm{G_E}\,\Delta_\sigma\mathbf{U} = \mathbf{U}^b,\\ &\mathbf{U}^b = \mathrm{P_{N,N_p}}\,\mathbf{E}^b.\end{aligned} \tag{4}$$

The first equation in (4) is nothing but the system of linear equations for expansion coefficients U_α^{n,n_x,n_y,n_z}, where the coefficients of system matrix K are the double volumetric integrals of the multiplication of Green's tensor components and functions $\Psi_n^{n_x,n_y,n_z}$

$$\begin{aligned}&\hat{K}_{n,k} = \int_{\Omega_n}\int_{\Omega_k} \Psi_n^{n_x,n_y,n_z} G_{\alpha\beta}\Psi_k^{k_x,k_y,k_z}dv_n dv_k,\\ &\alpha,\beta \in \{x,y,z\}.\end{aligned} \tag{5}$$

Here $G_{\alpha\beta}$ are the components of Green's tensor, and $\hat{K}_{n,k}$ are the $3N_p$-th order sub-matrices of K.

Using solution of the (4) one obtains the following formulas for the total EM field in any point $M \in \mathrm{R}^3$

$$\begin{aligned}&\mathbf{E} = \mathbf{E}^b + \mathrm{G_E}\,\Delta_\sigma\mathbf{U},\\ &\mathbf{H} = \mathbf{H}^b + \mathrm{G_H}\,\Delta_\sigma\mathbf{U}.\end{aligned} \tag{6}$$

Here $\mathrm{G_H}$ is the "magnetic" Green operator., i.e "magnetic" fundamental solution of Maxwell's equation in 1-D background media. Note, that in contrast to the high-order FE methods, the condition number of system matrix in (4) is independent of the polynomials order.

Main computational challenges

The main challenges of any IE method are the computation of matrix coefficients (5), and the matrix storage. These challenges have been addressed by using the ideas from (Kruglyakov & Bloshanskaya, 2017). The integrals in vertical direction are computed analytically, whereas for the horizontal integration the special digital filters are constructed. Note, that the computer algebra system is used at this stage because of complexity of necessary transformations. To decrease memory requirements the standard IE scheme is used which is based on the regular discretization in horizontal direction to obtain block-Toeplitz matrices, along with the utilization of system matrix symmetries and anti symmetries.

Numerical experiment

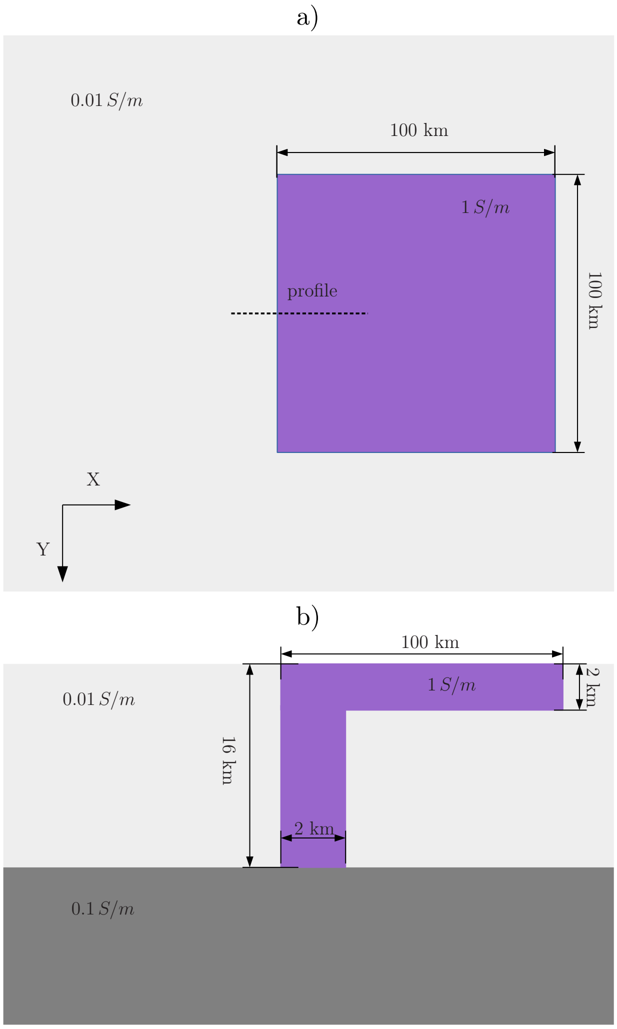

Figure 2: Example model. a)plan view, b)side view

To demonstrate the efficiency and importance of using high-order polynomial basis instead of piece-wise constant basis, the synthetic model from (Bakker et al., 2015) (shown in Fig. 2) is used. The results of magnetotellurics modelling at frequency 10^{-3}Hz obtained using the "piece-wise constant (PWC)" IE solver (solid curves) and new high-order IE solver (dashed curve) are presented in Fig. 1. One can see that the modeling by PWC IE solver with $N_z = 32$

produces an artifact in the apparent resistivity (blue curve). This artifact disappears, however, if rather excessive discretization with $N_z = 128$ is invoked (yellow curve). At the same time the usage of 3rd-order polynomial basis provides accurate results with $N_z = 2$ (dotted line). Taking into account that the 3-rd order polynomial basis requires four unknowns per cell, high-order IE solver allows *sixteen* times speed up and memory saving compared with PWC IE solver.

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