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Numerical calculation of singular integrals for different formulations of Boundary Element

***Abstract**. This paper presents a method of regularization for the numerical calculation of singular integrals used in different formulations of Boundary Element Method. The singular integrals arise when elements of order higher than zero are used for discretization. Very often in the Diffusive Optical Tomography for infant head modeling, triangular or square curvilinear boundary elements of the second order are used hence, our interest in the subject of effective and accurate calculation of singular integrals. Even for the classical formulation of BEM such a problem is extremely difficult. Some authors believe that the practical application possesses only flat triangular boundary elements of zero-order, and although there is some truth in this statement, Diffusion Optical Tomography elements of the second order show a significant advantage. This issue becomes even more interesting when we deal with the Galerkin BEM formulation offering the possibility of symmetrisation of the main matrix, which has fundamental importance for inverse problems. This matter becomes critical when we start to consider the Fourier BEM formulation, introduced by Duddeck. His approach provides the possibility of a solution in the case that there is no fundamental solution. The light propagation, which is described by the Boltzmann equation is such a case. Currently and most commonly, the Boltzman equation is approximated by the diffusion equation in strongly light scattering media. In the authors opinion, the problem of numerical integration of singular integrals has not yet been fully exhausted in the classic and Galerkin BEM formulation but the Fourier BEM formulation still expects the proposals of the solutions. Such an offer we would like to present in this paper*

Streszczenie.** W artykule przedstawiono metodę regularyzacji numerycznego obliczania całek osobliwych stosowanych w różnych rozwiązaniach Metody Elementu Brzegowego. Całki osobliwe powstają, gdy do dyskretyzacji zostaną użyte elementy wyższego rzędu niż zero. Bardzo często w dyfuzyjnej tomografii optycznej użytej do modelowania głowy dziecka używa się trójkątnych lub kwadratowych krzywoliniowych elementów brzegowych drugiego rzędu i dlatego nasze zainteresowanie dotyczy tematu skutecznego i dokładnego obliczenia całek osobliwych. Nawet w przypadku klasycznego sformułowania MEB ten problem jest wyjątkowo trudny. Niektórzy autorzy uważają, że praktyczne zastosowanie mają tylko płaskie trójkątne elementy brzegowe zerowego rzędu i chociaż w tym stwierdzeniu jest trochę prawdy, to dyfuzyjna tomografia optyczna stosując elementy brzegowe drugiego rzędu wykazuje znaczącą przewagę. Kwestia ta staje się jeszcze bardziej interesująca, gdy mamy do czynienia ze sformułowaniem Galerkina MEB, oferującym możliwość użycia symetrycznej macierzy współczynników, która ma fundamentalne znaczenie przy rozwiazywaniu problemów odwrotnych. Ta kwestia staje się krytyczna, gdy zastosujemy sformułowanie Fouriera w MEB, wprowadzoną przez Duddecka. Jego podejście daje szanse rozwiązania w przypadku braku rozwiązania fundamentalnego. Rozchodzenie światła, opisane przez równanie Boltzmanna jest takim przypadkiem. Obecnie, równanie Boltzmana jest przybliżane równaniem dyfuzji w ośrodkach silnie rozpraszających światło. W opinii autorów, problem numerycznego całkowania całek osobliwych nie został w pełni wyczerpany w klasycznej formule MEB i dla sformułowania Galerkina, ale formuła MEB Fouriera nadal oczekuje nowych rozwiązań. Propozycję takiego rozwiązania chcielibyśmy zaprezentować w tym artykule. **Metodę regularyzacji numerycznego obliczania całek osobliwych stosowanych w różnych rozwiązaniach Metody Elementu Brzegowego

Keywords: Boundary Element Method, Galerkin BEM, Fourier BEM, Numerical Integration of Singular Integrals.
Słowa kluczowe: Metoda Elementów Brzegowych (MEB), MEB Galerkina, MEB Fouriera, całkowanie numeryczne całek osobliwych.

Introduction

In the field of digital modeling, two methods are used at present: the Finite Element Method (FEM) and the Boundary Element Method (BEM). The latter is less common since there is much less the professional computer software that uses the BEM compared to FEM.

For a few decades rapid development of BEM can be observed [1, 5-7,9-12,14,15] resulting in an increase in BEM's application over time to, among other things, electromagnetic, thermal, and optical analysis [1, 5–7, 11]. Nevertheless it is not easy to find ready-to-use BEM implementations. The situation becomes even more difficult if we try to find free open source software and worse still if we need specialized BEM software applicable, for example, to Diffusion Optical Tomography. One of the reasons why this state is maintained might be the complexity of integration (in particular singular integrals) which needs to be done using BEM calculations. Of course, this is not a problem which cannot be overcome [12,14,15]. The need for the BEM calculations software exists and is unquestionable, but it has been only insignificantly implemented (Table 1 [10,11,12]). The other software packages for Boundary Element Methods is listed in Tab. 1. It is worth emphasizing that by no means the list is not complete.

Table 1. Commercial software implementing BEM [11,12].

Library (programme)	Environment (language)	Application
BEASY	Windows or Unix	Construction engineering
Integrated Engineering Software	Windows only	fields, wave, thermal analysis
GPBEST	Windows or Unix	acoustics, thermal analysis
Concept Analysis	Windows	stress analysis

It appears that industrial and scientific groups would like to have a well-designed platform for BEM calculations which should be universal but at the same time have modularity that easily enables application [8,14, 15].

Table 2. Free software implementing BEM [8,14, 15].

Library	Language	Distribution conditions	Application
ABEM (by Kirkup)	Fortran	commercial, open source	acoustics, Laplace and Helmholz problems
LibBem	C++	semi-commercial	Laplace equation
BEMLIB (Pozrikidis)	Fortran	GPL	Laplace, Helmholtz equations and Stokes flow
BIEPACK	Fortran	free open source	Laplace equation
BEA	Fortran	Distributed with the book	acoustics
MaiProgs [8]	Fortran	copyright © 2007 Matthias Maischak. Designed by Free CSS	Galerkin BEM for Laplace, Helmholtz, Lamé and Stokes

		Templates All templates are licensed under the Creative Commons Attribution 3.0 license	equations
HyENA (Hyperbolic and Elliptic Numerical Analysis [16])	C++	provided under the GNU Lesser General Public License	Laplace, Helmholtz and Lamé equations in 2D and 3D using the Galerkin or collocation approaches.
BETL (Boundary Element Template Library [Hiptmair and Kielhorn 2012; Kielhorn 2012])	C++	BETL is free for academic use in research and teaching	Laplace, Helmholtz and Maxwell equations in 3D using the Galerkin approach.
BEM++ [13]	C++ Phyton	open-source	Laplace, Helmholtz and Maxwell problems in three space dimensions.

The plan of this article is as follows. In section 2, a review of the foundations of boundary element methods and standard methods for integration of singular integrals is presented. Section 3 is devoted to a presentation of the major features of Numerical integration for Galerkin formulation of Boundary Element Method (GBEM) in 2D space only. The practical use of Fourier Boundary Element Method (FBEM) and numerical integration is demonstrated in section 4. Finally, in section 5, we discuss plans for further directions of our research.

A. Standard 3D Boundary Element Method and numerical integration of singular integrals

Let us consider Poisson's equation in three–dimensional space:

(1) $$\nabla^2 \Phi(r) = b,$$

where Φ stands for the arbitrary potential function for temperature or electric potential.

On the surface Γ of the volume under consideration Ω, the Robin boundary conditions are imposed:

(2) $$\frac{\partial \Phi(\mathrm{r})}{\partial n} = m_R \Phi(\mathrm{r}) + n_R$$

where m_R and n_R are known coefficients for the Robin boundary condition [2].

The fundamental solution for 3D space is:

(3) $$G\left(\left|\mathrm{r}-\mathrm{r}'\right|\right) = \frac{1}{4\pi R}$$

where $R = |\mathbf{r} - \mathbf{r}'|$ is a distance between **r** (the source point) and **r'** (the field point).

The integral form for the Eq. (1) is:

(4) $$c(\mathrm{r})\Phi(\mathrm{r}) + \int_\Gamma \frac{\partial G\left(\left|\mathrm{r}-\mathrm{r}'\right|\right)}{\partial n}\Phi(\mathrm{r}')d\Gamma(\mathrm{r}') = $$
$$= \int_\Gamma G\left(\left|\mathrm{r}-\mathrm{r}'\right|\right)\frac{\partial \Phi(\mathrm{r}')}{\partial n}d\Gamma(\mathrm{r}') + \int_\Omega bG\left(\left|\mathrm{r}-\mathrm{r}'\right|\right)d\Omega(\mathrm{r}')$$

When the distance between the source point and the element over which the integration is performed is sufficiently large relative to the element size, the standard Gauss–Legendre quadrature formula works efficiently. But when the distance tends to zero then integrals become singular and special integration strategy should be applied. Let us consider quadrilateral boundary elements. The strategy used for integration rectangular boundary elements is as follows: mapping them at first onto 2D curvilinear coordinates and then dividing them into two or three triangles and subsequently onto the standardized square. The whole procedure is shown in Fig. 1.

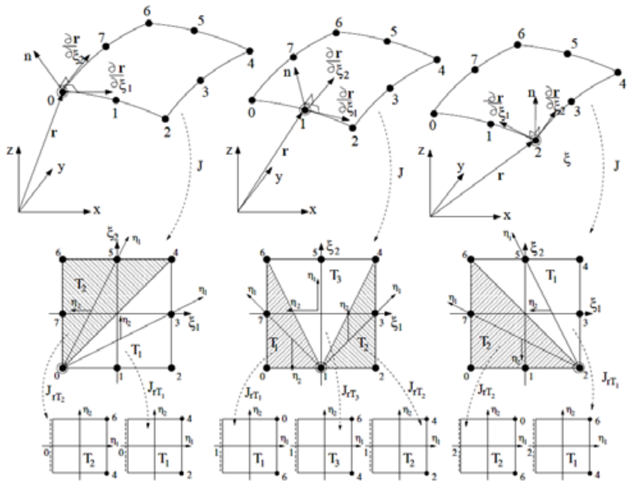

Fig. 1. Local coordinates of the quadrilateral boundary element and a mapping strategy [12].

Finally, in all the above cases the Gauss – Legendre method of numerical integration was used [4]. The coordinates of the numerical integration points and the weights are available in the literature or in the internet, for example, [4,12].

Fourier Boundary Element Method (FBEM) and numerical integration

Let us briefly introduce some elements of basics of Fourier approach to BEM [5].

To obtain the Fourier transform of the Galerkin BEM, all quantities have to be extended from domain Ω to the space $\mathbb{R}^n$. This can be achieved by defining a cutoff distribution χ [5], multiplying all quantities by χ and finally transforming the quantities into Fourier space.

$$F(u) = u, \qquad u \in L_1\left(R^n\right), \qquad i = \sqrt{-1}$$

The n-dimension Fourier transform is defined as:

(5) $$\hat{u}\left(\hat{x}\right) = \int_{R^n} u(x)\, e^{-i\langle x,\hat{x}\rangle}dx,$$

(6) $$\left\langle x, \hat{x}\right\rangle = \sum_{k=1} x_k \hat{x}_k.$$

The discretized Fourier BEM leads to an algebraic system identical to that obtained in the original space:

(7) $$\sum_i K_u^{ji}u^i = F_u^j + \sum_i H_u^{ji}t^i - \sum_i G_u^{ji}u^i$$

where now, the matrices and vectors are computed in the transformed space:

(8)
$$F_u^j = \frac{1}{\left(2\pi\right)^n}\left\langle \hat{\Phi}_t^j\left(-\hat{x}\right), \hat{f}\left(\hat{x}\right)\hat{U}\left(\hat{x}\right)\right\rangle,$$
$$G_u^{ji} = \frac{1}{\left(2\pi\right)^n}\left\langle \hat{\Phi}_t^j\left(-\hat{x}\right), \hat{\Phi}_u^i\left(\hat{x}\right)\hat{A}_t^i\,\hat{U}\left(\hat{x}\right)\right\rangle,$$

$$H_u^{ji} = \frac{1}{(2\pi)^n}\left\langle \hat\Phi_t^j(-\hat x), \hat\Phi_t^i(\hat x)\hat U(\hat x)\right\rangle,$$

$$K_u^{ji} = \frac{1}{(2\pi)^n}\left\langle \hat\Phi_t^j(-\hat x), \hat p_u^i(\hat x)\right\rangle.$$

The meaning of the $\hat{\mathrm{A}}_t$ and $\hat p_u(x)$ in the equations (8) is the following one:

- $\hat{\mathrm{A}}_t = -\nu \cdot \nabla$ (where: ∇, ν - the gradient and the outer unit normal) is the boundary operator transformed to $\hat{\mathrm{A}}_t$ in the Fourier space,
- $\hat p_u(x)$ is the transformed polynomial trial functions.

The main advantage of the FBEM is that the integrals extend formally over the entire R_n and therefore the Fourier transformation can be applied to these integral equation.

A. Numerical example

The Fourier formulation of BEM is only presented for the boundary integral equations limited to constant elements and 2D space (Fig. 2). As the test example, the Dirichlet problem of the Poisson equation is considered:

(9) $\Delta u(x) = -f(x), \quad x\in\Omega, \quad u(x) = u_\Gamma = 0, \quad x\in\Gamma.$

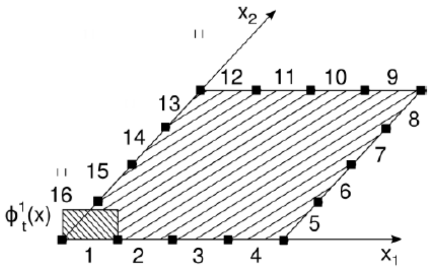

Fig. 2. Quadratic domain under consideration.

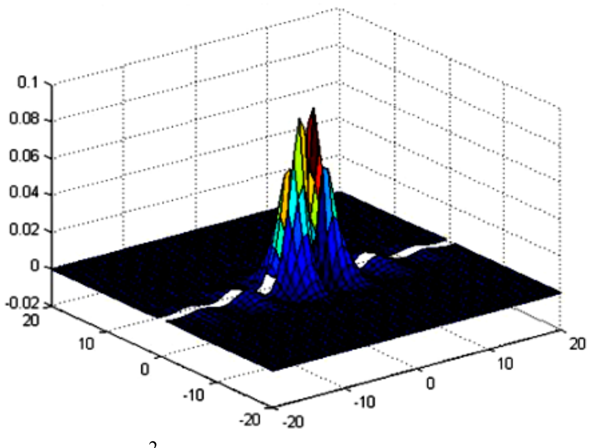

Fig. 3. Function $\mathbb{R}^2$ space.

The Dirichlet problem is solved in a quadratic two-dimensional domain Ω [0, 1]x[0, 1]. At the boundaries, u=0 is imposed. The interior is subjected to stationary heat source f. The boundary Γ is divided into 16 elements. In our case when the source function f=1 the exemplary entries are:

$$H^{12} = \frac{1}{(2\pi)^2}\left\langle \hat\Phi_t^1(-\hat x), \hat\Phi_t^2(\hat x)\hat U(\hat x)\right\rangle =$$

$$= \frac{1}{(2\pi)^2}\int_{R^2} \frac{\left[i\left(e^{i\hat x_1/4}-1\right)\right]\left[i\left(e^{-i\hat x_1/2}-e^{-i\hat x_1/4}\right)\right]}{-\hat x_1\hat x_1\left(-\hat x_1^2-\hat x_2^2\right)} d\hat x_1 d\hat x_2,$$

(10)

$$F^1 = \frac{1}{(2\pi)^2}\int_{R^2} \hat\Phi_t^2(-\hat x)\hat U(\hat x)\, d\hat x =$$

$$= \frac{-1}{(2\pi)^2}\int_{R^2} \frac{\left[i\left(e^{i\hat x_1/4}-1\right)\right]}{-\hat x_1\left(-\hat x_1^2-\hat x_2^2\right)} d\hat x_1 d\hat x_2, \quad \text{for } f_0 = 1.$$

B. The integration in $\mathbb{R}^2$ space

The integrand (see Eq. (10)) has a singularity along the axis of the coordinate system x_1, x_2 as it is shown in Fig. 3. Therefore, in order to successfully integrate such a function numerically, we divide the space R^2 into four quarters in accordance with Fig. 4.

After dividing the area into four infinite subareas and unifying the limits of integration (for easier algorithmization) we have:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x_1,x_2)dx_1dx_2 =$$

$$\int_0^{\infty}\int_0^{\infty} f(x_1,x_2)dx_1dx_2 + \int_0^{\infty}\int_{-\infty}^{0} f(x_1,x_2)dx_1dx_2 +$$

(11) $$+\int_{-\infty}^{0}\int_{-\infty}^{0} f(x_1,x_2)dx_1dx_2 + \int_{-\infty}^{0}\int_0^{\infty} f(x_1,x_2)dx_1dx_2 =$$

$$\int_0^{\infty}\int_0^{\infty} f(x_1,x_2)dx_1dx_2 + \int_0^{\infty}\int_0^{\infty} f(-x_1,x_2)dx_1dx_2 +$$

$$+\int_0^{\infty}\int_0^{\infty} f(-x_1,-x_2)dx_1dx_2 + \int_0^{\infty}\int_0^{\infty} f(x_1,-x_2)dx_1dx_2$$

Every subarea was transformed into a local coordinate system using the transformation ***T*** (the same for both x_1 and x_2 coordinates):

(12) $$x(\xi) = \frac{2\xi}{(1-\xi)^2}$$

where ξ is the local coordinate.

Unfortunately, such transformation introduced an oscillatory behavior of the function near to the boundary (Fig. 5). That will demand a very careful numerical integration.

After the transformation, the integral in the local coordinate system over each boundary element is equal to:

(13) $I = \int_{-1}^{1}\int_{-1}^{1} f\left(x_1(\xi_1), x_2(\xi_2)\right)\, J(\xi_1)J(\xi_2)\, d\xi_1 d\xi_2$

where: f means any function and

(14) $$J(\xi) = \frac{dx}{d\xi} = \frac{2(1+\xi)^2}{\left(1-\xi^2\right)^2}$$

is the Jacobian of transformation.

To achieve a satisfactory precision of integration the 80 integration points were used (see Fig. 6).

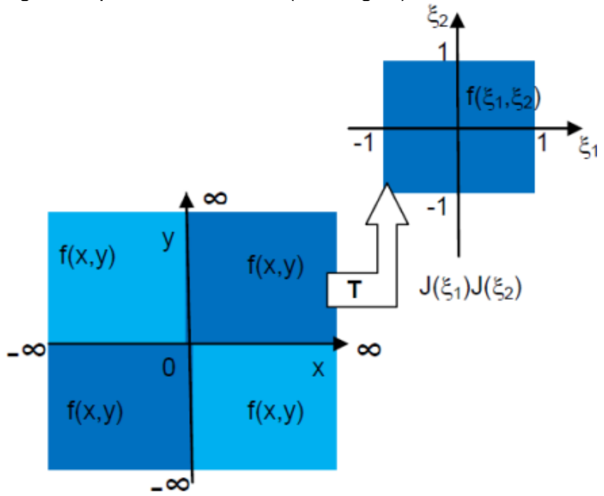

Fig. 4. One of the quarter after mapping into the square.

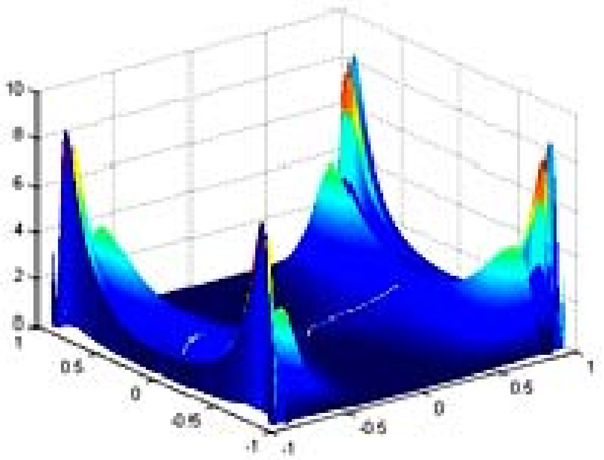

Fig. 5. Function after mapping into square.

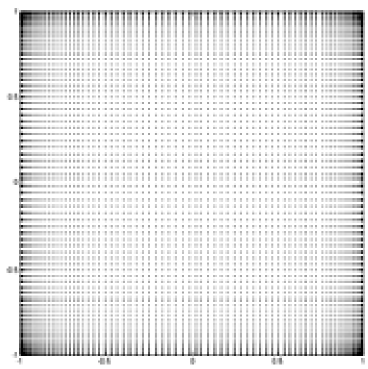

Fig. 6. For numerical calculation - the 80 integration points were used.

Table 3. Comparison between exact and numerical integration

Exact solution	Numerical solution	Relative error [%]
0.166736	0.166059	0.41
0.336249	0.343520	2.16
0.336249	0.343520	2.16
0.166736	0.166059	0.41

In the table 3 results of numerical calculations are presented for the region and it discretization shown in Fig. 2. As we can see the discretization is not particularly dense – only 16 elements. As an exact solution, the analytical integration was treated (see Table 3).

Conclusion

This paper presents the regularization method for the integration of singular integrals for three different formulations of BEM: classical, Galerkin's and Fourier. With the help of numerical experimentation the effectiveness of the proposed method of integration was proven. Additionally, the authors tried to demonstrate that the degree of difficulty increases in the direction from the classical to the Fourier approach.

A very interesting formulation of the BEM was presented by Duddeck in his monograph [5], however the problem of integration was not looked into thoroughly. One of the main goals of this paper was to address this gap. Without effective numerical integration the Fourier approach to BEM becomes useless.

The authors believe that the Fourier's formulation holds great potential, in particular for the Diffusion Optical Tomography. The light propagates in accordance with the Boltzman equation [2]. The Boltzman equation does not have a fundamental solution. Therefore classical formulation of BEM becomes useless. Usually in case of environments strongly dissipative the Boltzmann equation is approximated by the diffusion equation [2, 12].

The authors are aware that this work on numerical integration particularly in the R2 space still require further work in order to improve the accuracy and reduce the number of integration points. This will be a critical issue for real discretization with the aid of thousands of boundary elements.

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