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General Closed-Form Asymptotic Boundary Conditions for Finite Element Analysis of Exterior Electrical Field Problems

***Abstract**. This paper presents general closed-form asymptotic boundary conditions (ABCs) on circular, elliptical and spherical boundaries suitable for the finite element modeling of 2D and 3D electrical field problem with open boundaries. To the best knowledge of the authors of this paper, the ABCs (in such forms) have not yet been reported in the literature. The 1st and 2nd order ABCs, which can be easily implemented into existing finite element codes, are discussed in details, also for an arbitrary shape of the finite element region in 2D and for box-shaped boundaries in 3D.*

***Streszczenie.** Artykuł przedstawia zwarte postaci asymptotycznych warunków brzegowych na kołowych, eliptycznych i sferycznych brzegach. Warunki te mogą być wykorzystane do modelowania zagadnień pola elektrycznego 2D i 3D w obszarach nieograniczonych metodą elementów skończonych. Według najlepszej wiedzy autorów nie były one przedstawiane w literaturze w takiej postaci. Warunki pierwszego i drugiego rzędu mogą być łatwo zaimplementowane do programów metody elementów skończonych i zostały szczegółowo omówione dla dowolnego kształtu obszaru 2D oraz prostopadłościennego 3D. (**Ogólna, zwarta postać asymptotycznych warunków brzegowych dla zagadnień pola elektrycznego analizowanych metodą elementów skończonych**).*

Keywords: Asymptotic boundary conditions, finite element method, open boundary problems, static fields.
Słowa kluczowe: asymptotyczne warunki brzegowe, metoda elementów skończonych, zagadnienia o otwartych brzegach, pola stacjonarne.

Introduction

Many 2D and 3D electrical field problems can be considered as being of the exterior form, that is the problem domain is unbounded. Since the finite element method is a finite domain method, special techniques must be employed when the solution domain is infinite. Over the last three decades various methods of analysis for the open boundary static and quasi-static electromagnetic field problems have been investigated [1]-[10]. The literature on the subject is vast and the cited references should only be taken as illustrative examples. Unfortunately, very often it is not quite obvious how to implement these methods into existing classical finite element programs. Among the methods, asymptotic boundary conditions (ABCs) seem to be very attractive from the numerical point of view. In the present paper we discuss different aspects of the ABCs for the finite element analysis of 2D and 3D open boundary electrical field problems. The closed-form expressions for the Nth order ABCs (generalization of formulas presented in [9]) on circular, elliptical and spherical boundaries have been derived. To the best knowledge of the authors of this paper, the expressions, in such forms, have not yet been reported in the literature. The 1st and 2nd order ABCs, which can be implemented into existing finite element codes, are discussed in details, also for an arbitrary shape of the finite element region in 2D and for box-shaped boundaries in 3D. Implementation of the ABCs into commercial finite element software COMSOL Multiphysics is presented. Numerical examples are given.

Asymptotic boundary conditions on circular, elliptical and spherical boundaries

To solve elliptic boundary value problems in an infinite domain by the finite element method, it is normal to divide the unbounded domain by an artificial boundary Γ into an interior region R_i (where sources, heterogeneities, anisotropies, etc. may exist) and a residual, uniform region R_e. When using the finite element method in R_i, some boundary conditions must be imposed on the artificial boundary Γ. The boundary conditions (called the ABCs) should mimic the behavior of the unknown potential V at infinity and give reasonably accurate results in the interior region R_i. The electric potential V in the exterior region R_e (and in the outermost part of R_i) satisfies the Laplace equation:

$$\nabla^2 V = 0 . \tag{1}$$

The general solutions to (1), if the potential tends to zero at infinity, can be expressed as follows:

2D, polar coordinates (r, φ)

$$V(r,\varphi) = \sum_{n=1}^{\infty} r^{-n} F_{1n}(\varphi) , \tag{2}$$

2D, elliptical coordinates (η,ξ)

$$V(\eta,\xi) = \sum_{n=1}^{\infty} \exp(-n\eta)\ F_{2n}(\xi) , \tag{3}$$

3D, spherical coordinates (R, θ, φ)

$$V(R,\theta,\varphi) = \sum_{n=1}^{\infty} R^{-n} F_{3n}(\theta,\varphi) , \tag{4}$$

where $F_{1n}(\varphi)$, $F_{2n}(\xi)$ and $F_{3n}(\theta,\ \varphi)$ are functions of angles measured in a standard way in polar (2D), elliptical (2D) and spherical (3D) coordinates, respectively.

The solutions (2), (3) and (4) can be used to obtain ABCs on the artificial boundary Γ. The conditions are exactly correct when imposed at infinity but only approximately correct when imposed at a finite boundary. We will show in detail how to obtain the closed form expression for the Nth order ABC on a spherical boundary Γ. The condition can be constructed as a linear combination of the electric potential and its radial derivatives. Taking the partial derivative of the electric potential (4) with respect to R yields

$$\frac{\partial V(R,\theta,\varphi)}{\partial R} = -\frac{1}{R} V(R,\theta,\varphi) - \sum_{n=2}^{\infty} (n-1) \frac{F_{3n}(\theta,\varphi)}{R^{n+1}} . \tag{5}$$

Thus we see that

$$\frac{\partial V(d,\theta,\varphi)}{\partial R} + \frac{1}{d} V(d,\theta,\varphi) = O\left(d^{-3}\right) \tag{6}$$

which is recognized as the first-order ABC on a sphere of radius d.

The second derivative of the potential V can be expressed as follows:

$$(7)\quad \frac{\partial^2 V(R,\theta,\varphi)}{\partial R^2}=\sum_{n=1}^{\infty} n(n+1)\frac{F_{3n}(\theta,\varphi)}{R^{n+2}}=$$

$$=-\frac{\alpha_1^{(2)}}{R^2}V-\frac{\alpha_2^{(2)}}{R}\frac{\partial V}{\partial R}+\sum_{n=1}^{\infty}\left[n(n+1)+\alpha_1^{(2)}-\alpha_2^{(2)}n\right]\frac{F_{3n}(\varphi)}{R^{n+2}}$$

where $\alpha_1^{(2)}$ and $\alpha_2^{(2)}$ are coefficients.

Now, we want the expression $[n(n+1)+\alpha_1^{(2)}-\alpha_2^{(2)}n]$ to be equal to zero for $n = 1$ and $n = 2$. This leads to the following system of algebraic equations

$$\begin{pmatrix}1 & -1\\ 1 & -2\end{pmatrix}\begin{pmatrix}\alpha_1^{(2)}\\ \alpha_2^{(2)}\end{pmatrix}=-\begin{pmatrix}1\cdot 2\\ 2\cdot 3\end{pmatrix}\text{ and the result is }\begin{pmatrix}\alpha_1^{(2)}\\ \alpha_2^{(2)}\end{pmatrix}=\begin{pmatrix}2\\ 4\end{pmatrix}.$$

We obtain the second-order ABC

$$(8)\quad \frac{\partial^2 V(d,\theta,\varphi)}{\partial R^2}+\frac{4}{d}\frac{\partial V(d,\theta,\varphi)}{\partial R}+\frac{2}{d^2}V(d,\theta,\varphi)=O\left(d^{-5}\right).$$

Similarly, we can obtain the ABCs of the third and higher-orders. The Nth order ABC has the form

$$(9)\quad \frac{\partial^N V(d,\theta,\varphi)}{\partial R^N}+\sum_{m=1}^{N}\frac{\alpha_m^{(N)}}{d^{N-m+1}}\frac{\partial^{m-1}V(d,\theta,\varphi)}{\partial R^{m-1}}=O\left(d^{-2N-1}\right)$$

where $\partial^0 V/\partial R^0 = V$ and the coefficients $\alpha_m^{(N)}$ can be found as the solution of the following system of N linear equations

$$(10)\quad \alpha_1^{(N)}-\sum_{m=2}^{N}(-1)^m\frac{(n+m-2)!}{(n-1)!}\alpha_m^{(N)}=(-1)^{N+1}\frac{(N+n-1)!}{(n-1)!}$$

$n = 1, 2, \ldots, N.$

The result is surprisingly simple

$$(11)\quad \alpha_m^{(N)}=\binom{N}{m-1}\frac{N!}{(m-1)!},\ m = 1, 2, \ldots, N.$$

Curiously enough, the coefficients $\alpha_m^{(N)}$ arise in many different areas of mathematics and physics. They are known as coefficients of the Laguerre polynomials (e.g.: $N = 6 \Rightarrow \alpha_m^{(6)} = \{720, 4320, 5400, 2400, 450, 36\}$, where $m = \{1, 2, \ldots, 6\}$). To the best knowledge of the authors of this paper, the Nth order ABC (9) with coefficients (11) has not yet been reported in the literature in such a form.

In a similar way one can find the Nth order ABCs on circular and elliptical boundaries in 2D. Comparing (2) and (4), it is evident that the Nth order ABC on a circle of radius d can be obtained from (9) by replacing R with r and omitting θ. The Nth order ABC on an ellipse, $\eta = \eta_0$, is as follows

$$(12)\quad \frac{\partial^N V(\eta_0,\xi)}{\partial \eta^N}+\sum_{m=1}^{N}\beta_m^{(N)}\frac{\partial^{m-1}V(\eta_0,\xi)}{\partial \eta^{m-1}}=O\left\{\exp[-(N+1)\eta_0]\right\}$$

where $\beta_m^{(N)}=\begin{bmatrix}N+1\\ m\end{bmatrix}.$

The coefficients $\beta_m^{(N)}$ are known as the unsigned Stirling numbers of the first kind (well-known in combinatorics) and can be calculated by the recurrence relation

$$\begin{bmatrix}N+1\\ m\end{bmatrix}=N\begin{bmatrix}N\\ m\end{bmatrix}+\begin{bmatrix}N\\ m-1\end{bmatrix}$$

for $m > 0$, with the initial conditions:

$$\begin{bmatrix}1\\ 1\end{bmatrix}=1,\ \begin{bmatrix}N\\ 0\end{bmatrix}=0,\ \begin{bmatrix}0\\ 0\end{bmatrix}=1.$$

No doubt, that the closed-form expressions for the Nth order ABCs are very interesting from the theoretical point of view, however, in fact only the first and second order ABCs can be relatively easily implemented into existing finite element codes. The boundary contribution in the finite element method enters into a line integral representation over the outer boundary Γ, where the integrand is a product of the weighting function (shape function) and the normal derivative of the unknown function V. Hence, the ABCs need to be imposed on the normal derivative of V.

In the case of circular and spherical boundaries the radial derivatives are equivalent to the normal ones, but in an elliptic system of co-ordinates (η, ξ) the normal derivative is given by

$$(13)\quad \frac{\partial V}{\partial n}=\frac{1}{c\sqrt{\cosh^2\eta-\cos^2\xi}}\frac{\partial V}{\partial \eta}.$$

The Cartesian co-ordinates (x, y) are related to the elliptic co-ordinates (η, ξ) via $x = c\cosh\eta\cos\xi$ and $y = c\sinh\eta\sin\xi$. The semi-major and semi-minor axes of the ellipse $\eta = \eta_0$ are $a = c\cosh\eta_0$ and $b = c\sinh\eta_0$. Therefore, the first order ABC on an ellipse $\eta = \eta_0$ for the normal derivative is as follows

$$(14)\quad \left.\frac{\partial V}{\partial n}\right|_{\eta_0}=-\frac{1}{c\sqrt{\cosh^2\eta_0-\cos^2\xi}}V(\eta_0,\xi).$$

If we substitute the second order ABCs into the Laplace equation in polar, elliptical and spherical co-ordinates, we can eliminate the second order derivatives $\partial^2V/\partial r^2$, $\partial^2V/\partial\eta^2$ and $\partial^2V/\partial R^2$, respectively. Therefore, the second order ABCs can be expressed in required forms for the normal derivatives as

2D, polar co-ordinates (r, φ), $r = d$

$$(15)\quad \frac{\partial V}{\partial r}=-\frac{1}{3d}\left(2V-\frac{\partial^2 V}{\partial\varphi^2}\right)$$

2D, elliptical co-ordinates (η, ξ), $\eta = \eta_0$

$$(16)\quad \left.\frac{\partial V}{\partial n}\right|_{\eta_0}=-\frac{1}{3c\sqrt{\cosh^2\eta_0-\cos^2\xi}}\left(2V-\frac{\partial^2 V}{\partial\xi^2}\right)$$

3D, spherical co-ordinates (R, θ, φ), $R = d$

$$(17)\quad \frac{\partial V}{\partial R}=-\frac{1}{d}V+\frac{1}{2d\sin\theta}\left[\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V}{\partial\theta}\right)+\frac{1}{\sin\theta}\frac{\partial^2 V}{\partial\varphi^2}\right].$$

Asymptotic Boundary Conditions – Implementation

An implementation of the ABCs into the FEM program is relatively simple when the code of the program is available. However, commercial programs are usually closed-source software packages. Fortunately, in COMSOL Multiphysics software it is enough to choose so called *surface charge* boundary conditions, $-\boldsymbol{n}\cdot\boldsymbol{D} = \rho_s$ ($\boldsymbol{n}$ – unit normal vector, $\boldsymbol{D}$ – electric displacement, ρ_s – surface charge density), in the boundary conditions section. In the section modifications of typical boundary conditions are possible in an easy way by introducing user's own formulas.

The choice of the artificial boundary to be a circle or an ellipse in 2D, or a sphere in 3D, enabled simple derivation of the ABCs. However, such boundaries are uneconomical for problems with large aspect ratios. The ABCs can be relatively easily transferred for an arbitrary shape finite element region in 2D and box-shaped boundaries in 3D. It is, therefore, necessary to derive the appropriate normal derivative expressions for different sides/faces of the polygon/box representing the outer boundary. Using the relations between the Cartesian and polar/spherical coordinates, we have found the relevant ABCs.

2D, 1st order ABC, $u = d$, $u = r\cos\psi$, $v = r\sin\psi$ (Fig. 1)

$$-1_u \cdot \boldsymbol{D} = \varepsilon_0 \frac{\partial V}{\partial u} = -\varepsilon_0 \left(\frac{1}{d} V + \frac{v}{d} \frac{\partial V}{\partial v} \right) \tag{18}$$

3D, 1st order ABC, $x = d$

$$-1_x \cdot \boldsymbol{D} = \varepsilon_0 \frac{\partial V}{\partial x} = -\varepsilon_0 \left(\frac{1}{d} V + \frac{y}{d} \frac{\partial V}{\partial y} + \frac{z}{d} \frac{\partial V}{\partial z} \right) \tag{19}$$

3D, 2nd order ABC, $x = d$

$$\begin{aligned} -1_x \cdot \boldsymbol{D} &= \varepsilon_0 \frac{\partial V}{\partial x} = \\ &= \varepsilon_0 \left(\frac{-1}{2d} V + \frac{d^2 + y^2}{4d} \frac{\partial^2 V}{\partial y^2} + \frac{d^2 + z^2}{4d} \frac{\partial^2 V}{\partial z^2} + \frac{zy}{2d} \frac{\partial^2 V}{\partial y \partial z} \right) \end{aligned} \tag{20}$$

with the conditions on the other faces obtained by replacing x with y and y with x for $y = d$, and x with z and z with x for $z = d$ (in (20) we have used the 1st order ABC to approximate the terms $\partial^2 V/\partial x \partial y$ and $\partial^2 V/\partial x \partial z$; condition (20) differs from that given in [2]).

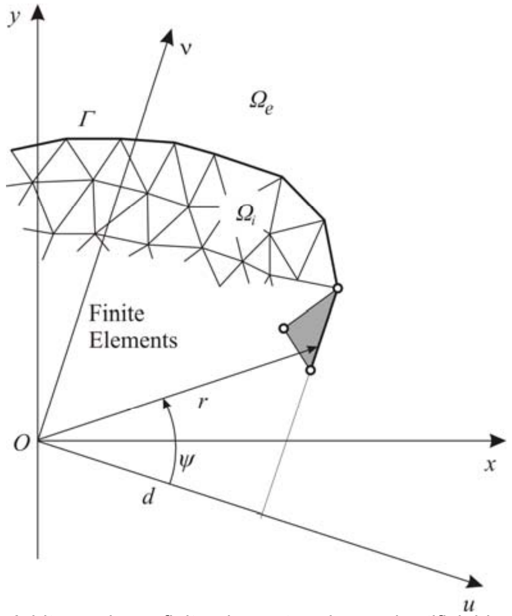

Fig. 1. Arbitrary shape finite element region and artificial boundary Γ in 2D

Numerical Results

Two examples, for which the exact solutions exist, have been analyzed to test the performance of the proposed ABCs.

Test Case A (2D)

The example was chosen in [1] for testing infinite elements. It deals with the scalar potential distribution due to a dipole consisting of two lines with charge densities $\pm\lambda$ on the x-axis at positions $x = \pm a$, respectively. The problem was solved numerically with $a = 0.5$ and $\lambda = \varepsilon_0$. Due to symmetry, the domain of solution was only one-quarter of the plane. Solutions of the problem by different techniques are compared qualitatively in Fig. 2 (equipotential lines are shown in each case). To check if the methods work well, a strange form of the finite element region with cut-out was chosen for calculation.

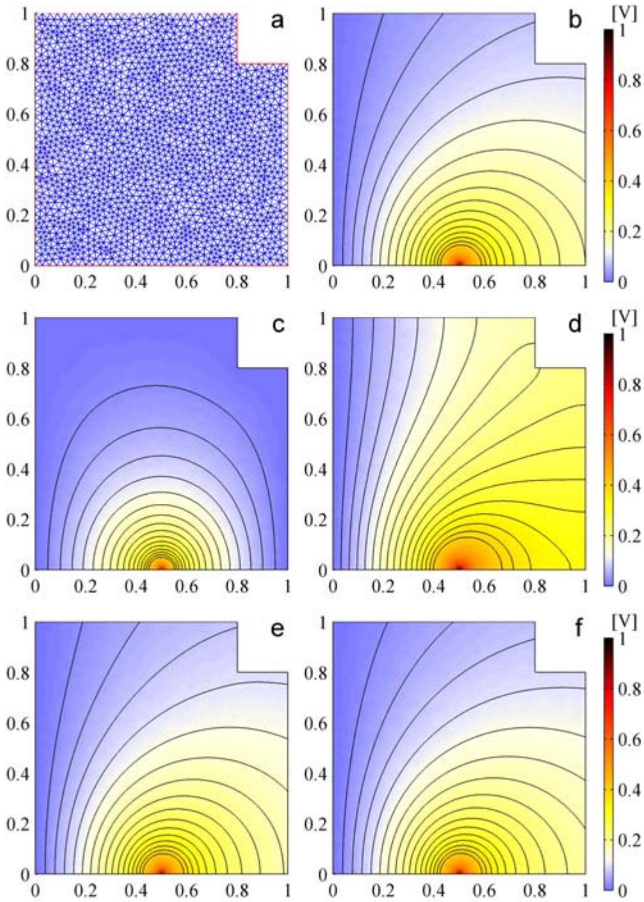

Fig. 2. Test problem A: a) finite element mesh, b) analytical solution, c) zero Dirichlet boundary condition, d) zero Neumann boundary condition, e) infinite elements [1], f) 1st order ABC

Test Case B (3D)

The test problem B is as follows [3]:

$$\nabla^2 V = 0\,, \quad -\infty < x < \infty\,, \quad -\infty < y < \infty\,, \quad -\infty < z < \infty$$

$$-\varepsilon_0 \left(\frac{\partial V}{\partial z} \right)_{z=0} = \begin{cases} \sigma & |x| \le h, \quad |y| \le h \\ 0 & |x| > h, \quad |y| > h \end{cases}$$

The test problem was solved numerically using finite elements and ABCs. The problem was also solved on the truncated mesh with zero Dirichlet boundary condition, $V = 0$, for comparison. For symmetry only the positive octant of three dimensional space was used with the homogeneous Neumann boundary condition on the symmetry planes. The domain R_i here is a cube $d \times d \times d$ and the planes $x = d$, $y = d$ and $z = d$ represent the artificial boundary Γ.

We compared exact and numerical solutions in the interior region R_i on the basis of the standard global error norm

$$\delta = \sqrt{\sum_{j=1}^{M} \left(V_j - V_{ej} \right)^2 \Big/ \sum_{j=1}^{M} V_{ej}^2} \;\; 100\%$$

where the subscripts "j" and "ej" refer to the computed values and the exact values obtained from the analytical solution. The summations were carried out over all nodes. The numerical values used were $h = 5$ mm, $d = 1$ cm, $\sigma/\varepsilon_0 = 1$ V/cm. Exemplary results are presented in Table I and in Figs. 3-5. It can be seen that Dirichlet boundary condition gives very inaccurate results but it is obvious that if the artificial boundary is moved far enough out the results must be better. In the case of the ABCs the outer boundary need not be far away from the source. The first and second order ABCs give similar results. The accuracy of the solutions is weakly dependent on the discretization. In the case of the 2nd order ABC a better mesh gives a more accurate solution.

TABLE 1. Global error norm, δ (%)

Boundary Condition	Predefined mesh size				
	Coarse	Normal	Fine	Finer	Extra fine
Dirichlet	68.77	68.032	67.852	68.056	68.12
1st order ABC, (19)	1.0448	1.0023	1.3598	1.1179	1.1773
2nd order ABC, (20)	1.6487	1.469	1.3936	1.1874	1.1345
Number of points	1346	3367	6441	19393	72592
Number of elements	6184	16872	33388	104773	407992

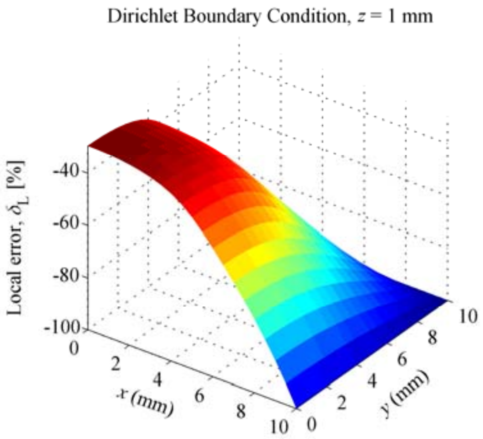

Fig. 3. Distribution of the local percentage error

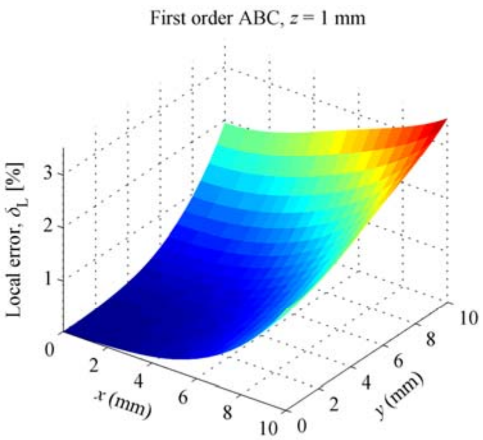

Fig. 4. Distribution of the local percentage error

Conclusions

New, previously unknown (to the best knowledge of the authors of this paper), general expressions for the Nth order ABCs, for both two- and three-dimensional electric field problems with open boundaries have been presented. Curiously enough, coefficients of the Nth order ABCs are known for as Laguerre and Stirling, and arise in many different areas of mathematics and physics. An implementation of the ABCs into commercial finite element software COMSOL Multiphysics via *surface charge* boundary conditions has been discussed.

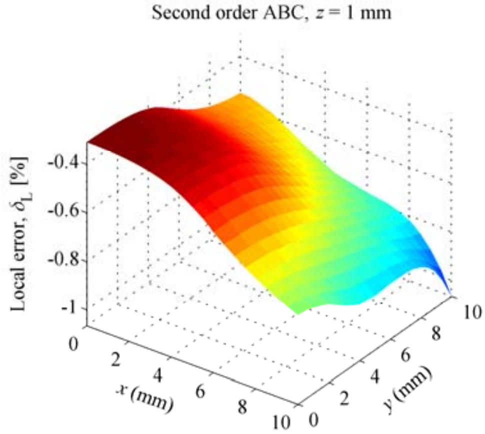

Fig. 5. Distribution of the local percentage error

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