



10.4 A NEW MAGNETOTELLURIC 3D MODELING ALGORTIHM: COMPARISON BASED ON DIFFERENT DIRECT AND ITERATIVE SOLVER PERFORMANCES

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ABSTRACT

The calculation time of the 3D magnetotelluric forward modeling algorithm is so large that traditional serial and parallel algorithms cost an extremely large computation time. Reducing the computation time in paralel computing is usually done by allocating threads to different cores for each discrete frequency. However, when sharing the threads, researchers completely focuses on different frequencies and on computers that do not have a sufficient number of cores, the total time is given in proportion to the threads that takes the longest processing workload. In those algorithms, the number of cores used is generally chosen depending on the number of frequencies in distributed computing algorithms. But, solving the Helmholtz equation by iterative methods for high frequencies can reach solution faster than solving it iteratively for low frequencies. When a very low relative residual value is selected, it is observed that the algorithms did not reach a solution in low frequencies and ended with the maximum number of iterations. It is not possible for iterative algorithms to reach a solution for very low frequencies because the amplitude difference between the imaginary and real components grows proportionately too much. For this reason, the solution is generally less sensitive to phase values compared to amplitude values. To overcome this, direct methods can be used instead of iterative methods. However, the excessive RAM usage of direct methods limits the use of the methods for large model meshes. Thanks to the recently developed multifrontal methods, RAM usage has been reduced and a solution has become possible even for large model networks. During this study, dynamic selection of direct and iterative methods are studied to reduce the solution time in 3D magnetotelluric modeling studies. Thus, it has been suggested to use iterative methods in solving high frequencies and to use direct solvers after the determined threshold frequency value. Additionally, due to the high solution speeds at high frequencies, additional recommendations are made when distributing it to the cores. At the and of the study, we also compared the CPU and GPU performances of the algorithm and their contribution to performance has been discussed.

KEY WORDS : Magnetotelluric, Modeling, Direct and Iterative Solvers, 3 Dimensional, Dynamic Selection, CPU and GPU computation

INTRODUCTION

3-D forward solution in the magnetotelluric method is one of the most important research topics in recent years. In this method, solving the Helmholtz equation takes a long time and require enormous RAM consumption. For this reason, it is extremely important to develop new and





rapid approaches to solving the method faster than previously developed algorithms. To do so, we need to calculate performance of the direct and iterative solvers on the solution of the Helmholtz equation.

In recent years, there have been many studies on 3-D forward solutions in frequency domain EM methods. As a forward solution method, Finite Differences (Newman and Alumbaugh, 1995, 2002; Streich, 2009), Finite Elements (Badea et al., 2001; Mitsuhata and Uchida, 2004; da Silva et al., 2012), Finite volume approach (Mackie et al., 1994; Haber and Ascher, 2001; Constable and Weiss, 2006) and integral equation (Wannamaker, 1991; Avdeev et al., 2002) methods are used. The finite element method is the most flexible method in terms of defining the model geometry (Avdeev, 2005, Erdoğan et al. 2008, Demirci et al., 2012). Although integral equation methods are very useful for simple models, there are difficulties in calculating them for complex models (Mackie et al. 1993). For this reason, the Finite Difference method and the closely related finite volume approach are preferred due to ease of calculation, application and solution stability.

To improve the efficiency of 3D flat solution algorithms, the general idea focuses mainly on the development of faster and more accurate numerical algorithms, parallelization of codes on the CPU and/or GPU-based algorithms with direct and iterative solvers. During this study, first iterative and direct solver performances were compared. Then, the combined and/or sequential use of the best solvers were tested on the CPU and their performance on the GPU was also discussed.

METHOD and APPLICATION

In MT method, the frequency domain equations of the forward solution is the Helmholtz equations obtained from Maxwell's equations. This equation cannot be solved analytically for complex models. For this reason, one of the numerical solution approaches must be used to solve the equation. The Finite Difference method (Newman and Alumbaugh, 1995; Alumbaugh et al., 1996; Champagne II et al., 2001; Weiss and Newman, 2002, Streich, 2009) is one of the most frequently preferred methods due to its ease of application and solution speed. In this study, the Finite Difference method was preferred to solve the Helmholtz equation. In the solution of method, the Finite Difference expression is obtained using the staggered grid approach of Yee (1966), scaled symmetrically and Dirichlet boundary conditions are used (Dirichlet boundary conditions were generally used in previous studies to ensure that the resulting equation is to be symmetric, see Newman and Alumbaugh, 1995; Streich, 2009). As a result, system of linear equations in the form given below is obtained.

KE=S

(1)

Here, K matrix defines a hermitian and sparse matrix with at most 13 non-zero elements in each row, and S defines the source term. E field values are obtained by solving the equation system, and H fields can be derived from electric fields using auxiliary equations. In solving the system of equations, the K matrix must be inverted (direct methods) or the system of equations must be solved with Krylov environment solvers (iterative methods).

The number of rows or columns of the K matrix in the system of equations to be solved can be expressed in hundreds of thousands or even millions, depending on the number of elements in





the designed 3-D model mesh. For this reason, the stationary and fast solvers used in the solution of the system of equations directly affect the speed of the method. Krylov environment solvers are frequently preferred because RAM usage is much lower than direct solvers. The main Krylov space solvers used in the forward solution in the 3-D MT method are CG (Zhdanov et al., 2000; Haber, 2004; Zhdanov et al., 2011), BICG (Sasaki et al., 2010; Farquharson and Miensopust, 2011; Sasaki, 2012), BICGSTAB (Xiao et al., 2018; Singh et al., 2017; Plessix and Mulder, 2008), QMR (Kelbert et al., 2014; Tang et al., 2015; Wang and Tan, 2017) and GMRES (Cox et al., 2010; Grayver, 2015). ; Grayver and Kolev, 2015). During this study, the performances of those iterative solvers were tested.

Recently, direct solvers have begun to be used for relatively small model networks. Since the matrix is inverted in direct solvers, there is no need to solve the equation again for each polarization and the solution speed increases. Due to developments in computer technology, the use of direct solution methods has increased in the last decades and the use of Multifrontal methods in the CPU environment has become widespread (Streich, 2009; da Silva et al., 2012; Kordy et al., 2015; Puzyrev et al., 2016; Mütschard et al., 2017). ; Liu et al., 2018). Although RAM usage of direct solvers is reduced with multifrontal methods, their use is not preferred for large model networks.

During the study, the solution sensitivities and calculation times of all iterative and direct solvers were tested and the obtained results were discussed.

DISCUSSION and RESULTS

In 2008 and 2011, during two workshops at the Dublin Institute for Advanced Studies over 40 people from academia and industry from around the world met to discuss 3-D MT modeling and inversion studies. In these workshops, to test the numerical forward solutions, a 3-D models were designed to compare the responses obtained by different codes and/or users. This model was called as Dublin Test Model-1 (DTM-1). The DTM1 test model which is used by the 3D algorithm developers in the MT method was used during the study. The results of the developed algorithm were discussed using Dublin Test Model-1 (DTM-1). In the comparison, whole algorithm reached same results and whole discussions made based on this test model.

During the study, the performances of the solvers were tested on the CPU and the BICGSTAB solver was found to be the fastest and most stable solver (Figure-1). However, it is seen that direct solvers reach the solution in the most effective solution time if more than one polarization is used. In Figure-1, the results are given according to the use of a single polarization. While it is necessary to make a new calculation for each polarization in iterative solvers, this is not necessary in direct solvers and there is no noticeable increase in calculation time. Therefore, as a result of the study, it was concluded that it would be efficient to use direct solvers, especially at low frequencies (0.01 Hz and lower), for small model meshes. Using iterative methods for frequencies of 0.01 Hz and larger allows the algorithm to reach faster results than direct solvers. For this reason, it has been observed that making this selection in the algorithms to be developed increases the solution speed. When we look at the CPU and GPU performances of the BICGSTAB algorithm (which is the selected iterative solver), it is observed that the acceleration in the solver is 2.5 times higher,





especially at low frequencies, for the algorithm developed on the GPU platform (Figure-2). However, due to GPU RAM usage restrictions, it has been observed that its use is not suitable for large model meshes.

CONCLUSIONS

The simultaneous use of direct and iterative solvers during 3D magnetotelluric modeling is important in terms of solution speed. Therefore, the use of BICGSTAB iterative solver for frequencies higher than 0.01 Hz and direct solvers for frequencies lower than 0.01 Hz makes a positive contribution to the solution speed. In addition, coding the entire algorithm in the GPU environment has shown that this selection may not be necessary in the future if there is no GPU RAM bottleneck. It has been observed that the best method for today's conditions is to use both direct and iterative methods together on the CPU.

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Figure1 Comparison of iterative and direct methods in terms of number of iterations, calculation time, relative error and speedup based on DTM-1



Figure2 CPU and GPU performances and relative acceleration graphs of the selected solver (BICGSTAB)