Symmetric BEM and Multiscale Fast Multipole Method for the E/MEG Problem

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Abstract

We use the novel symmetric boundary element method (BEM) for solving the direct E/MEG problem — computation of the electromagnetic field caused by a known distribution of sources. We generalize the classical shell model of the head and reformulate the symmetric BEM for this topology. We have derived a variant of the fast multipole method (FMM) for the symmetric BEM. Finally, we show how to solve the problem in a multiscale fashion, to reduce the computational complexity for large problems.

Introduction

Electro/magnetoencephalography [1–3] is a non-invasive medical technique for measuring neuronal activity in the brain. In our earlier work [4] we compared the classical BEM and FEM approaches for solving the direct problem — computation of the electrical field caused by a known distribution of sources; the magnetic field is then obtained by a simple integration [5]. Later on, we studied a new symmetrical integral formulation [6, 7] and found it to be much more accurate than the previously used alternatives.

The first problem we address in this paper is the limitation of the classically used head model consisting of a set of nested closed surfaces. It fails for example to model the openings present in the skull (eyes), or the junction between the two hemispheres via the corpus callosum. We therefore propose a new formulation that can handle arbitrary partitioning of the space into volumes corresponding to different tissue types.

Since the realistic models involved are very large, the second issue we deal with here is the reduction of computational complexity. To this end, we modify the single-level variant of the Fast Multipole Method (FMM) [8] for the new, symmetric BEM formulation and extend it from one level to the full hierarchy of scales. We also propose to use the multipole technique to obtain lower-resolution versions of the problem and thus enable a solution in a hierarchical fashion.

Problem definition

The quasi-static approximation of Maxwell equations [9] yields the fundamental Poisson equation

$$\nabla \cdot \big(\sigma \nabla V\big) = f = \nabla \cdot \mathbf{J}^{\mathrm{p}} \quad \text{in } \mathbb{R}^3 \tag{1}$$

with conductivity σ, current source density $\mathbf{J}^{\mathrm{p}}$, and unknown electric potential V.

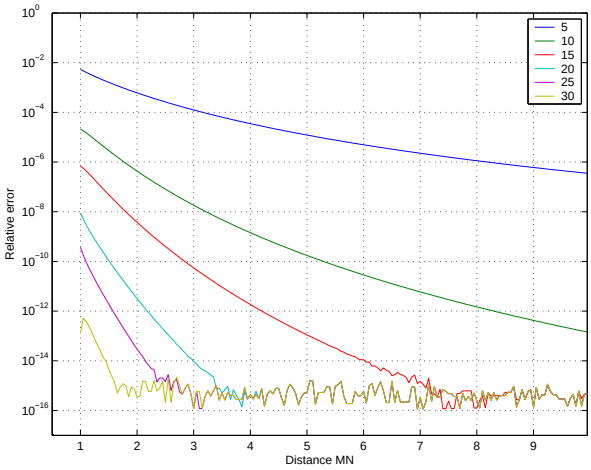

Figure 1: A typical relative error of the multipole approximation with respect to order L and the inter centre distance $\mathbf{MN}$.

Head model

Consider a piecewise constant conductivity head model partitionining the space into $N+1$ disjoint connected open sets $\Omega_1, \ldots, \Omega_{N+1}$ such that $\bigcup_{\alpha=1}^{N+1} \overline{\Omega}_\alpha = \mathbb{R}^3$. The volumes $\Omega_1, \ldots, \Omega_N$ with conductivities σ_α correspond to head tissues and are bounded, while Ω_{N+1} represents the air, has conductivity $\sigma_{N+1} = 0$ and extends to infinity.

For each pair $\Omega_\alpha, \Omega_\beta$ their common boundary $S_{\alpha\beta} = \partial\Omega_\alpha \cap \partial\Omega_\beta$ is either empty or can be decomposed into a finite number of connected regular surfaces, their normals pointing by definition from Ω_α to Ω_β. Note that each $S_{\alpha\beta}$ is regular almost everywhere.

Connected Laplace problems

Since the conductivity is supposed to be piecewise constant, we can factor out σ from (1) to yield a set of Laplace problems connected by boundary conditions imposing the continuity of potential V and current $p = \sigma\partial_{\mathbf{n}} V$ across the interfaces:

$$\begin{aligned} \sigma_\alpha \Delta V &= f \quad \text{in all } \Omega_\alpha \\ \big[V\big]_{S_{\alpha\beta}} = \big[p\big]_{S_{\alpha\beta}} &= 0 \quad \text{on all } S_{\alpha\beta} \end{aligned} \tag{2}$$

Symmetric BEM

Symmetric boundary element method [7] transforms the differential equations (2) for V in $\mathbb{R}^3$ into a set of integral equations with unknowns V and p on the boundaries $S_{\alpha\beta}$. Their discretization leads to a symmetric system of linear equations.

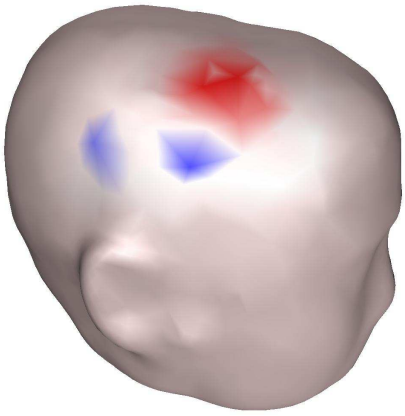

Figure 2: A typical skin potential due to a dipole close to the cortex.

Free-space solution

A free-space solution of $\sigma_\alpha \Delta v_\alpha = f_\alpha$ is given by $v_\alpha = -\big(f_\alpha * G\big)/\sigma_\alpha$ in each Ω_α with $\sigma_\alpha \neq 0$, where f_α is the subset of the sources localized in Ω_α and $G(\mathbf{r}) = 1/\big(4\pi\|\mathbf{r}\|\big)$ is the Green function. In Ω_{N+1} (air), where $\sigma_{N+1} = 0$, we choose $v_{N+1} = 0$, a valid solution of the Poisson equation which is compatible with our boundary condition of "zero at infinity" ($\mathscr{H}$, [7]) that shall be needed to apply the Representation Theorem [7].

Continuous form of the symmetric BEM

In each Ω_α we define a function

$$u_\alpha = \begin{cases} V - v_{\Omega_\alpha} & \text{in } \Omega_\alpha \\ -v_{\Omega_\alpha} & \text{elsewhere} \end{cases}$$

harmonic in $\mathbb{R}^3 \backslash \partial\Omega_\alpha$ and jumping on the boundary $\partial\Omega_\alpha$ as $[u_\alpha]_{\partial\Omega_\alpha} = V_\alpha$ and $\sigma_\alpha [\partial_{\mathbf{n}} u_\alpha]_{\partial\Omega_\alpha} = p_\alpha$, where V_α is the restriction of V on the boundary and p_α is defined by the previous equation.

Let us now consider the surface $S_{\alpha\beta} = \Gamma$. First, we apply the Theorem to calculate the limit of $u_\alpha = V - v_\alpha$ from Ω_α towards Γ, using the values of V and p on all the boundary $\partial\Omega_\alpha$:

$$\begin{aligned} \big(V - v_\alpha\big)^-_\Gamma &= \frac{[u_\alpha]_\Gamma}{2} - \mathcal{D}\big[u_\alpha\big]_{\partial\Omega_\alpha} + \mathcal{S}\big[\partial_{\mathbf{n}} u_\alpha\big]_{\partial\Omega_\alpha} \\ &= \frac{V_\Gamma}{2} - \sum_{\Theta = S_{\alpha\delta}} \big(\mathcal{D}_{\Gamma\Theta} V_\Theta - \sigma_\alpha^{-1} \mathcal{S}_{\Gamma\Theta} p_\Theta\big) \end{aligned}$$

where $\mathcal{D}$ and $\mathcal{S}$ are the double resp. single layer potential integral operators [7], the subscripts indicate the target and source surfaces it operates upon, and we sum over all surfaces adjacent to Ω_α. Second, we apply the Theorem to the limit of $u_\beta = V - v_\beta$ from Ω_β towards Γ:

$$\begin{aligned} \big(V - v_\beta\big)^+_\Gamma &= \frac{[u_\beta]_\Gamma}{2} - \mathcal{D}\big[u_\beta\big]_{\partial\Omega_\beta} + \mathcal{S}\big[\partial_{\mathbf{n}} u_\beta\big]_{\partial\Omega_\beta} \\ &= \frac{V_\Gamma}{2} + \sum_{\Theta = S_{\beta\delta}} \big(\mathcal{D}_{\Gamma\Theta} V_\Theta - \sigma_\beta^{-1} \mathcal{S}_{\Gamma\Theta} p_\Theta\big) \end{aligned}$$

where the sign change is caused by the "inward" orientation of Γ with respect to Ω_β; this changes the sign of the normal derivative $\partial_{\mathbf{n}}$ involved in $\mathcal{D}$ and p. Thanks to the continuity of v_α,v_β, and V across Γ we can subtract the two previous equations:

$$\begin{aligned} \big(v_\beta - v_\alpha\big)_\Gamma = -2\mathcal{D}_{\Gamma\Gamma} V_\Gamma + (\sigma_\beta^{-1} + \sigma_\alpha^{-1}) \mathcal{S}_{\Gamma\Gamma} p_\Gamma \\ - \sum_{(\Theta,\gamma)} \big(\mathcal{D}_{\Gamma\Theta} V_\Theta - \sigma_\gamma^{-1} \mathcal{S}_{\Gamma\Theta} p_\Theta\big) \end{aligned} \quad (3)$$

with $(\Theta,\gamma) \in \big\{(S_{\alpha\delta},\alpha); \delta \neq \beta\big\} \cup \big\{(S_{\delta\beta},\beta); \delta \neq \alpha\big\}$. Similarly, by evaluating $\big(\sigma\partial_{\mathbf{n}} u\big)$ on both sides of Γ we get:

$$\begin{aligned} \big(\sigma_\beta \partial_{\mathbf{n}} v_\beta - \sigma_\alpha \partial_{\mathbf{n}} v_\alpha\big)_\Gamma = -(\sigma_\alpha + \sigma_\beta) \mathcal{N}_{\Gamma\Gamma} V_\Gamma + 2\mathcal{D}^*_{\Gamma\Gamma} p_\Gamma \\ - \sum_{(\Theta,\gamma)} \big(\sigma_\gamma \mathcal{N}_{\Gamma\Theta} V_\Theta - \mathcal{D}^*_{\Gamma\Theta} p_\Theta\big) \end{aligned} \quad (4)$$

with the same (Θ,γ). We have obtained a set of equations for V and p that must hold on all surfaces. Note that since $\sigma_{N+1} = 0$ the flow p across the external surfaces is 0 and the corresponding terms disappear.

Discretization of unknowns and surfaces

The surfaces $S_{\alpha\beta}$ are triangulated, with boundary vertices shared. To balance approximation errors, the potential V is discretized on the surfaces using piecewise linear P1 basis $\{\varphi_k\}$ and the flow p using the piecewise constant P0 basis $\{\psi_l\}$. Unlike the ψ_l, the P1 functions φ_k span several triangles. We shall therefore decompose them as $\varphi_k = \sum_{k'(k)} \varphi'_{k'}$, each of the partial functions $\varphi'_{k'}$ supported only on one (oriented) triangle $T_{k'}$ and hence belonging only to one surface. We approximate $V = \sum_{k=1}^{N_v} \sum_{k'(k)} x_k \varphi'_{k'}$ and $p = \sum_{l=1}^{N_t} y_l \psi_l$, where N_v, resp. N_t are the total numbers of vertices, resp. triangles across all surfaces.

Discretizing the equations by Galerkin method

We take scalar products of (4) with basis functions $\varphi'_{i'}$ and of (3) with basis functions ψ_j, on $S_{\alpha\beta} = \Gamma$:

$$\begin{aligned} &\big\langle (\sigma_\beta \partial_{\mathbf{n}} v_\beta - \sigma_\alpha \partial_{\mathbf{n}} v_\alpha), \varphi'_{i'} \big\rangle = \\ &\qquad \sum_k x_k \sum_{k'(k)} \delta_{i'k'} \big(\mathsf{N}\big)_{i'k'} + \sum_l y_l \mu_{i'l} \big(\mathsf{D}^*\big)_{i'l} \\ &\big\langle (v_\beta - v_\alpha), \psi_j \big\rangle = \sum_k x_k \sum_{k'(k)} \gamma_{jk'} \big(\mathsf{D}\big)_{jk'} + \sum_l y_l \nu_{jl} \big(\mathsf{S}\big)_{jl} \end{aligned}$$

with $\varphi'_{k'}$, ψ_l on Θ adjanced to Ω_α or Ω_β and

$$\big(\mathsf{N}\big)_{i'k'} = \big\langle \mathcal{N}_{\Gamma\Theta} \varphi'_{k'}, \varphi'_{i'} \big\rangle, \ \big(\mathsf{S}\big)_{jl} = \big\langle \mathcal{S}_{\Gamma\Theta} \psi_l, \psi_j \big\rangle$$
$$\big(\mathsf{D}\big)_{jk'} = \big(\mathsf{D}^*\big)_{k'j} = \big\langle \mathcal{D}_{\Gamma\Theta} \varphi'_{k'}, \psi_j \big\rangle = \big\langle \mathcal{D}^*_{\Theta\Gamma} \psi_j, \varphi'_{k'} \big\rangle$$

$\delta_{i'k'}$	$\mu_{i'l}$	$\gamma_{jk'}$	ν_{jl}	condition
$-(\sigma_\alpha + \sigma_\beta)$	2	-2	$(\sigma_\alpha^{-1} + \sigma_\beta^{-1})$	$\Theta = \Gamma$
$-\sigma_\alpha$	1	-1	$-\sigma_\alpha^{-1}$	$\Theta = S_{\alpha\delta}, \delta \neq \beta$
$-\sigma_\beta$	1	-1	$-\sigma_\beta^{-1}$	$\Theta = S_{\delta\beta}, \delta \neq \alpha$
0	0	0	0	otherwise

with the obvious sign changes for $S_{\delta\alpha}$ instead of $S_{\alpha\delta}$, etc. Note that if we order the equations as written above and the unknowns as in $\mathsf{A}\,[\mathbf{x}\ \mathbf{y}]^T$, the resulting matrix is A symmetric and sparse with block structure.

Fast Multipole Method and Multiresolution

FMM accelerates the calculation of the inner product Az from $O(N^2)$ to $O(N \log N)$, where $N = N_v + N_t$. The product Az is used for iterative resolution of the system, e.g. by GMRES, possibly using a multiresolution approach from coarser to finer levels.

Multipole approximation

We use the inner and outer spherical harmonics $I_n^m(\mathbf{r})$, $O_n^m(\mathbf{r})$ [8, 10] to approximate the discretized operators $\mathcal{S}$, $\mathcal{D}$ and $\mathcal{N}$. Let us define the outer-field expansion coefficients $\mathtt{a}$ and $\mathtt{b}$ with respect to some center $\mathbf{M}$

$$
\begin{aligned}
{}^{i}\mathtt{a}_n^m(\mathbf{M}) &= \left\langle I_n^m(\mathbf{M}-\mathbf{r}), \psi_i(\mathbf{r}) \right\rangle_{\mathbf{r}} \\
{}^{j'}\mathtt{b}_n^m(\mathbf{M}) &= \left\langle \nabla I_n^m(\mathbf{M}-\mathbf{r}) \cdot \mathbf{n}_{j'}, \varphi'_{j'}(\mathbf{r}) \right\rangle_{\mathbf{r}}
\end{aligned}
$$

and the outer-outer, inner-inner, and outer-inner translation operators (can be further accelerated using FFT [10])

$$
\begin{aligned}
\mathtt{x}_{n'}^{-m'}(\mathbf{M}) &= \left(\mathrm{R}_{\mathbf{NM}}\,\mathtt{x}\right)_{n'}^{-m'} = \sum_{n=0\ldots n', m=-n\ldots n} I_{n'-n}^{m-m'}(\mathbf{N}-\mathbf{M})\,\mathtt{x}_n^{-m}(\mathbf{N}) \\
\widetilde{\mathtt{x}}_{n'}^{-m'}(\mathbf{M}) &= \left(\mathrm{S}_{\mathbf{NM}}\,\widetilde{\mathtt{x}}\right)_{n'}^{-m'} = \sum_{n=n'\ldots L, m=-n\ldots n} I_{n-n'}^{m'-m'}(\mathbf{N}-\mathbf{M})\,\widetilde{\mathtt{x}}_n^{-m}(\mathbf{N}) \\
\widetilde{\mathtt{x}}_{n'}^{m'}(\mathbf{M}) &= \left(\mathrm{T}_{\mathbf{NM}}\,\mathtt{x}\right)_{n'}^{m'} = \sum_{n=0\ldots L, m=-n\ldots n} O_{n+n'}^{m+m'}(\mathbf{N}-\mathbf{M})\,\mathtt{x}_n^{-m}(\mathbf{N})
\end{aligned}
$$

where L controls the truncation order. The operator approximations around $\mathbf{M}$ are

$$
\begin{aligned}
4\pi \left\langle \mathcal{S}\psi_i, \psi_j \right\rangle &= \sum\nolimits_{n,m} {}^{i}\mathtt{a}^{-m,n}(\mathbf{M})\; {}^{i}\widetilde{\mathtt{a}}^{m,n}(\mathbf{M}) \\
4\pi \left\langle \mathcal{D}\varphi'_{i'}, \psi_j \right\rangle &= \sum\nolimits_{n,m} {}^{i'}\mathtt{b}^{-m,n}(\mathbf{M})\; {}^{j}\widetilde{\mathtt{a}}^{m,n}(\mathbf{M}) \\
4\pi \left\langle \mathcal{N}\varphi'_{i'}, \varphi'_{j'} \right\rangle &= \sum\nolimits_{n,m} {}^{i'}\mathtt{b}^{-m,n}(\mathbf{M})\; {}^{j'}\widetilde{\mathtt{b}}^{m,n}(\mathbf{M})
\end{aligned}
$$

for $n = 0\ldots L, m = -n\ldots n$. For operator $\mathcal{D}$, ${}^{j}\mathtt{a} \cdot {}^{i}\widetilde{\mathtt{b}}$ works too. The truncation error can be crudely estimated as $C\left(\|\mathbf{M}-\mathbf{r}'\|/\|\mathbf{M}-\mathbf{r}\|\right)^{L+1}$ for the above formulas and as $C\left(\max\{\|\mathbf{M}-\mathbf{r}'\|, \|\mathbf{N}-\mathbf{r}\|\}/\|\mathbf{M}-\mathbf{N}\|\right)^{L+1}$ when the outer-inner translation $\mathrm{T}_{\mathbf{NM}}$ is used, for elements at $\mathbf{r}$,$\mathbf{r}'$.

Tree structure and traversal

Consider the task of calculating all $\mathcal{S}$ interactions $y_i = \sum_j x_j\,(\mathsf{S})_{ij}$ between two sets A, B of P0 elements. (The $\mathcal{N}$, $\mathcal{D}$ cases are analogous). We first partition the space into volume cells organized in hierarchical tree structures and assign the elements from A,B to these trees. Classically, a regular octtree common for A,B is used; other options are possible. The algorithm proceeds in three steps:

1. *Preparation*: Calculate the inner coefficients $\mathtt{a}_n^m(\mathbf{M}_\mathcal{C})$ for A,B and sum them in each cell $\mathcal{C}$ in tree A as ${}^{\mathcal{C}}\mathtt{a}_n^m(\mathbf{M}_\mathcal{C}) = \sum_{\psi_j \in \mathcal{C}} x_j\; {}^{j}\mathtt{a}_n^m(\mathbf{M}_\mathcal{C})$.

2. *Up-sweep*: For each cell $\mathcal{C}$ in tree A, translate coefficients ${}^{\mathcal{C}}\mathtt{a}_n^m$ to its parent cell $p(\mathcal{C})$ using the operator $\mathrm{R}_{\mathbf{M}_\mathcal{C}\mathbf{M}_{p(\mathcal{C})}}$ and sum the contributions there.

3. *Down-sweep*: For each cell $\mathcal{C}$ in tree B, translate outer coefficients ${}^{p(\mathcal{C})}\widetilde{\mathtt{a}}_n^m$ from parent $p(\mathcal{C})$ to $\mathcal{C}$ using the operator $\mathrm{S}_{\mathbf{M}_{p(\mathcal{C})}\mathbf{M}_\mathcal{C}}$. Add contributions from all cells $\mathcal{D}$ from tree A that were not accounted for in $p(\mathcal{C})$ but can be treated in $\mathcal{C}$ within a prescribed error bound, converting and translating them with $\mathrm{T}_{\mathbf{M}_\mathcal{D}\mathbf{M}_\mathcal{C}}$.

4. *Evaluation*: For each element ψ_i in each leaf cell $\mathcal{C}$ in tree B, $y_i = \sum_{m,n} {}^{i}\mathtt{a}^{\mathcal{C}}\widetilde{\mathtt{a}} + \sum_j x_j\,(\mathsf{S})_{ij}$, summing over all (local) ψ_j not accounted for in ${}^{\mathcal{C}}\widetilde{\mathtt{a}}$.

Multiresolution

We can take advantage of the spatial smoothness of the solution to produce a hierarchy of progressively lower dimensional approximations of the problem, each providing an initial guess for a finer level solution. Instead of a difficult multiresolution mesh generation, we choose to aggregate elements, forming a cluster from each cell on a certain level Q of the FMM tree. We generate aggregate basis functions such as $\psi^{(Q)} = \sum_{\psi_i \in \mathcal{C}} \psi_i$ (P0-like approximation) and discretize the continuous problem using them. Interaction between aggregate basis function, e.g. $\left\langle \mathcal{S}\psi_i^{(Q)}, \psi_j^{(Q)} \right\rangle$ can be calculated easily by starting the up-sweep at level Q and summing the contributions y_i in a cluster $\psi_i^{(Q)}$ after the evaluation phase. Local interactions at level Q can be precalculated.

Conclusions and experiments

We have provided a complete framework for accurate and computationally efficient solution of the forward E/MEG problem using the FMM accelerated symmetric BEM, directly applicable for the inverse problem as well. Only two examples are shown due to a lack of space.

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