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SINGULAR INTEGRATION IN BOUNDARY ELEMENT METHOD FOR HELMHOLTZ EQUATION FORMULATED IN FREQUENCY DOMAIN

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Abstract. Two ways of approximation of the BEM kernel singularity are presented in this paper. Based on these approximations extensive error analysis was carried on. As a criterion the preciseness and simplicity of approximation were selected. Simplicity because such approach would be applied for the tomography problems, so time of execution plays particularly significant role. One of the approximations which could be applied for the wide range of the arguments of the kernel were selected.

Keywords: partial differential equations, numerical analysis, function approximation, integral equations

CAŁKI OSOBLIWE W METODZIE ELEMENTÓW BRZEGOWYCH DLA RÓWNIANIA HELMHOLTZA SFORMUŁOWANEGO W PRZESTRZENI CZĘSTOTLIWOŚCI

Streszczenie. Dwie metody aproksymacji osobliwości funkcji Greena zaproponowano w tej pracy. Bazując na tych aproksymacjach dokonano wnikliwej analizy błędów. Jako kryterium wybrano dokładność i prostotę zaproponowanych aproksymacji. Prostotę dlatego, że takie podejście będzie proponowane w zagadnieniach tomograficznych. Tak więc czas odgrywa zasadniczą rolę. Wybrano aproksymację, która może być stosowana dla szerokiego zakresu argumentów.

Słowa kluczowe: równania różniczkowe cząstkowe, analiza numeryczna, aproksymacja funkcji, równania całkowe

Introduction

Singular integrals are an especially important question for the Boundary Element Method. Only for the Laplace's equation and for the basic boundary elements of the zero order, such an integral could be calculated analytically (see for example [11]). But the second order boundary element demands a special treatment [11]. Many technical problems described by Helmholtz equation [5, 7] demands integration of difficult functions like for example the Green function. Then, particularly useful is the procedure of approximation. In this paper some difficulties associated with this procedure will be presented. Unfortunately, there is no one single universal approximation for the Green function. Below, following [1, 6] we will show a simple approximation which could be useful for Helmholtz integral formulation in a frequency domain. As simple as possible because the approximation function should be easily integrable. But the kind of approximation depend on the value of the Green function arguments as it will be presented in this paper.

1. Treatment of singularity

For the small arguments $|x| \rightarrow 0$ the modified Bessel function (see for example Diffuse Optical Tomography (DOT) [2]) becomes, asymptotically simple power of their arguments [1]: for $n = 0$:

$$K_0(x) \cong -\ln(x) = \ln \frac{1}{x} \quad (1)$$

and for $n > 0$:

$$K_n(x) \cong \frac{(n-1)!}{2} \left(\frac{x}{2}\right)^{-n} \quad (2)$$

So, for the first order we will get:

$$K_1(x) \cong \frac{(1-1)!}{2} \left(\frac{x}{2}\right)^{-1} = \frac{1}{x} \quad (3)$$

Modified Bessel functions and their approximation for the small arguments are shown in Fig. 1.

As we can see in the next figure – Fig. 2 the approximation of the modified Bessel function of the second kind and first order is much better than for the same function but zero order. So, the small parameter in the case of the Helmholtz equation (DOT problems for example) mean that the arguments should not exceed value of 0.1.

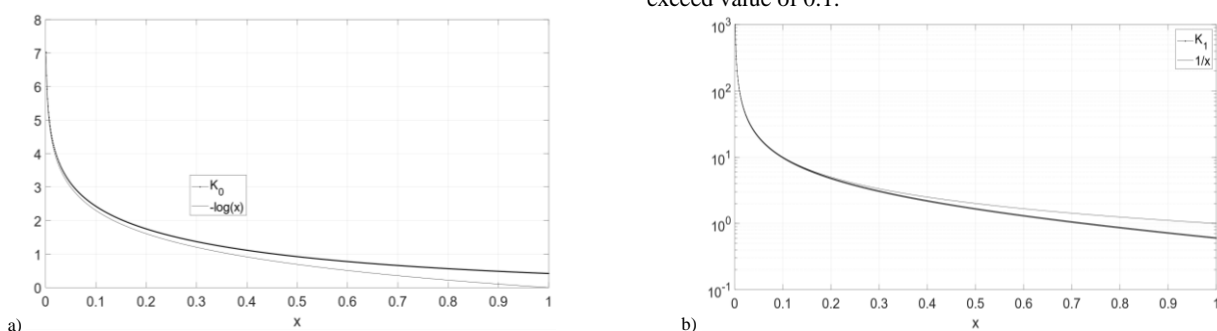


Fig. 1. Comparison for the small arguments between the modified Bessel function of the second kind and their approximation for a) zero order and b) first order (in semi-logarithmic scale)

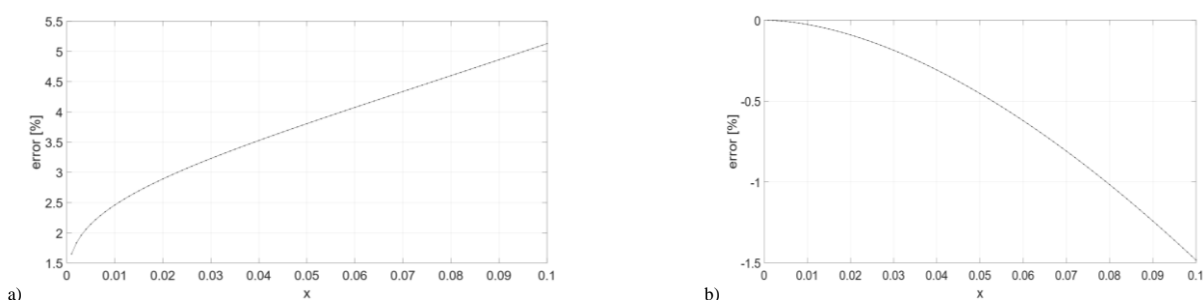


Fig. 2. Relative error of approximation for the small arguments for the modified Bessel function of the second kind a) zero order and b) first order

If the arguments become higher than more sophisticated approximations are required. Exists plenty of excellent approximations, for example in [1, 6, 12]. Following the [1] we have selected simple but effective approximation:

$$\tilde{K}_0(x) = -\left\{\ln\left(\frac{1}{2}x\right) + \gamma\right\}I_0(x) + \frac{\frac{1}{4}x^2}{(1!)^2} + \left(1 + \frac{1}{2}\right)\frac{\left(\frac{1}{4}x^2\right)^2}{(2!)^2} + \left(1 + \frac{1}{2} + \frac{1}{3}\right)\frac{\left(\frac{1}{4}x^2\right)^3}{(3!)^2} + \dots \quad (4)$$

where: \tilde{K}_0 and \tilde{I}_0 stands for approximation, γ is the Euler-Mascheroni constant [12].

The approximation of the function \tilde{I}_0 is the modified Bessel function of the first kind and zero order which could be approximated by [1]:

$$\tilde{I}_0(x) = 1 + \frac{\frac{1}{4}x^2}{(1!)^2} + \frac{\left(\frac{1}{4}x^2\right)^2}{(2!)^2} + \frac{\left(\frac{1}{4}x^2\right)^3}{(3!)^2} + \dots \quad (5)$$

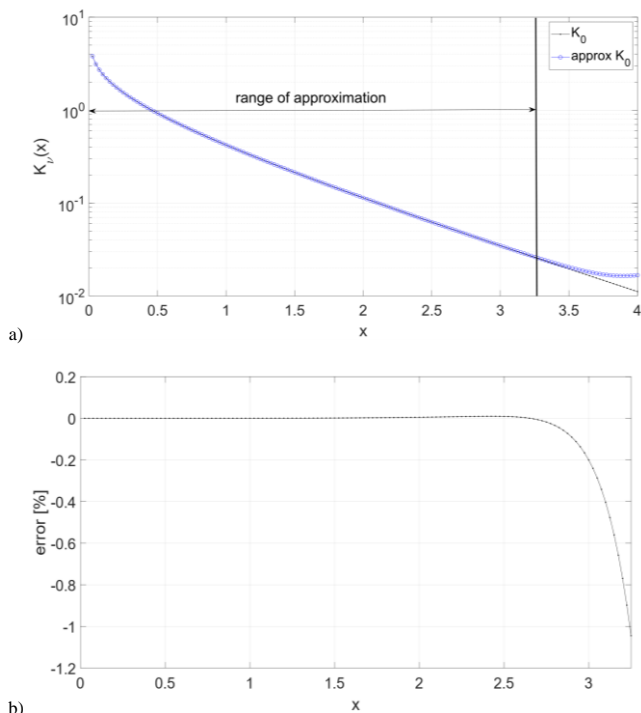


Fig. 3. a) approximation of the modified Bessel function of the second kind and zero order for the arguments less than 4 in a semilogarithmic scale and b) relative error of such approximation

The approximation proposed by Eq. (4) and (5) extend the range of arguments significantly and the approximation error does not exceed low value for example 0.3% as it is shown in Fig. 3b.

2. Governing equations

As an example of the problem leading to the Helmholtz equation let us consider the light transport in biological tissue [2].

The governing equation describing the light transport is a Boltzman equation approximated by diffusion equation (see for example [2]). For harmonic excitation it could be formulated in a frequency domain:

$$\nabla^2 \varphi(\mathbf{r}, \omega) - k^2 \varphi(\mathbf{r}, \omega) = q \quad (6)$$

where $k = \sqrt{\frac{\mu_a}{D} - i \frac{\omega}{cD}}$ [mm] – is the wave number, c speed of light, ω angular frequency, $D = \frac{1}{2(\mu_s + \mu_a)}$ [mm] for 2D space, μ_s, μ_a the optical parameters of the tissue and $q = \frac{q_s}{D}$ right hand side of Eq. (6) containing source of light.

On the external boundary the Robin boundary conditions are imposed:

$$\varphi(\mathbf{r}, \omega) + 2Dn \cdot \nabla \varphi(\mathbf{r}, \omega) = 0 \quad \forall \mathbf{r} \in \Gamma \quad (7)$$

After discretization for the Boundary Element Method, one must deal with a couple of unknowns in one node – $\varphi(\mathbf{r}, \omega)$ and $\frac{\partial \varphi(\mathbf{r}, \omega)}{\partial n}$, so it is convenient to present the boundary conditions in the following form:

$$\frac{\partial \varphi(\mathbf{r}, \omega)}{\partial n} = -\frac{1}{2D} \varphi(\mathbf{r}, \omega) \quad \forall \mathbf{r} \in \Gamma \quad (8)$$

The fundamental solution for BEM of the problem described by Eq. (6) is given by the Green function of the form (consult [2,3,6]):

$$G(|\mathbf{r} - \mathbf{r}'|, \omega) = \frac{1}{2\pi} K_0(k|\mathbf{r} - \mathbf{r}'|, \omega) \quad (9)$$

where K_0 – is the modified Bessel function of the second kind of zero order.

Using the Green's second identity to arrive at a boundary integral equation:

$$\begin{aligned} c(\mathbf{r})\varphi(\mathbf{r}, \omega) + \int_{\Gamma} \frac{\partial G(|\mathbf{r} - \mathbf{r}'|, \omega)}{\partial n} \varphi(\mathbf{r}', \omega) d\Gamma \\ = \int_{\Gamma} G(|\mathbf{r} - \mathbf{r}'|, \omega) \frac{\partial \varphi(\mathbf{r}', \omega)}{\partial n} d\Gamma + \\ - \int_{\Gamma} G(|\mathbf{r}_{is} - \mathbf{r}'|, \omega) q d\Omega \end{aligned} \quad (10)$$

where \mathbf{r} and $\mathbf{r}' \in \Gamma$, $\mathbf{r}_{is} \in \Omega$, and $G(|\mathbf{r}_{is} - \mathbf{r}'|, \omega)$ is the value of the fundamental solution at the point \mathbf{r}_{is} .

In optical tomography, concentrated light (point) sources are frequently used and modelled by Dirac delta function in a following way:

$$q = Q_{is} \delta_{is} \quad (11)$$

where Q_{is} is the magnitude of the light source and $\delta_{is}(|\mathbf{r}_{is} - \mathbf{r}'|, \omega)$ is the Dirac delta function which integral is equal to 1 at the point \mathbf{r}_{is} and zero elsewhere.

Assuming that there are no light sources, the equation (10) could be written:

$$\begin{aligned} c(\mathbf{r})\varphi(\mathbf{r}, \omega) + \int_{\Gamma} \frac{\partial G(|\mathbf{r} - \mathbf{r}'|, \omega)}{\partial n} \varphi(\mathbf{r}', \omega) d\Gamma = \\ = \int_{\Gamma} G(|\mathbf{r} - \mathbf{r}'|, \omega) \frac{\partial \varphi(\mathbf{r}', \omega)}{\partial n} d\Gamma \end{aligned} \quad (12)$$

Now the boundary integral equation (12) for constant boundary elements can be written in terms of local coordinate ξ instead of the boundary line Γ , as follows:

$$\begin{aligned} c(\mathbf{r})\varphi(\mathbf{r}) + \sum_{j=1}^M \varphi_j(\mathbf{r}') \int_{-1}^{+1} \frac{\partial G(|\mathbf{r} - \mathbf{r}'|)}{\partial n} J(\xi) d\xi = \\ = \sum_{j=1}^M \frac{\partial \varphi_j(\mathbf{r}')}{\partial n} \int_{-1}^{+1} G(|\mathbf{r} - \mathbf{r}'|) J(\xi) d\xi \end{aligned} \quad (13)$$

where M – is the total number of constant elements, and $J(\xi)$ – is the Jacobian of transformation:

$$\begin{aligned} J(\xi) = \frac{d\Gamma}{d\xi} = \sqrt{\left(\frac{dx(\xi)}{d\xi}\right)^2 + \left(\frac{dy(\xi)}{d\xi}\right)^2} = \\ = \sqrt{\left(\frac{x_3 - x_1}{2}\right)^2 + \left(\frac{y_3 - y_1}{2}\right)^2} = \frac{1}{2} L \end{aligned} \quad (14)$$

where x_3, y_3 and x_1, y_1 are the coordinates of the edge points of the zero-order boundary element and x_2, y_2 is a middle node when state function and its derivative is fixed, L is the length of element.

The functions under integral sign which contain the kernels can be substituted by the functions $A_{i,j}$ and $B_{i,j}$ as follows:

$$\begin{aligned} c(\mathbf{r})\varphi(\mathbf{r}) + \sum_{j=1}^M \varphi_j(\mathbf{r}') A_{i,j}(\mathbf{r}, \mathbf{r}') = \\ = \sum_{j=1}^M \frac{\partial \varphi_j(\mathbf{r}')}{\partial n} B_{i,j}(\mathbf{r}, \mathbf{r}') \end{aligned} \quad (15)$$

To form a set of linear algebraic equations, we take each node in turn as a load point \mathbf{r} and perform the integrations indicated in Eq. (13). This will result in the following system of algebraic equations:

$$[\mathbf{A}][\boldsymbol{\varphi}] = [\mathbf{B}] \left[\frac{\partial \boldsymbol{\varphi}}{\partial n} \right] \quad (16)$$

where the matrices $[\mathbf{A}]$ and $[\mathbf{B}]$ contain the integrals of the kernel's normal derivative $\frac{\partial G(|\mathbf{r} - \mathbf{r}'|)}{\partial n}$ and the kernels $G(|\mathbf{r} - \mathbf{r}'|)$ respectively, i.e. the functions $A_{i,j}$ and $B_{i,j}$ of Eq. (15).

It is apparent that the kernels in Eq. (12) may be written in more explicit form:

$$\begin{aligned} \frac{\partial G(|\mathbf{r}-\mathbf{r}'|, \omega)}{\partial n} &= \frac{\partial}{\partial n} \left(\frac{1}{2\pi} K_0(k|\mathbf{r}-\mathbf{r}'|, \omega) \right) = \\ &= -\frac{k}{2\pi} K_1(k|\mathbf{r}-\mathbf{r}'|, \omega) \frac{\partial R}{\partial n} \end{aligned} \quad (17)$$

where K_1 is the modified Bessel function of the second kind of order one.

The derivative of the radius R with respect to the unit outward normal n at the point \mathbf{r}' is calculated as follows:

$$\frac{\partial R}{\partial n} = \frac{\partial R}{\partial x} \frac{\partial x}{\partial n} + \frac{\partial R}{\partial y} \frac{\partial y}{\partial n} = \frac{\partial R}{\partial x} n_x + \frac{\partial R}{\partial y} n_y \quad (18)$$

where

$$\frac{\partial R}{\partial x} = \frac{x'-x}{R} \quad \text{and} \quad \frac{\partial R}{\partial y} = \frac{y'-y}{R}.$$

Now, the kernel from Eq. (13) can be rewritten more explicitly:

$$\frac{\partial G(|\mathbf{r}-\mathbf{r}'|, \omega)}{\partial n} = -\frac{k}{2\pi} K_1(k|\mathbf{r}-\mathbf{r}'|, \omega) \left(\frac{x'-x}{R} n_x + \frac{y'-y}{R} n_y \right) \quad (19)$$

When we put Eq. (17) into Eq. (13) than it can be solved numerically. However, the problem arises when the $\mathbf{r}' \rightarrow \mathbf{r}$ than the singularity of the integrand must be specially treated.

3. Singular integration for constant element

The singular integrals are a particularly important problem for integral formulation for the partial differential equations [4]. For the Dirichlet problem and for the Diffuse Optical Tomography (DOT) it was already solved [6,10,11]. However, for DOT integrand singularity only in case a small argument of the kernel, where successfully solved. Then the function in Eq. (10) which is the Bessel function was approximated by a quite simple equation (see for example Eq. (1)).

For many other problems like for example the acoustic ones [7, 8] it is insufficient and more sophisticated approximation is necessary (see for example Eq. (4) and Eq. (5)). After some mathematical operations Eq. (4) could be presented in the following form [1]:

$$\begin{aligned} \tilde{K}_0(x) &= -\ln\left(\frac{1}{2}x\right) I_0(x) - \gamma + 0.42278420 * \left(\frac{x}{2}\right)^2 + \\ &+ 0.23069756 * \left(\frac{x}{2}\right)^4 + 0.03488590 * \left(\frac{x}{2}\right)^6 + 0.00262698 * \\ &* \left(\frac{x}{2}\right)^8 + 0.00010750 * \left(\frac{x}{2}\right)^{10} + 0.00000740 * \left(\frac{x}{2}\right)^{12} + \epsilon \end{aligned} \quad (20)$$

where $|\epsilon| < 10^{-8}$.

The Bessel function of the first kind and zero order $I_0(x)$ appearing in the first term of Eq. (20) has the following shape and is completely covered by its approximation – Fig. 4.

In Fig. 4 it is clearly visible that function $I_0(x)$ it is not singular within the interesting us range of independent variable and its approximation is very precise (consult Fig. (4b)).

So, still we are facing the problem of integration of singular integrals because the first term of approximation is the logarithmic one. Some term of the kernel could be integrated in an analogous

way as for the Laplace's equation, but the rest term of integrand could be calculated using the Gauss quadrature. For this case, the $A_{i,j}$ coefficients are equal zero and the $B_{i,j}$ integrals can be calculated analytically and numerically as well. The distance between point \mathbf{r} and point $\mathbf{r}'(\xi)$ depends on local coordinate system in a following way: $R(\xi) = |\mathbf{r} - \mathbf{r}'(\xi)|$.

The entries of the matrices in Eq. (13) are:

$$\begin{aligned} B_{i,j}(\mathbf{r}, \mathbf{r}') &= \int_{-1}^{+1} G(|\mathbf{r}-\mathbf{r}'|) J(\xi) d\xi = \\ &= \int_{-1}^{+1} \tilde{K}_0(kR(\xi)) J(\xi) d\xi \end{aligned} \quad (21)$$

where \mathbf{r} depends on index i and \mathbf{r}' depends on index j and $J(\xi) = \frac{L}{2}$ is a Jacobian of transformation defined by Eq. (14), so:

$$\begin{aligned} B_{i,j}(kR(\xi)) &= \int_{-1}^{+1} \tilde{K}_0(kR(\xi)) J(\xi) d\xi = \\ &= \frac{L}{2} \int_{-1}^{+1} \left[-\ln\left(\frac{1}{2}kR(\xi)\right) I_0(kR(\xi)) - \gamma + \right. \\ &+ 0.42278420 * \left(\frac{kR(\xi)}{2}\right)^2 + 0.23069756 * \left(\frac{kR(\xi)}{2}\right)^4 + \\ &+ 0.03488590 * \left(\frac{kR(\xi)}{2}\right)^6 + 0.00262698 * \left(\frac{kR(\xi)}{2}\right)^8 + \\ &+ 0.00010750 * \left(\frac{kR(\xi)}{2}\right)^{10} + 0.00000740 * \left(\frac{kR(\xi)}{2}\right)^{12} \left. \right] d\xi \end{aligned} \quad (22)$$

To simplify consideration let us divide the integrand on two parts. The first one consists of the logarithmic term and the second one consists of the rest of the Eq. (20) as follows:

$$\begin{aligned} B_{i,i}(kR(\xi)) &= \frac{L}{2} \int_{-1}^{+1} \left[-\ln\left(\frac{1}{2}kR(\xi)\right) I_0(kR(\xi)) - \gamma \right] d\xi = \\ &= \frac{L}{2} \int_{-1}^{+1} \left[0.42278420 * \left(\frac{kR(\xi)}{2}\right)^2 + \right. \\ &+ 0.23069756 * \left(\frac{kR(\xi)}{2}\right)^4 + 0.03488590 * \left(\frac{kR(\xi)}{2}\right)^6 + \\ &+ 0.00262698 * \left(\frac{kR(\xi)}{2}\right)^8 + 0.00010750 * \left(\frac{kR(\xi)}{2}\right)^{10} + \\ &+ 0.00000740 * \left(\frac{kR(\xi)}{2}\right)^{12} \left. \right] d\xi \end{aligned} \quad (23)$$

The integral of the first part is the logarithmic type so we could calculate it analytically in the similar (integration by parts must be involved) way as for the Laplace's equation but for more complex cases a special logarithmically weighted numerical integration formula can be used [11]. Note that the limits of integration are from 0 to 1 instead of the -1 to $+1$ range used in the non-singular integrals of Boundary Integral Equations (BIE).

The remained part is not singular so it could be calculated numerically by the standard Gaussian rule.

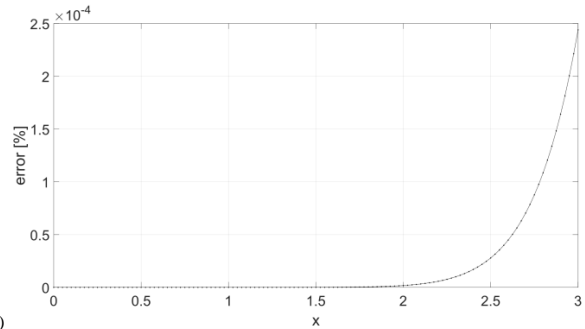
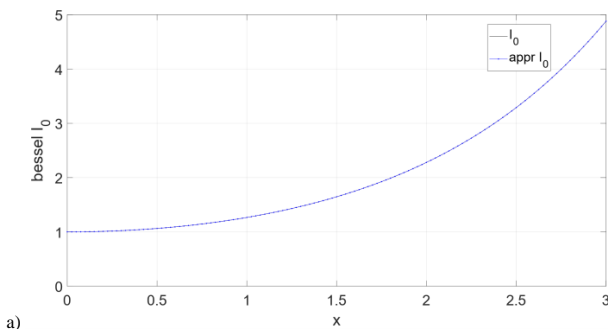


Fig. 4. a) The modified Bessel function of the first kind of zero order for the small arguments and b) relative error of approximation (see Eq. (5))

4. Benchmark solution

To solve the Helmholtz equation in the frequency domain, let us consider the excellent benchmark problem suggested by P. Jablonski in his monograph [6].

Inside the domain which is the interior of a rectangle of the width a and the height b as it is denoted in Fig. 5. On the boundary the following Neumann boundary conditions are imposed:

$$\frac{\partial \varphi}{\partial n} = \begin{cases} 0 & \text{when } y = 0, \\ 100 & \text{when } x = a, \\ 0 & \text{when } y = b, \\ 0 & \text{when } x = 0. \end{cases} \quad (24)$$

The analytical solution of the state function φ (see Eq. (6) and boundary conditions Eq. (7) and Eq. (24)) is equal to:

$$\varphi(\mathbf{r}(x, y)) = \frac{100 \cosh(2k)}{k \sinh(ak)} \quad (25)$$

where k is the wavelength, $a=4$ is the length of the rectangular area (Fig. 5).

Solutions of the problem (6) with the boundary conditions (7) for different wavelength are presented in the Fig. 6 and in the Fig. 7.

The bigger wave number the more rapid state function diminishing along the x axis direction.

Interesting is the error distribution of the state function along the boundary. In Fig. 9 it can be observed as the error rapidly erase on two corners where the Neumann boundary conditions were imposed. But only up to the value of 1.17%. It is quite satisfactory especially that no special treatment of the sharp corners was applied.

As the exact analytical solution exists it is possible to control exactness of the numerical solution within the internal points of the region.

In Fig. 9 for different wave numbers relative error was calculated for the point in the centre of the region. Coordinates of this point were: $(a/2, b/2)$. The error was calculated for two cases:

- 1) for the logarithmic approximation of the kernel,
- 2) for the approximation by the series suggested in [1].

The second case is much more precise for the Helmholtz equation than the simple logarithmic approximation as it is visible in the Fig. 9.

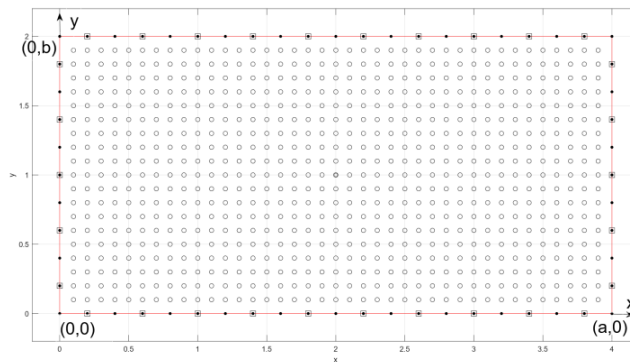


Fig. 5. Discretization of the region of interest with the internal points where the state function is calculated

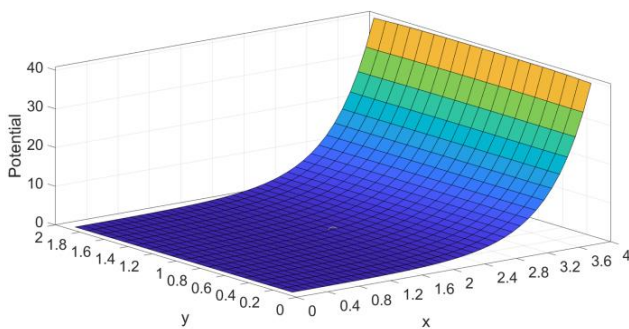


Fig. 6. Numerical solution for $k = \sqrt{4}$

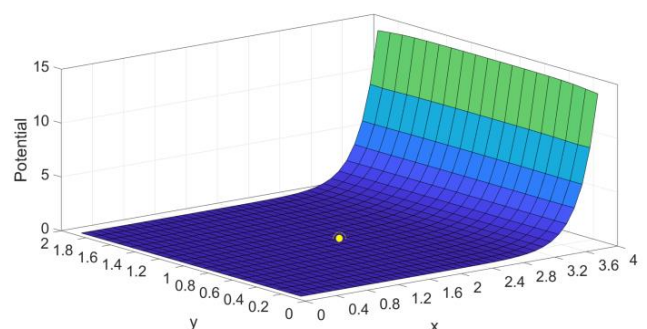


Fig. 7. Numerical solution for $k = \sqrt{20}$

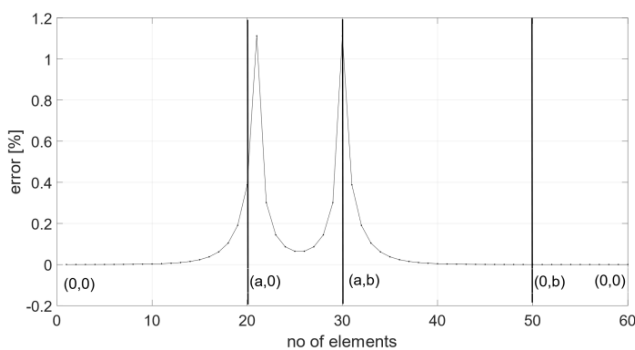


Fig. 8. Relative error distribution along the boundary

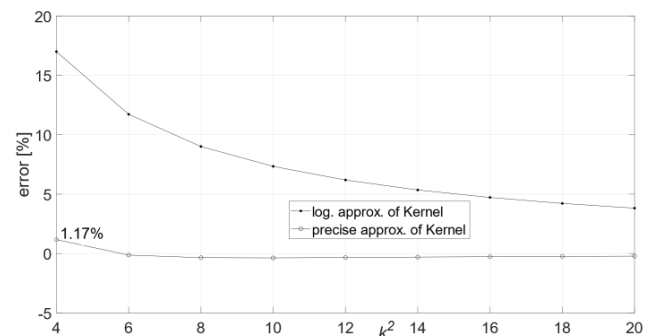


Fig. 9. Relative error distribution as a function of the wavelength with power two

5. Conclusions

Two ways of approximation of the kernels for the Helmholtz equation in the frequency domain were presented in this paper. Based on the benchmark provided in [6] error analysis was carried on for two cases of approximation of BEM singular integrands. The second one represents exceedingly high precision so it could be suitable for the imaging method for the different kind of tomography [9].

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