We investigate the use of different preconditioning within the framework of the Anisotropic-Finite-Difference based Solution for the EEG Forward Problem. Provided the minimal error of representation, comparison of the convergence rate and computational cost is carried out for several competitive numerical solver combinations. From the testing on real data, we obtain that combination of the biconjugate gradient solver and incomplete LU factorization results in a numerical solution that outperforms the other considered approaches in terms of reducing the computational cost significantly. We validate this numerical solution combination against analytical spherical mode. Also, testing on realistic head models (with high anisotropic areas and heterogeneous tissue conductivities) shows high accuracy and low computational cost.

1. Introduction

There are many recent advanced applications that had been reported for spatiotemporal distributed source analysis, such as for presurgical evaluation of the epileptogenic zone, investigation of evoked-related potentials in brain computer interface, and, generally, in task where the localization information for the active sources in the brain helps to diagnose pathological, physiological, mental and functional abnormalities related to the brain. Therefore, an accurate and fast forward solver has to be employed. In order to solve the forward problem, there are several approaches, each one having its own advantages and weaknesses depending on the necessity of the user, among others the following: spherical models, Boundary Finite Elements (BEM) [6], Finite Elements Method (FEM) [8], Finite Difference Method (FDM) [2], and Finite Volumetric Method. Since image data (MRI, CT) are usually acquired in regular formats of digitalization (mostly, 1×1×1), aFDM can be straightforwardly adapted to the grid.

Using FDM numerical approximations, the solution of the Poisson equation in a volume conductor medium (forward problem) derives in a large linear system with an ill-posed coefficient matrix. Furthermore, the numerical stability and computational burden of this type of problem highly depends on the conditional number of the coefficient matrix. Therefore, suitable preconditioners must be applied to improve the numeric properties of the solution. To this end, [4] introduces an anisotropic FDM formulation for the SOR solver. But, due to the stationary nature of the solver, this technique takes much time to solve realistic head models. In contrast, [7] proposes a fictitious domain data ordering allowing Fourier type preconditioning and obtaining fast and accurate realistic forward model calculations. Yet, this numerical approach may not reach the minimal error of representation to accurate forward solution.

In this work, we analyse several numerical solutions for the anisotropic FDM problem, finding a suitable iLU preconditioning-solver combination, allowing accurate and fast forward calculations in highly anisotropic and heterogeneous realistic head models.

2. Methods

2.1. Anisotropic-Finite-Difference based Solution of the EEG Forward Problem

The forward problem consists in the calculation of the electrical potential field on the scalp surface (provided the geometry and electrical conductivity of the head volume) for a given position, orientation, and magnitude of the dipole current sources. Due to measured EEG/MEG frequencies are usually below 100 Hz and electric and magnetic field time derivatives are typically much smaller than ohmic currents, we can neglect the nonstationary electromagnetic field terms [3]. Therefore, in order to determine the electrode potential field, \( V \in \mathbb{R}^m \) (being \( m \) the number of electrodes) generated by a brain current dipole with volumetric conductivity \( \Sigma \in \mathbb{R}^{3\times3} \), we make use of the quasi-static approximation of the Maxwell’s and Poisson equations as follows:

\[
\nabla \cdot (\Sigma(r) \nabla V(r)) = \nabla J(r),
\]
where \( J \in \mathbb{R}^m \) is the electric current density and \( r \in \mathbb{R}^3 \) is the point of detection holding the direction and position dipole. \( \Sigma(r) \) is the conductivity tensor with the direction-dependent conductivity that for isotropic conductivity becomes a diagonal matrix.

For the anisotropic case, however, \( \Sigma(r) \) varies according to the position in the anisotropic compartment. Namely, at the interface between two different conducting compartments, two boundary conditions take place. Particularly, if assuming all current leaving one compartment with conductivity \( \sigma_1 \in \mathbb{R}^{3} \) through the interface enters the neighboring compartment with conductivity \( \sigma_2 \in \mathbb{R}^{3} \), the current density at the head surface reads (termed Neumann boundary condition):

\[
\left\{ \begin{array}{l}
J_1 \cdot e_n = J_2 \cdot e_n \\
(\sigma_1 \nabla V_1) \cdot e_n = (\sigma_2 \nabla V_2) \cdot e_n
\end{array} \right. \tag{2}
\]

where \( e_n \) is the normal component on the interface. Likewise, another boundary condition also holds for interfaces not connected with air, stating that by crossing the interface the potential cannot have discontinuities (Dirichlet boundary condition), i.e.: \( V_1 = V_2 \).

Generally, the electrical forward problem means solving the Poisson 1 for the inhomogeneous anisotropic version holding spatial dependence in any direction. Thus, in the Cartesian coordinate system, 1 becomes for anisotropic conductivities:

\[
\sum_{i \in \{x,y,z\}} \sigma_{ii} \frac{\partial^2 V}{\partial i^2} + 2 \sum_{j \in \{x,y,z\}} \sigma_{ij} \frac{\partial^2 V}{\partial i \partial j} + \sum_{i,j \in \{x,y,z\}} \frac{\partial \sigma_{ji}}{\partial j} V = J_i \tag{3}
\]

with no-flux Neumann boundary conditions on the scalp. Notation \( l \) stands for the cardinal number of the argument \( l \).

For numerical solving, 3 can be transformed into a set of linear equations modeling the volume conduction. For this end, we use a cubic grid in which each cube (or element) has a conductivity tensor that can vary between neighbouring elements, so that the directions of the anisotropy are changed along the coordinate system axes of the head model. In [4], an approach (termed finite difference method in anisotropic media – aFDM) is presented to handle anisotropic properties of tissues, where a finite difference formulation for the Laplace’s equation is extended to the Poisson’s equation (see 1) that is valid everywhere in a piecewise inhomogeneous anisotropic medium. Since image data (MRI,CT) are usually acquired in regular formats of digitalization (mostly, \( 1\times1\times1 \)), aFDM can be straightforwardly adapted to the grid. Thus, we use a set of finite-difference approximations of the spatial derivatives on the uniform rectangular grid with a 19-point stencil made of 8 voxels. The grid has one common node (node labeled as 0) that represents the intersection of eight neighbouring cubic elements. From the 26 conductivity neighbouring nodes at node 0, the formulation uses the 18 nearest neighbours, with rectilinear distance \( \leq 2 \), yielding:

\[
\sum_{i=1}^{18} \alpha_i V_i - \left( \sum_{i=1}^{18} \alpha_i \right) V_0 = I \tag{4}
\]

where \( V_i \in \mathbb{R} \) is the scalar-valued potential at the \( i \)-th node, \( I \in \mathbb{R} \) is the dipole current, and \( \alpha_i \in \mathbb{R} \) are the coefficients depending on the conductivity tensor and the internode distance, which are fixed to ensure the Neumann and Dirichlet boundary conditions [5].

### 2.2. Solving large, sparse LES for Anisotropic-Finite-Difference Methods

The finite difference formulation derived in 4 results in nodal equations forming together a linear equation system (LES), \( Ax = b \), with \( A \in \mathbb{C}^{n \times n} \) nonsingular and \( b \in \mathbb{C}^n \), which can be solved using any standard technique. For the purpose of numerical implementation, however, the above anisotropic-finite-difference based solution of the EEG forward problem imposes the following properties on the coefficient matrix \( A \):

- The number of the rows is the amount of voxels of the skull and soft tissues (several thousands), leading to a high-dimensional matrix \( A \). The numerical approximation of the problem (solver) leads to solving a large LES with the square 19-diagonal matrix of dimension \( N \times N \), where \( N \) is the discretization number. Moreover, due to every matrix row contains a very few non-zero off-diagonal elements, the matrix \( A \) holds high sparseness.

- The coefficients connecting the same pair of neighbouring voxels are identical, resulting in a symmetric matrix \( A \) having weak diagonal dominance.

- The LSE \( Ax = b \) possesses infinite solutions differing only in an additive constant.

To date, several iterative solvers have been developed for a regular LES that can also be extended to the system matrix \( A \) holding the above-described restrictions. Yet, the choice of the solver depends to a large extent on two considerations: the convergence speed to achieve a given accuracy and the computational complexity of each iteration. The baseline stationary solver is the Successive Over-Relaxation (SOR) introducing a relaxation factor that reduces errors of succeeding approximations until all errors are within specified limit. This factor depends strongly upon the properties of the matrix, \( A \), and its choice is not necessarily easy, resulting in algorithms that are not quite efficient in terms of their computational cost.
For the case of symmetric positive definite matrices, the widely-known conjugate gradient (CG) iterative method takes advantage of the steepest descent method searching for orthogonal directions, which are constructed by conjugation of the residuals. The CG is a non-stationary iterative method that provides high convergence rate and is also suited for use with sparse matrices, as an additional plus for our case. In turn for a nonsymmetric system matrix, the generalized version, termed biconjugate gradient (BiCG), is used that does not require the matrix $A$ to be self-adjoint. Since BiCG is numerically unstable, by performing one step of the generalized minimum residual (GMRES) algorithm after each BiCG step, the resulting iteration is stable; this is usually referred to as BiCG-Stab. However, either version, BiCG or BiCG-stab, requires more matrix-vector multiplications and more dot products, resulting in worse efficiency.

Regardless the solver, however, matrix convergence in finite-precision arithmetic remains a crucial issue. Namely, the more ill-conditioned the system matrix $A$ (that is, the larger its condition number defined as $||A|| ||A^{-1}||$), the slower the convergence of the steepest descent method. To cope with this drawback, preconditioning techniques are introduced to improve the condition number of a nonsingular matrix, $M$, making the resulting condition number $M^{-1}A$ much smaller than in the original matrix $A$. Thus, provided that $M$ is a symmetric, positive-definite matrix that approximates system matrix $A$, but having and affordable computational cost of the inverse matrix calculation. Therefore, We can solve $Ax=b$, indirectly as follows:

$$M^{-1}Ax = M^{-1}b$$  \hspace{1cm} (5)

In practice, the combination of solvers with preconditioning procedure (numerical solution combination – NSC) based on incomplete LU (iLU) factorizations constitutes an effective class of methods for solving the sparse linear systems arising from the numerical approximation of partial differential equations. iLU computes an incomplete factorization of the coefficient matrix and requires a solution of lower and upper triangular LES in every iteration of the iterative method.

3. Experimental Set-Up

In order to test the effectiveness of the iLU preconditioning within the Anisotropic-Finite-Difference based Solution for the EEG Forward Problem, we compare its convergence rate and numerical stability to other competitive numerical solution combinations, for a given accuracy. Then, we validate the best iLU-based numerical solution against a concrete analytic method to demonstrate the efficiency of the proposed numerical approach in the highly heterogeneous anisotropic case. All tests are carried out using a 6-shell spherical head model with anisotropic skull and white matter compartments. Lastly, we also validate the iLU numerical solution in a realistic head model white anisotropic skull and white matter derived from high-resolution MRI data.

3.1. Multi shell anisotropic spherical model

The validating spherical head model is a 6-shell anisotropic skull and white matter layers [1]. The shells represent the scalp, the skull, the cerebral spinal fluid (CSF), gray matter (external and thalamic inner sphere) and white matter. We use the following external radius [m]: 0.092 (scalp), 0.084 (skull), 0.076 (CSF), 0.068 (GM), 0.050 (WM), 0.020 (GM); all tissues having conductivity values [S/m]: 0.33 (scalp), 0.018 (anisotropic skull with 1:10 radial/tangential ratio), 1.79 (CSF), 0.33 (brain), and 0.14 (anisotropic white matter with 9:1 radial/tangential ratio). For the anisotropic skull and white matter, we apply rotational transformation to the local coordinate system for orienting the eigenvectors in a normal direction from the concentric spheres. Additionally, we carry out testing for 10 different values of image resolution in order to analyze the conditional number of the system matrix.

3.2. Testing of convergence rate and computational cost

We compare a set of Anisotropic-Finite-Difference based solutions that include combination of four widely-known preconditioners (Cholesky, LU, iLU, Fourier-Jacobi) together with two baseline non-stationary solvers (GMRES, BiCG-Stabilized) and the baseline stationary SOR solver (without any preconditioning). Besides, since the Cholesky preconditioner is just devoted to the GMRES solver and the Fourier Jacoby for BiCG solver, only these concrete combinations are considered, respectively. As a result, we get the following set of numerical solution combinations: SOR, GMRES, GMRES–Cholesky, GMRES–LU, GMRES–iLU, BiCG, BiCG–LU, BiCG–iLU, BiCG–Fourier-Jacoby. It must be noted that the used version of the BiCG is the stabilized one.

The convergence rate is calculated as the lowest number of iterations that each NSC at hand requires for reaching its minimal error of representation. Specifically, We calculate this amount as the residual error value assuming the more complex image resolution, that is, 6×6×6, mm. Another important aspect of comparison is the minimal amount of the residual set that each NSC must reach to make it workable in practical applications. Here, we fix this value as $10^{-13}$.

Numerical computation shows that the plain SOR gets the worse convergence since it needs 350 iterations to reach its lowest error of representation close to $1.8×10^{-7}$; this amount remains far from the fixed minimal residual set. As seen in 1 showing the achieved outcomes of residual error as dependence of the testing iteration number, the GMRES algorithm performs a bit better than SOR, and BiCG im-
Figure 1. Convergence rate of the compared NSC algorithms. Dashed line remarked in red stands for the fixed minimal residual set.

proves even better. Besides, the use of either preconditioning, iLU or LU, leads to a less number of iterations, improving the NSC convergence. Moreover, the latter preconditioner improves the convergence rate remarkably. In fact, the best NSC is the BiCG-Stabilized LU that reaches the needed residual value just after five iterations. Likewise, the Cholesky and Fourier Jacoby preconditioners improve the convergence rate of their corresponding solvers. Nevertheless, the use of preconditioning does not mean that the NSC algorithm should reach the fixed minimal amount of residual set error (dashed line remarked in red). Thus, the GMRES, BiCG, and BiCG–Fourier Jacoby algorithms hang up on some intermediate values close to $\sim 10^{-10}$. In turn, the GMRES–iLU, GMRES–Cholesky, and GMRES–LU converge towards a lower residual value ($\sim 10^{-12}$); still, that amount is not enough. Certainly, the BICG–LU and BICG–iLU are the only algorithms to reach the fixed minimal error of representation.

On the other hand, the computational cost of each iteration turns out to be different in dependence on the used preconditioning approach. For having a common base time to compare computational cost units, we make the time unit as the one spent by the baseline stationary SOR solver. Thus, the time unit is $20.1949\,s$ that is appraised in a workstation 8 core Intel Xeon CPU E5-2687W with 64Gb RAM, using the Matlab software environment. 1 shows the computational time that each NSC requires for reaching its intrinsic final condition stop. Thus, the second column displays the time that each preconditioning procedure spends. As expected, the LU is very much expensive than the other preconditioners, being the iLU the fastest one. The third column shows the time spent by the solver after preconditioning, where the GMRES employs more time that the BiCG. The total amount of time required by each NSC that is shown in the last column is the sum of the previous two columns. As a result, the most expensive NSC is the BiCG–LU, while the fastest – the BiCG–iLU (in as much as 860 times!). Although there are two NSC providing also small computational (BiCG and BiCG–Fourier Jacoby), they do not fit with needed minimal amount of residual error. As a consequence, the BiCG–iLU is the best NSC in terms of computational cost under fixed value of error representation.

$$\begin{array}{c|c|c|c}
\text{NSC} & \text{Preconditioning} & \text{Solver} & \text{Total cost} \\
\hline
\text{SOR} & - & 1.0000 & 1.00 \\
\text{GMRES} & - & 4.1998 & 4.20 \\
\text{GMRES–Cholesky} & 3.4400 & 1.0826 & 4.52 \\
\text{GMRES–LU} & 257.0000 & 0.5903 & 258 \\
\text{GMRES–iLU} & 0.0018 & 4.2279 & 4.23 \\
\text{BiCG} & - & 0.3543 & 0.35 \\
\text{BiCG–LU} & 257.0000 & 0.4153 & 258.00 \\
\text{BiCG–Fourier Jacoby} & 0.0540 & 0.3223 & 0.37 \\
\text{BiCG–iLU} & 0.0018 & 0.2991 & 0.30 \\
\end{array}$$

Table 1. Achieved computational time. Notation * stands for the algorithms reaching the fixed minimal residual error.

Further, we test the BiCG–iLU for 10 different values of numerical resolution, where $N$ is the number of divisions in one direction in the cubic fictitious domain (being $N^3$ the number of rows of the system squared matrix). As seen in 2, the highest the resolution – the large the number of needed iterations. This fact may be explained by the conditional number that is computed for the studied range of numerical resolution. As shown in 3, the conditional number grows exponentially when increasing the division number $N$. Therefore, for high resolutions, the coefficient matrix size becomes bigger and is most difficult to solve due to the obtained larger conditional number. However, the BiCG–iLU remains stable even under the largest conditional number $1.63 \times 10^{14}$, achieved for $N=61$.

Figure 2. Conditional number of BiCG-iLU for different values of numerical resolution.

### 3.3. Validation of BiCG–iLU Numerical Solution

We validate the concordance of the NSC to a suitable analytical solution. To this end, we make use of the spherical
head model having $6 \times 6 \times 6 \text{ mm}$ voxel size. 4 shows the Potential ($\mu V$) versus the electrode channel number computed for the proposed 7-layered spherical head model. The continuous line displays the BiCG–iLU employing aFDM while the circles show the analytical potentials calculated employing the multishell anisotropic spherical model described above. Both, the numerical and analytical, solutions match correctly in computing the potentials for a single source placed at the gray matter area in the normal disposition to the gray matter sphere. Here, the electrodes are placed in 6 different rings covering the entire surface of the scalp surface.

Validation of BiCG–iLU is also carried out on realistic head models. Particularly, we the chosen NSC on realistic head models comprising an isotropic representation with a highly anisotropic head model. Image preprocessing is carried out using 3D Slicer built-in modules. The preprocessing steps included: MRI bias correction (N4 ITK MRI bias correction) and registration (BRAINS) for movement correction. We obtain detailed tissue models from the T1-weighted and TOF volumes by using the pipeline described in [?]. The model contain WM, GM, CSF, skull, eyes, muscle, fat, arteries, and skin. The arteries segmentation mask is processed to estimate the direction of blood flow, obtaining a normalized vector map describing the maximum anisotropy inside the arteries. The MRI segmentation holds 9 different tissues with different conductivity values [S/m]: (scalp = 0.33; fat = 0.4; muscle = 1.1112; skull = 0.020; eye = 0.0505; CSF = 1.538; GM = 0.3333; WM = 0.14; blood vessels = 0.28). Since the skull and white matter have strongly anisotropic behavior [2], we use a 1:10, radial:tangential anisotropic setup for the skull, based on the volume constraint of the isotropic value. For the anisotropic white matter, DWI are corrected for motion, eddy currents and field inhomogeneities. Diffusion tensor images (DTI) are reconstructed with Diffusion-Toolkit. Finally, registration of DTI images to the anatomical T1 image space is performed using the FSL tool with the preprocessed DWI b0 image.

Performance of the BiCG–iLU in highly anisotropic aFDM formulations is carried out for two different realistic head models. The 5 shows a simplify 5-tissues head model that we set to be completely isotropic. In contrast, we define a 9-tissues head model with anisotropic skull and white matter, including fat, muscle, eyes and even blood vessels tissues. In accordance to [4], we calculate the dipole estimation errors due to neglect multiple tissue segmentation including the anisotropic skull and white matter. The solver takes about 4 minutes to solve the coefficient matrix for a given source for a $1 \times 1 \times 1 \text{ mm}$ resolution with $N=256$. Therefore, the algorithm shows a feasible numerical stability even in the presence of highly anisotropic areas, and larger heterogeneity tissues.
4. Discussion and concluding remarks

We discuss the use of the iLU preconditioning within the framework of the Anisotropic-Finite-Difference based Solution for the EEG Forward Problem. To this end, we carry out the comparison of several numerical solver combinations in terms of convergence rate and computational cost. Since there is a need for fast, but accurate forward solver, the minimal error of representation is also included as an additional consideration. From the obtained results of the comparison on real data, we infer that the BiCG solver outperforms the other considered approaches: GMRES and SOR. Furthermore, the BiCG is the only one to reach the fixed amount of residual error. In order to reduce the computational cost significantly, however, a proper choice of the preconditioner for a particular matrix is probably more important than using the optimal outer-level iterative solver. We show that the LU preconditioners is not efficient under the considered settings. On the contrast, the incomplete LU preconditioner improves the solver performance. Thus, the BiCG–iLU results in the best NSC in terms of computational cost within a wide range of numerical resolution. However, if the amount of residual error is relaxed down to $\sim 10^{-10}$, the use of BiCG–Fourier Jacoby leads to a workable NSC.

Validation process comparing numerical and analytical models is carried out and shows that the BiCG–iLU as a numerical approximation accurately matches the potentials over the scalp. Specifically, we select a source placed in the outer gray matter sphere in a 76 artificial electrode configuration covering the entire surface of the sphere with 6 parallel rings. BiCG–iLU performs high accuracy and low computational cost even for realistic head models with high anisotropic areas and heterogeneous tissue conductivity considerations. As a result, the calculation time for a $1\times1\times1\,mm$ is under 1 minute; this amount of time is very competitive in comparison to other aFDM solution techniques reported in literature.

One of the promising approaches for improving the solver performance is the use of the fictitious domain enclosing the data in a redundant low zero voxelization, allowing a straightforward data ordering in the coefficient matrix. Instead of using the fictitious domain, we hypothesize that an inhomogeneous data ordering considering only the non-zero entries of the volumetric model should reduce the size of the coefficient matrix and the number of potential unknowns. As a result, we may improve memory allocation and, at the same time, reduce the whole amount of numerical operations.

As future work, the authors plan to test the discussed NSC in realistic head data extracted from EEG recordings, in order to measure the influence of volumetric anisotropic medium on the performance of the source localization problem.

References


