

A Fast Method to Compute the Potential in the Multisphere Model

J. C. de Munck and Maria J. Peters

Abstract—A series expansion is derived for the potential distribution, caused by a dipole source in a multilayered sphere with piecewise constant conductivity. When the radial coordinate of the source approaches the radial coordinate of the field point the spherical harmonics expansion converges only very slowly. It is shown how the convergence can be improved by first calculating an asymptotic approximation of the potential and using the so-called addition-subtraction method. Since the asymptotic solution is an approximation of the true solution, it gives some insight on the dependence of the potential on the conductivities. The formulas will be given in Cartesian coordinates, so that difficulties with coordinate transformations are avoided. Attention will be paid to the (fast) computation of the partial derivatives of the potential, which is useful for inverse algorithms.

I. INTRODUCTION

IT is commonly accepted that the mechanism underlying the generation of the electroencephalogram (EEG) can be physically described as a set of current sources embedded in a conductive medium. The position and orientation of these sources can be estimated from the observed potential differences on the skin by constructing mathematical models that describe the geometry of the sources and the geometry of the medium. Since the head is approximately spherically symmetric, a concentric sphere model has been developed to describe the head, with different levels of complexity: the homogeneous sphere model [1], the three sphere model [2], the four sphere model [3], the isotropic multisphere model [4], and the anisotropic multi sphere model [5]. The computation of the potential distribution, when the geometry of the sources and the medium are given is called the forward problem. The inverse problem is to estimate the sources, for a given medium and a known potential distribution on a set of electrodes. The inverse problem is a parameter estimation problem in which the unknown source parameters are varied until the difference between the measured and calculated potential is as small as possible. Since for the inverse algorithm the solution of the forward problem has to be known for many different combinations of source parameters, it is of prime importance to calculate the potential as fast as possible. When the Marquardt algorithm is used in the inverse problem then also the partial derivatives of the potential have to be calculated in a fast way.

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In this paper the forward problem is solved for the general anisotropic multisphere model. The solution method which is used is based on the derivation given in [5]. However, the derivation is slightly adapted to obtain an expression in Cartesian coordinates (Section II). The new formulation of the solution also makes it possible to derive an asymptotic approximation of the terms of the spherical harmonics expansion. This approximation is used to accelerate the speed of convergence of the series. In Section III it is shown how the improvement of the convergence works in general and in Section IV the asymptotic approximation of the multisphere potential is derived. In Section V an explicit expression for the dipole potential and its partial derivatives is given. Finally, in Section VI the merits of the convergence acceleration are demonstrated with some numerical examples.

II. REFORMULATION OF THE SOLUTION

If the quasi-static approximation is valid, the potential ψ is a solution of a boundary value problem with Neuman conditions [6],

$$\begin{cases} \operatorname{div}(\vec{\gamma} \operatorname{grad} \psi) = s, & \vec{x} \in V \\ (\vec{\gamma} \cdot \operatorname{grad} \psi) \cdot \vec{n} = f, & \vec{x} \in \partial V \end{cases} \quad (1)$$

where $\vec{\gamma}(\vec{x})$ is the conductivity tensor, V is the volume conductor, ∂V is the volume conductor boundary with outer normal $\vec{n}(\vec{x})$ and $s(\vec{x})$ is the current source density. From Gauss' identity it follows that a solution of the Neuman problem can only exist if

$$\int_V s d\vec{x} = \oint_{\partial V} f dS. \quad (2)$$

For a current dipole in an isolated volume conductor this condition is automatically satisfied, since then $f \equiv 0$. It can be shown that the solution is unique up to an additive constant.

The current dipole potential can be expressed in terms of the gradient of the monopole potential $\psi_{\text{mon}}(\vec{x}_0, \vec{x}_e)$:

$$\psi(\vec{x}_0, \vec{x}_e) = \vec{Q} \cdot \nabla_0 \psi_{\text{mon}}(\vec{x}_0, \vec{x}_e) \quad (3)$$

where \vec{x}_0 is the source point and \vec{x}_e is the field point, and \vec{Q} is the dipole vector. The symbol ∇_0 indicates that the gradient has to be taken with respect to the source point. The monopole potential ψ_{mon} is the solution of (1), with $s = \delta(\vec{x}_0 - \vec{x})$ and $f = A^{-1}$, and A is the area of the volume conductor. It will next be assumed that the volume conductor is spherically symmetric, and therefore the conductivity $\vec{\gamma}(\vec{x})$ is completely defined by its radial and tangential conductivity, which in turn

both depend only on r . Obviously, the monopole potential is only a function of the radial coordinate of the source r_0 , the radial coordinate of the electrode r_e and on the angular distance ω_{0e} between electrode and source point. Therefore, ψ_{mon} can be expressed as follows

$$4\pi\psi_{\text{mon}} = \sum_{n=0}^{\infty} (2n+1)R_n(r_0, r_e)P_n(\cos \omega_{0e}). \quad (4)$$

Here, P_n are the Legendre polynomials and the coefficients R_n are solutions of the following differential equation [5],

$$\frac{\partial}{\partial r} \left(r^2 \epsilon(r) \frac{\partial}{\partial r} R_n(r_0, r) \right) - n(n+1)\eta(r)R_n(r_0, r) = \delta(r_0 - r) \quad (5)$$

where $\epsilon(r)$ is the radial and $\eta(r)$ the tangential conductivity. The solution of the inhomogeneous (5) can be expressed as the product of two linear independent solutions of the homogeneous equation [7]:

$$R(r_0, r_e) = \frac{1}{r^2 \epsilon W(H_n^{(1)}, H_n^{(2)})} \cdot \begin{cases} H_n^{(2)}(r_0)H_n^{(1)}(r_e), & r_0 > r_e \\ H_n^{(1)}(r_0)H_n^{(2)}(r_e), & r_0 < r_e \end{cases} \quad (6)$$

where

$$W(H_n^{(1)}, H_n^{(2)}) \equiv H_n^{(1)}(r) \frac{d}{dr} H_n^{(2)}(r) - H_n^{(2)}(r) \frac{d}{dr} H_n^{(1)}(r) \quad (7)$$

is the Wronskian determinant. The functions $H_n^{(i)}$ satisfy the homogeneous equation

$$\frac{d}{dr} \left(r^2 \epsilon(r) \frac{d}{dr} H_n^{(i)}(r) \right) - n(n+1)\eta(r)H_n^{(i)}(r) = 0, \quad i = 1, 2. \quad (8)$$

It follows from straightforward differentiation that the denominator in (6) is independent of r , so that $R(r_0, r_e)$ is symmetric in r_0 and r_e .

To specify the boundary conditions, it is convenient to make a small caving in the center of the volume conductor, with radius r_{N+1} . On this spherical surface it is required that the potential is constant. For the solution so obtained the limit $r_{N+1} \rightarrow 0$ is taken, yielding the solution for the "massive" conductor. The functions $H_n^{(1)}$ are determined up to a multiplicative constant. However, when they are substituted into (6), this factor cancels. Therefore, the derivative of $H_n^{(1)}$ may be put equal to 1 at $r = r_{N+1}$. Hence,

$$\begin{aligned} H_n^{(1)}(r_{N+1}) &= 0 \\ H_n^{(1)'}(r_{N+1}) &= 1, \quad n \neq 0 \end{aligned} \quad (9)$$

where $H_n^{(1)'}(r_{N+1})$ denotes the derivative of $H_n^{(1)}(r)$, evaluated at $r = r_{N+1}$.

It follows from (8) that $H_0^{(1)}(r) \equiv 1$ is a solution of the homogeneous equation for $n = 0$. With this choice for $H_0^{(1)}(r)$

we find, with $r = r_1$ is the outer surface of the volume conductor:

$$\begin{aligned} & ((\vec{\gamma} \cdot \text{grad } \psi) \cdot \vec{n})_{\vec{x} \in \partial V} \\ &= \frac{\epsilon(r_1)}{4\pi} \sum_{n=0}^{\infty} (2n+1) \frac{d}{dr_e} R_n(r_0, r_1) P_n(\cos \omega_{0e}) \\ &= \frac{\epsilon(r_1)}{4\pi} \sum_{n=0}^{\infty} \frac{(2n+1)H_n^{(1)}(r_0)H_n^{(2)'}(r_1)}{r_1^2 \epsilon(r_1) (H_n^{(1)}(r_1)H_n^{(2)'}(r_1) - H_n^{(2)}(r_1)H_n^{(1)'}(r_1))} \\ &\quad \cdot P_n(\cos \omega_{0e}) \\ &= \frac{1}{4\pi r_1^2} \end{aligned} \quad (10)$$

provided that $H_n^{(2)}(r_1)$ satisfies the following boundary condition at $r = r_1$:

$$\begin{aligned} H_n^{(2)}(r_1) &= 1 \\ H_n^{(2)'}(r_1) &= 0, \quad n \neq 0. \end{aligned} \quad (11)$$

In (3) the derivative is taken and, since the term $n = 0$ is independent of \vec{x}_0 , this term has no influence on the dipole potential. In the following the zeroth term will not be considered anymore.

As in [5] the solutions of (8) will be expressed as a series of matrix multiplications. For this purpose it is noted that finding a solution of the homogeneous equation is equivalent to finding a 2×2 matrix $M(r_a, r_b)$, which transfers $H_n^{(i)}(r_a)$ and its derivative into $H_n^{(i)}(r_b)$ (and its derivative):

$$\begin{pmatrix} H_n^{(i)}(r_a) \\ \epsilon(r_a)H_n^{(i)'}(r_a) \end{pmatrix} = M(r_a, r_b) \begin{pmatrix} H_n^{(i)}(r_b) \\ \epsilon(r_b)H_n^{(i)'}(r_b) \end{pmatrix}. \quad (12)$$

For, if we have $M(r_a, r_b)$ then the variables r_1 or r_{N+1} , which appear in the boundary conditions (9) and (11), can be substituted for r_b and simultaneously r can be substituted for r_a . In this way the solution at arbitrary r is expressed in terms of the values at the boundaries.

For piecewise constant $\epsilon(r)$ and $\eta(r)$ an explicit expression for $M(r_a, r_b)$ can easily be found. Therefore it is assumed that the conductivities change abruptly at $r = r_{N+1}, r_N, \dots, r_1$, with $r_{N+1} < r_N < \dots < r_1$ and that

$$\begin{aligned} \epsilon(r) &= \epsilon_j \\ \eta(r) &= \eta_j, \quad r_{j+1} < r < r_j. \end{aligned} \quad (13)$$

It can be verified that for $r_{j+1} < r < r_j$, the functions r^{v_j} and r^{-v_j-1} are two linear independent solutions of (8), with

$$v_j = \frac{1}{2}(-1 + \sqrt{1 + 4n(n+1)\eta_j/\epsilon}). \quad (14)$$

Note that if $\epsilon_j = \eta_j$ then $v_j = n$. So for isotropic shells the two linear independent solutions of (8) become the well-known functions r^n and r^{-n-1} . When r_a and r_b are in the same shell, so that $r_{j+1} < r_a, r_b < r_j$, the transfer matrix will be denoted by $M_j(r_a, r_b)$. To find this matrix it is noted that $H_n^{(i)}(r)$ is a linear combination of r^{v_j} and r^{-v_j-1} , and in particular for $r = r_b$,

$$H_n^{(i)}(r_b) = Ar_b^{v_j} + Br_b^{-v_j-1} \quad (15)$$

$$R_n(r_0, r_e) = - \frac{\left\{ \prod_{J_e-1}^1 M_j(r_j, r_{j+1}) M_{J_e}(r_{J_e}, r_e) \right\}_{22} \left\{ M_{J_0}(r_0, r_{J_0+1}) \prod_N^{J_0+1} M_j(r_j, r_{j+1}) \right\}_{12}}{r_e^2 \left\{ \prod_{j=N}^1 M_j(r_j, r_{j+1}) \right\}_{22}} \quad (26)$$

for certain A and B . By simple differentiation it is found that

$$\epsilon(r_b) H_n^{(i)}(r_b) = \epsilon_j (A v_j r_b^{v_j-1} - B(v_j + 1) r_b^{-v_j-2}). \quad (16)$$

Similarly we conclude that

$$H_n^{(i)}(r_a) = A r_a^{v_j} + B r_a^{-v_j-1} \quad (17)$$

and

$$\epsilon(r_a) H_n^{(i)}(r_a) = \epsilon_j (A v_j r_a^{v_j-1} - B(v_j + 1) r_a^{-v_j-2}). \quad (18)$$

By eliminating A and B from (15)–(18) the following expression for M_j is found:

$$M_j(r_a, r_b) = \begin{pmatrix} r_a^{v_j} & r_a^{-v_j-1} \\ \epsilon_j v_j r_a^{v_j-1} & -\epsilon_j (v_j + 1) r_a^{-v_j-2} \end{pmatrix} \cdot \begin{pmatrix} r_b^{v_j} & r_b^{-v_j-1} \\ \epsilon_j v_j r_b^{v_j-1} & -\epsilon_j (v_j + 1) r_b^{-v_j-2} \end{pmatrix}^{inv} \quad (19)$$

From the definition of the transfer matrix it follows that

$$M_j^{inv}(r_a, r_b) = M_j(r_b, r_a) \quad (20)$$

and it can also be verified that

$$\det M_j(r_a, r_b) = \frac{r_b^2}{r_a^2} \quad (21)$$

By substituting r_2 and r_1 for r_a and r_b respectively, (19) can be used to transfer the boundary condition (11) to a solution at the interface of the first and the second shell. Since both elements in the column vectors in (12) are continuous functions, $M_2(r, r_2)$ transfers this solution into the solution for the second shell. By applying this argument repeatedly and expressing (11) as the first column of the identity matrix, we find for $r_{J+1} \leq r \leq r_J$:

$$\begin{pmatrix} H_n^{(2)}(r) & * \\ \epsilon_J H_n^{(2)}(r) & * \end{pmatrix} = M_J(r, r_J) M_{J-1}(r_J, r_{J-1}) \cdots M_1(r_2, r_1). \quad (22)$$

Application of (20) and (21) yields

$$\begin{pmatrix} * & * \\ -\epsilon_J H_n^{(2)}(r) & H_n^{(2)}(r) \end{pmatrix} = \frac{r_1^2}{r_2^2} M_1(r_1, r_2) \cdots M_{J-1}(r_{J-1}, r_J) M_J(r_J, r). \quad (23)$$

In a similar way it is found that $H_n^{(1)}(r)$ can be expressed as a matrix element as follows

$$\begin{pmatrix} * & H_n^{(1)}(r) \\ * & \epsilon_J H_n^{(1)}(r) \end{pmatrix} = M_J(r, r_{J+1}) M_{J+1}(r_{J+1}, r_{J+2}) \cdots M_N(r_N, r_{N+1}). \quad (24)$$

Here we see the use of the assumption that $r_{N+1} \neq 0$. For if we had specified the boundary condition at $r = 0$, then in (19) we had to divide by zero.

Finally, it is noted that the denominator in (6) can also be expressed as a matrix element, by applying (22) and (24) to (7):

$$\begin{pmatrix} * & * \\ * & r^2 \epsilon(r) W(H_n^{(1)}, H_n^{(2)}) \end{pmatrix} = -r_1^2 M_1(r_1, r_2) \cdots M_N(r_N, r_{N+1}). \quad (25)$$

(25) shows that $r^2 \epsilon(r) W(H^{(1)}, H^{(2)})$ does not depend on r , indeed.

Substituting (23)–(25) into (6) yields the coefficients of the spherical harmonics expansion and in this way the potential is expressed in terms of the radii and conductivities of the multi layer model (see top of page), for

$$r_0 < r_e < r_1 \quad r_{J_0+1} < r_0 \leq r_{J_0} \quad r_{J_e+1} \leq r_e < r_{J_e} \quad (27)$$

and similarly for $r_0 > r_e$. From now on only the case $r_0 < r_e$ will be considered. Note the difference in the definitions of J_e and J_0 . Also note that if $r_e = r_1$ then the 22-matrix element in the numerator has to be replaced by unity.

With (4) and (26) the boundary value problem (1) is solved formally. An interesting aspect of the solution method is that it automatically yields the solution of the “dual” problem, i.e. the case that the inner sphere is isolated whereas the outer sphere is kept at a constant potential. Since in this case the boundary conditions (9) and (11) are interchanged, its solution results from interchanging the asterisks and the functions in (22)–(25).

Although we now have a formal solution of our problem, when r_0 approaches r_e , the series converges only very slowly and therefore many terms are needed to obtain accurate results. The convergence behavior becomes apparent when $R_n(r_0, r_e)$ is written in a different way. By carrying out the matrix product in (19), it is found that

$$M_j(r_a, r_b) = \left(\frac{r_a}{r_b}\right)^{-v_j-2} S_j^-(r_a, r_b) + \left(\frac{r_a}{r_b}\right)^{v_j} S_j^+(r_a, r_b) \quad (28)$$

with

$$S_j^-(r_a, r_b) = \frac{1}{2v_j + 1} \begin{pmatrix} v_j \frac{r_a}{r_b} & -\frac{r_a}{r_b} \\ -\epsilon_j \frac{v_j(v_j + 1)}{r_b} & \epsilon_j v_j + 1 \end{pmatrix} \quad (29)$$

$$R_n(r_0, r_e) = \frac{\left\{ \prod_{j=1}^{J_e-1} U_j(r_j, r_{j+1}) U_{J_e}(r_{J_e}, r_e) \right\}_{22} \left\{ U_{J_0}(r_0, r_{j_0+1}) \prod_N^{J_0+1} U_j(r_j, r_{j+1}) \right\}_{12}}{-r_e^2 \left\{ \prod_{j=N}^1 U_j(r_j, r_{j+1}) \right\}_{22}} \cdot \prod_{j_e}^{J_0-1} \lambda_j^{v_j} \frac{\lambda_0^{v_{j_0}}}{\lambda_e^{v_{j_e}}} \quad (32)$$

and

$$S_j^+(r_a, r_b) = \frac{1}{2v_j + 1} \cdot \begin{pmatrix} v_j + 1 & r_b \\ \epsilon_j \frac{v_j(v_j + 1)}{r_a} & \frac{\epsilon_j r_b}{v_j r_a} \end{pmatrix}. \quad (30)$$

The matrix $U_j(r_a, r_b)$ is defined as follows

$$U_j(r_a, r_b) = \left(\frac{r_a}{r_b} \right)^{-2v_j-2} S_j^-(r_a, r_b) + S_j^+(r_a, r_b), \quad (31)$$

so that $M_j = (r_a/r_b)^{v_j} U_j$. Finally, $R_n(r_0, r_e)$ is expressed in terms of the matrix elements of U_j (see top of page) with

$$\lambda_e \equiv \frac{r_e}{r_{J_e}} < 1 \quad \lambda_0 \equiv \frac{r_0}{r_{J_0}} < 1 \quad \lambda_j \equiv \frac{r_{j+1}}{r_j} < 1. \quad (33)$$

In the derivation of (32), (31) has been applied with $r_a > r_b$. Therefore, for large n , the term with S_j^+ is dominating, and the matrix products in (32) tend to a rational function of v_j . The convergence of the spherical harmonics expansion is therefore determined by the behavior of the product of the λ_j . If all layers between the source and the electrode are isotropic, this product equals

$$\prod_{j_e}^{J_0-1} \lambda_j^{v_j} \frac{\lambda_0^{v_{j_0}}}{\lambda_e^{v_{j_e}}} = \left(\frac{r_{J_e+1}}{r_{J_e}} \right)^n \left(\frac{r_{J_e+2}}{r_{J_e+1}} \right)^n \dots \left(\frac{r_{J_0}}{r_{J_0-1}} \right)^n \cdot \left(\frac{r_0}{r_{J_0}} \right)^n \left(\frac{r_e}{r_{J_e}} \right)^{-n} = \left(\frac{r_0}{r_e} \right)^n \quad (34)$$

from which the poor convergence for $r_0 \approx r_e$ is obvious. In Section IV it is demonstrated that for anisotropic layers, the λ_j -product tends to $\Lambda \lambda^n$, with $\Lambda \rightarrow 1$, for $r_0 \rightarrow r_e$, so that also in the general case the convergence of the spherical harmonics expansion is determined by the ratio of r_0 and r_e .

For the massive sphere, the limit of $r_{N+1} \rightarrow 0$ has to be taken of (32). The dependence of (32) on r_{N+1} is only through the second column of the matrix $U_N(r_N, r_{N+1})$. Since for $r_{N+1} = 0$, both the numerator and the denominator vanish, l'Hôpital's rule has to be applied to calculate the limit. Therefore, instead of using $U_N(r_a, 0)$,

$$\lim_{r_b \rightarrow 0} \frac{d}{dr_b} U_N(r_a, r_b) = \frac{1}{2v_N + 1} \begin{pmatrix} 1 \\ 0 \\ \frac{\epsilon_N}{v_N} \\ \frac{v_N}{r_a} \end{pmatrix} \quad (35)$$

has to be applied for the computation of $R_n(r_0, r_e)$.

III. ADDITION-SUBTRACTION METHOD

In the previous section the functions ψ and ψ_{mon} have been expressed as an infinite series of spherical harmonics which have poor convergence for $r_0 \approx r_e$. This implies that, in particular for superficial sources, many terms are needed to obtain accurate results. A strategy to reduce computation time is to approximate the spherical harmonics expansion as well as possible with a formula which is known both in analytically closed form and as a spherical harmonics expansion. This approximation is added to the solution in closed form and subtracted in the form of the infinite series. In this way a series of differences results with a higher speed of convergence, provided that the approximation is properly weighed.

To demonstrate the method, it is assumed that the function ψ is expanded as follows,

$$\psi(\Lambda, \omega) = \sum_{n=1}^{\infty} f_n \Lambda^n P_n(\cos \omega) \quad (36)$$

where the coefficients f_n are known and Λ is a function of r_0 and r_e . Furthermore, it is assumed that these coefficients can be expanded in a finite number K of positive powers of n and an infinite number of negative powers of n ,

$$f_n = \sum_{k=-K}^{\infty} n^{-k} f^{(k)} + O(n^{-\infty}). \quad (37)$$

In the next section it is shown that $O(n^{-\infty})$ result from terms with $\lambda^n, \lambda < 1$. These terms are of order infinity, because $\lim_{n \rightarrow \infty} \lambda^n / n^{-k} = 0$, for any finite k . Therefore these terms tend to zero very quickly for large n and they contribute only to the first few terms of (36).

The k th asymptotic approximation is defined as

$$\phi^{(k)}(\Lambda, \omega) = \sum_{n=1}^{\infty} \frac{\Lambda^n}{n^k} P_n(\cos \omega) \quad (38)$$

and $f^{(-K)} \phi^{(-K)} + f^{(-K+1)} \phi^{(-K+1)} + \dots + f^{(0)} \phi^{(0)} + f^{(1)} \phi^{(1)} + \dots$ is called asymptotic expansion of ψ . For $k < 2$ we can express $\phi^{(k)}(\Lambda, \omega)$ in closed form by taking appropriately chosen partial derivatives and integrals of the infinite medium potential. For instance, we obtain,

$$\phi^{(-1)}(\Lambda, \omega) = \frac{\Lambda \cos \omega - \Lambda^2}{R^3}, \quad (39a)$$

$$\phi^{(0)}(\Lambda, \omega) = R^{-1} - 1 \quad (39b)$$

$$\phi^{(1)}(\Lambda, \omega) = -\ln \frac{1}{2} (1 - \Lambda \cos \omega + R) \quad (39c)$$

where R is

$$R = \sqrt{1 - 2\Lambda \cos \omega + \Lambda^2}. \quad (40)$$

When $K = 0$ is the first nonvanishing term in (37) and if $f^{(0)}$ and $f^{(1)}$ are known, ψ can be calculated as

$$\psi(\Lambda, \omega) = f^{(0)}\phi^{(0)} + f^{(1)}\phi^{(1)} + \sum_{n=1}^{\infty} (f_n - f^{(0)} - n^{-1}f^{(1)})\Lambda^n P_n(\cos \omega) \quad (41)$$

Since $P_n(\cos \omega) = O(n^0)$, the series of differences converges as $\Sigma n^{-2}\Lambda^n$, instead of as $\Sigma \Lambda^n$, which represents the convergence of the original series. Therefore, much fewer terms are necessary to compute (41) than (36), with the same precision. The method is based on the knowledge of the expansion coefficients $f^{(k)}$, and therefore it will be considered in the next section how to calculate them for the multilayer model.

IV. THE ASYMPTOTIC APPROXIMATION

In this section it will first be considered how the λ -product in (32) behaves for large n . For this purpose v_j is expanded in powers of n ,

$$v_j = \frac{1}{2}(-1 + \sqrt{1 + 4n(n+1)\alpha_j^2}) \approx \alpha_j n + \frac{1}{2}(\alpha_j - 1) + \frac{1}{4}(\alpha_j^{-1} - \alpha_j)n^{-1} + O(n^{-2}) \quad (42)$$

with

$$\alpha_j \equiv \sqrt{\eta_j/\epsilon_j}. \quad (43)$$

Hence we have for large n ,

$$\lambda_j^{v_j} \rightarrow \lambda_j^{1/2(\alpha_j - 1)} \lambda_j^{\alpha_j n}$$

and therefore

$$\prod_{J_e}^{J_0-1} \lambda_j^{v_j} \frac{\lambda_0^{v_{J_0}}}{\lambda_e^{v_{J_e}}} \rightarrow A \Lambda^n$$

with

$$A = \prod_{J_e}^{J_0-1} \lambda_j' \frac{\lambda_0'}{\lambda_e'}, \quad \Lambda = \prod_{J_e}^{J_0-1} \lambda_j' \frac{\lambda_0'}{\lambda_e'} \quad (44)$$

$$\lambda_j' \equiv \lambda_j^{\alpha_j} \quad \lambda_j'' \equiv \lambda_j^{1/2(\alpha_j - 1)}. \quad (45)$$

In Section II it has been shown that if all shells between the source and the electrode are isotropic, $A = 1$ and $\Lambda = r_c/r_e$.

The behavior of the U_j matrix product in (32) will be studied next. It was already noted that in the application of (32), we have $r_a > r_b$, so that

$$\prod_{j=J_2}^{J_1} U_j(r_j, r_{j+1}) = \prod_{j=J_2}^{J_1} S_j^+(r_j, r_{j+1}) + O(n^{-\infty}). \quad (46)$$

Here, the $O(n^{-\infty})$ term results from $(r_{j+1}/r_j)^{2n+1}$. From (46) it becomes apparent that for large n we need to consider products of S_j^+ instead of products of U_j . It is easily verified from the definition of S_j^+ (30) that $\text{rank}(S_j^+) = 1$. This notion makes it possible to write the matrix element of a product as a product of matrix elements, and therefore the approximation of (32) can be largely simplified. We can express S_j^+ as

$$S_j^+(r_a, r_b) = \frac{1}{2v_j + 1} a_j b_j^T \quad (47)$$

with

$$a_j = \begin{pmatrix} \epsilon_j^{-1} \\ v_j r_a^{-1} \end{pmatrix} \quad b_j = \begin{pmatrix} (v_j + 1)\epsilon_j \\ r_b \end{pmatrix}. \quad (48)$$

When (47) is substituted into (46) the associative property of matrix multiplication can be applied:

$$\begin{aligned} \prod_{j=J_2}^{J_1} S_j^+(r_j, r_{j+1}) &= \prod_{j=J_2}^{J_1} \frac{1}{2v_j + 1} a_j b_j^T \\ &= \left(\prod_{j=J_2}^{J_1} \frac{1}{2v_j + 1} \right) \\ &\quad \cdot ((a_{J_1} b_{J_1}^T)(a_{J_1+1} b_{J_1+1}^T) \cdots (a_{J_2} b_{J_2}^T)) \\ &= \left(\prod_{j=J_2}^{J_1} \frac{1}{2v_j + 1} \right) \\ &\quad \cdot ((b_{J_1}^T a_{J_1+1}) \cdots (b_{J_2-1}^T a_{J_2})) a_{J_1} b_{J_2}^T \\ &= \frac{1}{2v_{J_1} + 1} \prod_{j=J_2}^{J_1+1} \frac{(v_{j-1} + 1)\epsilon_{j-1} + \epsilon_j v_j}{\epsilon_j(2v_j + 1)} \\ &\quad \cdot \begin{pmatrix} (v_{J_2} + 1)\epsilon_{J_2} & r_{J_2+1} \\ \frac{\epsilon_{J_1}}{v_{J_1}(v_{J_2} + 1)\epsilon_{J_2}} & \frac{\epsilon_{J_1} r_{J_2+1}}{r_{J_1}} \end{pmatrix}. \end{aligned} \quad (49)$$

In the derivation of (49) it has been found that $b_j^T a_{j+1}$ is a scalar, and for this reason it can be put in front of the matrix.

An important consequence of (49) is that the asymptotic approximation of $R_n(r_0, r_e)$ only depends on the conductivities of the layers between source and electrode. The dependence on the radii disappears, because this dependence is canceled in $b_j^T a_{j+1}$. Moreover, when (49) is substituted into (32), many factors of the denominator cancel to factors of the numerator. The only surviving factors depend on the conductivities of the shells between r_{J_0+1} and r_{J_e} . We find for $r_e = r_1$ and $J_0 > 1$

$$R_n(r_0, r_e) = -A \Lambda^n \left(\frac{1}{\epsilon_{J_0} r_e v_1} \frac{2v_1 + 1}{2v_{J_0} + 1} \cdot \prod_{j=0}^{J_1-1} \frac{\epsilon_{j+1}(2v_{j+1} + 1)}{(v_j + 1)\epsilon_j + \epsilon_{j+1}v_{j+1}} + O(n^{-\infty}) \right). \quad (50)$$

If $J_0 = 1$ the product has to be replaced by 1, so that in this case $R_n(r_0, r_e) = -A \Lambda^n / (\epsilon_1 r_e v_1)$. When v_j are expanded in powers of n , we finally arrive at

$$\begin{aligned} &(2n + 1)R_n(r_0, r_e) \\ &= -A \Lambda^n \left(\frac{2}{r_e \beta_{J_0}} \prod_{j=0}^{j=1} \frac{2\beta_{j+1}}{\beta_j + \beta_{j+1}} + O(n^{-1}) \right) \\ &\quad r_e = r_1 \end{aligned} \quad (51)$$

and

$$\begin{aligned} &(2n + 1)R_n(r_0, r_e) \\ &= -A \Lambda^n \left(\frac{1}{r_e \beta_{J_0}} \prod_{j=0}^{j=J_e} \frac{2\beta_{j+1}}{\beta_j + \beta_{j+1}} + O(n^{-1}) \right) \end{aligned}$$

$$r_e < r_1 \quad (52)$$

with

$$\beta_j \equiv \sqrt{\eta_j \epsilon_j}. \quad (53)$$

The reason why (51) and (52) are different is that for $r_e = r_1$ by definition $M_j(r_1, r_e)$ is the identity, so that the approximation presented in (46) is not valid for this case.

V. COMPUTATION OF THE DIPOLE POTENTIAL

In this section the theory derived in Sections II–IV will be applied to the computation of the dipole potential and its partial derivatives. The formulas will be presented in a way which circumvents coordinate transformations from Cartesian coordinates to spherical ones, and backwards. For this purpose it is noted that

$$\nabla_0 r_0 = \frac{\vec{x}_0}{r_0} \equiv \hat{x}_0 \quad (54)$$

and

$$\nabla_0 \cos \omega_{0e} = \nabla_0 \frac{\vec{x}_0 \cdot \vec{x}_e}{r_0 r_e} = \frac{1}{r_0} (\hat{x}_e - \cos \omega_{0e} \hat{x}_0) \quad (55)$$

and where \hat{x}_e is the unit vector in the direction of the electrode. When these two equations are applied to (3) and (4) it is found that

$$4\pi\psi = \vec{Q} \cdot \{ \hat{x}_0 (S_1 - \cos \omega_{0e} S_0) + \hat{x}_e S_0 \} \quad (56)$$

with

$$S_0 = \frac{1}{r_0} \sum_{n=1}^{\infty} (2n+1) R_n(r_0, r_e) P'_n(\cos \omega_{0e}) \quad (57)$$

and

$$S_1 = \sum_{n=1}^{\infty} (2n+1) R'_n(r_0, r_e) P_n(\cos \omega_{0e}). \quad (58)$$

Here P'_n denotes the derivative of the Legendre polynomial and it can be computed recursively by [7]

$$P'_n(\cos \omega) \equiv \frac{d}{d \cos \omega} P_n(\cos \omega) \\ = n P_{n-1}(\cos \omega) + \cos \omega P'_{n-1}(\cos \omega). \quad (59)$$

In (58) $R'_n(r_0, r_e)$ denotes the derivative of $R_n(r_0, r_e)$ with respect to r_0 . Obviously, S_0 can be interpreted as the potential caused by a unit dipole pointing in the radial direction, and similarly S_1 corresponds to a tangential dipole.

The computation of $R'_n(r_0, r_e)$ is rather easy, because it appears as one of the matrix elements in (24). Therefore, to compute $R'_n(r_0, r_e)$ we only need to change the 12-matrix element in (32) into a 22-matrix element and to divide the result by the local conductivity ϵ_{J_0} (see bottom of page). The computation of the derivative of ψ with respect to \vec{Q} follows immediately from (56). For the calculation of the derivatives with respect to the dipole position we find, by applying (54) and (55) systematically to (56):

$$4\pi \frac{\partial \psi}{\partial \vec{x}_0} = \hat{x}_0 \left\{ \vec{Q} \cdot \hat{x}_0 \left(3 \cos \omega_{0e} \frac{S_0}{r_0} - \frac{S_1}{r_0} \right. \right. \\ \left. \left. + S_2 - 2 \cos \omega_{0e} S_3 + \cos^2 \omega_{0e} S_4 \right) \right. \\ \left. + \vec{Q} \cdot \hat{x}_e \left(-\frac{S_0}{r_0} + S_3 - \cos \omega_{0e} S_4 \right) \right\} \\ + \vec{Q} \left\{ \frac{S_1}{r_0} - \cos \omega_{0e} \frac{S_0}{r_0} \right\} \\ + \hat{x}_e \left\{ \vec{Q} \cdot \hat{x}_0 \left(-\frac{S_0}{r_0} + S_3 - \cos \omega_{0e} S_4 \right) \right. \\ \left. + \vec{Q} \cdot \hat{x}_e S_4 \right\} \quad (61)$$

with

$$S_2 = \sum_{n=1}^{\infty} (2n+1) R''_n(r_0, r_e) P_n(\cos \omega_{0e}) \quad (62)$$

$$S_3 = \frac{1}{r_0} \sum_{n=1}^{\infty} (2n+1) R'_n(r_0, r_e) P'_n(\cos \omega_{0e}) \quad (63)$$

and

$$S_4 = \frac{1}{r_0^2} \sum_{n=1}^{\infty} (2n+1) R_n(r_0, r_e) P''_n(\cos \omega_{0e}). \quad (64)$$

Here, the double primes denote the second derivative. The second derivative of the Legendre polynomial can be easily calculated by differentiating (59):

$$P''_n(\cos \omega) = n P'_{n-1}(\cos \omega) + \cos \omega P''_{n-1}(\cos \omega). \quad (65)$$

For the computation of the second derivative of $R_n(r_0, r_e)$ it is convenient to return to the definition of $R_n(r_0, r_e)$ by the differential equation. When ϵ and η are constant, it follows from (5) that (since $r_0 \neq r_e$)

$$R''_n(r_0, r_e) = \frac{\eta J_0}{\epsilon_{J_0} r_0^2} n(n+1) R_n(r_0, r_e) \\ - \frac{2}{r_0} R'_n(r_0, r_e). \quad (66)$$

$$R'_n(r_0, r_e) = \frac{\left\{ \prod_{j=1}^1 U_j(r_j, r_{j+1}) U_{J_e}(r_{J_e}, r_e) \right\}_{22} \left\{ U_{J_0}(r_0, r_{J_0+1}) \prod_N^{J_0+1} U_j(r_j, r_{j+1}) \right\}_{22}}{-\epsilon_{J_0} r_e^2 \left\{ \prod_{j=N}^1 U_j(r_j, r_{j+1}) \right\}_{22}} \prod_{J_e}^{J_0-1} \lambda_j^{v_j} \frac{\lambda_{J_0}^{v_{J_0}}}{\lambda_e^{v_{J_e}}}. \quad (60)$$

With the above formulas the dipole potential can be calculated. To reduce the number of terms required for the computation of S_0 to S_4 asymptotic approximations will be derived next. Similar to (51) we find for $r_e = r_1$:

$$(2n+1)R_n(r_0, r_e) \rightarrow_0^f \Lambda^n; \\ F_0 = -\frac{2A}{r_e \beta_{J_0}} \prod_{j=0}^{j=1} \frac{2\beta_{j+1}}{\beta_j + \beta_{j+1}} \quad (67)$$

$$(2n+1)R'_n(r_0, r_e) \rightarrow nF_1\Lambda^n; \quad F_1 = \frac{\beta_{J_0}}{r_0 \epsilon_{J_0}} F_0 \quad (68)$$

and

$$(2n+1)R''_n(r_0, r_e) \rightarrow n^2 F_2 \Lambda^n; \quad F_2 = \frac{\eta_{J_0}}{r_0^2 \epsilon_{J_0}} F_0. \quad (69)$$

If $r_e < r_1$ then F_0 has to be replaced by

$$F_0 = -\frac{A}{r_e \beta_{J_0}} \prod_{j=0}^{j=J_e} \frac{2\beta_{j+1}}{\beta_j + \beta_{j+1}}. \quad (70)$$

With these equations the sums S_0 to S_4 can conveniently be computed as

$$S_0 = \frac{1}{r_0} \sum_{n=1}^{\infty} \{(2n+1)R_n - F_0 \Lambda^n\} P'_n \\ + \frac{F_0 \Lambda \cos \omega - \Lambda^2}{r_0 R^3}, \quad (71)$$

$$S_1 = \sum_{n=1}^{\infty} \{(2n+1)R'_n - F_1 n \Lambda^n\} P_n + F_1 \Lambda R^{-3} \quad (72)$$

$$S_2 = \sum_{n=1}^{\infty} \{(2n+1)R_n - F_2 n(n+1)\Lambda^n\} P_n \\ + F_2 \Lambda \frac{(2 \cos \omega - 3\Lambda)R^2 + 3\Lambda(\cos \omega - \Lambda)^2}{R^5} \quad (73)$$

$$S_3 = \frac{1}{r_0} \sum_{n=1}^{\infty} \{(2n+1)R'_n - F_1 n \Lambda^n\} P'_n \\ + \frac{F_1 \Lambda}{r_0} \frac{3\Lambda(\cos \omega - \Lambda) + R^2}{R^5} \quad (74)$$

and

$$S_4 = \frac{1}{r_0^2} \sum_{n=1}^{\infty} \{(2n+1)R_n - F_0 \Lambda^n\} P''_n + \frac{3F_0 \Lambda^2}{r_0^2 R^5} \quad (75)$$

where R is defined by (40).

Finally it is noted that when the algorithm presented here is used as a part of an inverse algorithm, many dipole potentials have to be calculated with the same volume conductor parameters and the same electrode grid. In that case it is useful to take advantage from the fact that the quantities $\{\Pi_{J_e-1}^1 U_j(r_j, r_{j+1}) U_{J_e}(r_{J_e}, r_e)\}_{22}$ and $\{\Pi_{j=N}^1 U_j(r_j, r_{j+1})\}_{22}$, which appear in (32), are independent of the dipole position, and therefore they need to be calculated

TABLE I
VOLUME CONDUCTOR PARAMETERS USED IN SIMULATIONS

	shell index j	r_j	ϵ_j	η_j
white matter	5	63	5	1
cortex	4	88	2	1
fluid	3	91	3	3
skull	2	95	0.004	0.04
skin	1	100	1	1

only once. Similarly, the quantities $\{\Pi_N^{J_0+1} U_j(r_j, r_{j+1})\}_{12}$ and $\Pi_{J_e}^{J_0-1} \lambda_j^{v_j}$ need to be calculated only when the dipole jumps from one shell to another. Thus, the calculation of the potential in the multisphere model can be performed in approximately the same amount of time as the potential in the three sphere model, even when the addition-subtraction method is not applied.

VI. RESULTS

In this section the use of convergence acceleration is demonstrated by the application to a special example of a multilayered volume conductor. It has been assumed that the volume conductor consists of an anisotropic sphere representing the white matter, surrounded by four concentric spherical shells, representing respectively the cortex, the cerebrospinal fluid, the skull, and the skin. The outer radii of the shells r_j and the conductivity parameters ϵ_j and η_j are given in Table I. These parameters are in arbitrary units, but they correspond roughly to figures given in literature [10]–[13].

It has been assumed furthermore that the dipole was on the z -axis, at a distance of 85 from the origin, and that it is directed half radially, half tangentially. Four different positions of the electrode have been assumed: on the z -axis with $r_e = 100$ (A), on the x -axis with $r_e = 100$ (B), on the z -axis with $r_e = 90$ (C), and on the x -axis with $r_e = 90$ (D). In each of the cases (A–D) the potential ψ_n was calculated using n terms and the addition subtraction algorithm. We also calculated the quantity ψ'_n , which is similar to ψ_n , but omitting the addition subtraction algorithm. Finally, we plotted (fig. 1) for each of the cases A–D the relative errors $|\psi_{200} - \psi_n|/|\psi_{200}|$ (solid line) and $|\psi_{200} - \psi'_n|/|\psi_{200}|$ (dotted line) on a logarithmic scale as a function of the number of terms n .

The dashed horizontal line in Fig. 1 denotes a relative error of 10^{-3} . It appears that in case A (where $r_e = 100$) about 30 terms are needed to obtain an accuracy of 99.9% when no convergence acceleration is used. With acceleration of convergence this accuracy is obtained in 20 terms, and therefore the decrease in computer time is about 30%. A similar gain in computer time is obtained in case B. In case C and D, where $r_e = 90$, the gain in computer time is more substantial. The figure shows that without convergence acceleration 100 terms are far from enough to compute the potential more accurate than 99.9%. However, when acceleration of convergence is used, 100 terms are enough for a precision of 99.9%.

VII. DISCUSSION

Compared to the derivation followed in [5], the present derivation contains some important modifications. First, the

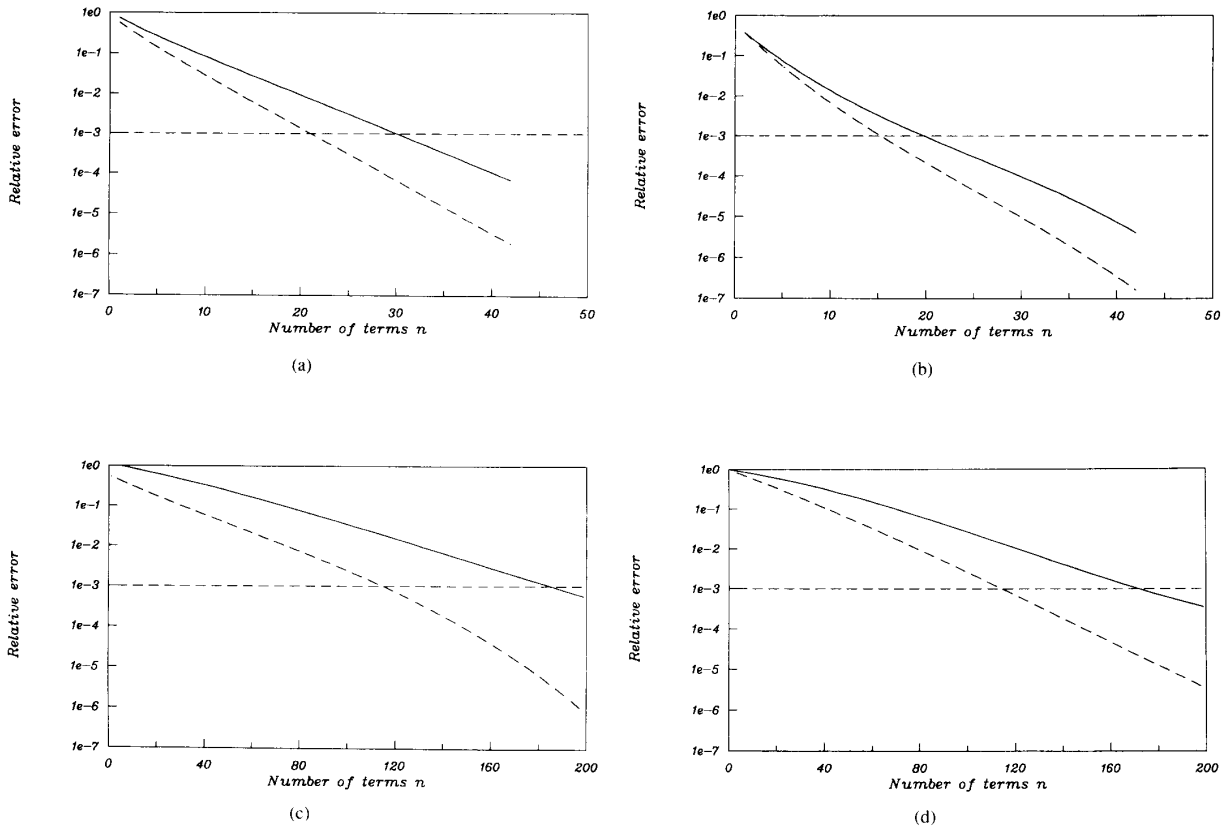


Fig. 1. The relative error in the potential is plotted on a logarithmic scale, against the number of terms used in the series expansion. The dotted lines refer to the cases where the additional subtraction algorithm was used. In case A and B the electrode had a distance of 100 from the origin. In case C and D this distance was 90. The electrode was either on the z -axis (case A and C) or on the x -axis (case B and D). In all cases the dipole was on the z -axis, at a distance of 85 from the origin.

formulas are presented in such a way that they are valid for any dipole position. In [5] the dipole was rotated to the z -axis first, which makes it difficult to perform the partial derivatives with respect to the dipole position, because in the formula for the rotated dipole, the dependence on \vec{x}_0 is not explicitly present anymore. The second modification of [5] is that in the present derivation the radii of the layers appear in the formulas only as a ratio (see (33)). Therefore, these quantities are automatically scaled so that "overflow errors," which could occur when r_j is raised to the power n , are avoided. The most important advantage of the present formulation is, however, that the speed of convergence of the series expansions is increased using the addition-subtraction method and the asymptotic approximation.

The asymptotic approximation has some interesting properties concerning the dependence of ψ on r_j , ϵ_j , and η_j . From Section IV these properties occur.

- 1) The finite order approximation is a local one, since it depends only on the radii and conductivities of the shells between (and including) the source layer and the layer containing the electrode.
- 2) When all layers between the source and the field point are isotropic then the matching Λ is given by r_0/r_c : if

one (or more) of those layers are anisotropic then the Λ is distributed by that layer(s).

- 3) Under the conditions of 2), the finite order approximation is independent of the radii.
- 4) When the dipole is in an anisotropic layer, the weighing coefficient of the first order approximation is different for a radial and a tangential dipole. It follows from (68) that their ratio equals the square root of the ratio of the radial and tangential conductivity.

Since the asymptotic expansion is devised as an approximation of the true potential, properties 1)–4) shed some light on the dependence of the potential on the volume conductor. Note, however, that in this expansion the infinite order terms are omitted, whereas they do have an influence on the lower order terms of the spherical harmonic expansion.

It is possible to increase the speed of convergence still further, by taking higher order approximations of (50). This is worked out for the three sphere model in [8]. Another possibility is to add and subtract the potentials of appropriately chosen mirror sources. A third possibility is to apply additional transformations to the series of differences (71)–(75). Examples of this are given in [9].

Apart from dipole source estimation, the theory presented in this paper can be used to estimate the conductivities of

the different layers by applying a known current to two of the electrodes and measuring the potential distribution on the remaining electrodes. This potential distribution depends on the conductivities of the different layers and therefore the conductivities can be estimated by a least squares fit with the theoretical distribution given by the formulas derived here. In this application, the current sources and the field points have exactly the same radial coordinate, and hence the spherical harmonics expansion does not converge if no precautions are taken. With the addition-subtraction method this problem can be solved adequately.

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