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ON THE ACCURACY OF ADAPTIVE QUADRATURES IN THE NUMERICAL INTEGRATION OF SINGULAR GREEN'S FUNCTIONS FOR LAYERED MEDIA

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Abstract. *This work investigates methods for the numerical evaluation of definite integrals of singular functions. Such integrals arise in the solution of many problems by the boundary element method (BEM). Influence functions describing time-harmonic axisymmetric loads within half-spaces, for example, which occur in many soil-foundation interaction problems, can be derived in terms of Hankel integral transforms. These integrals contain a number of singularities corresponding to shear, pressure and Rayleigh wave numbers. This work investigates integration schemes to deal with singular integrands, taking as a representative example the aforementioned influence function. A normalization of the integration interval according to Hankel's wave number causes the singularities to fall within a predictable region, after which only an oscillatory-decaying behavior of the integrand remains. The interval where the singularities fall is divided at the singularities into a number of subintervals. The singularities were located by direct mathematical manipulation of the integrands for the case at hand. A technique of regularizing the singularities by the synthetic division of polynomials and its subsequent integration with a modified Legendre quadrature was used to solve the integral. A straightforward adaptive Gaussian quadrature was used for comparison. The results are compared with the analytical integration in representative cases. The findings in this article contribute to the accuracy in the numerical solution of integrals that are common in many branches of mathematical physics, remarkably in Green's functions and their applications in the BEM.*

Keywords: *Numerical integration, Singular integrands, Adaptive Quadratures, Greens functions.*

1 INTRODUCTION

The numerical integration of singular functions is a routine task within the boundary element method (BEM). Most Green's functions required as fundamental solutions by the BEM demand some kind of singularity to be integrated. Attempts to deal with this issue resort to substituting the fundamental solution by a non-singular one, or by improving directly the numerical methods for dealing with these functions (Dumont, 1994).

One such substitution of the singular integrand consists in smoothing out the singularities by introducing a small damping to the elastic constants. This is a reasonable hypothesis in the modeling of unbound media, for example, since they present a significant geometric damping (Gaul, 1999; Christensen, 2010). This approach is not useful for perfectly elastic media.

The second approach to deal with singular integrands is to design numerical techniques tailored specifically for singular integrands. Standard quadratures, such as Gauss or Simpson rules, are no longer practical, since a large number of integration points are needed to achieve the required accuracy (Luo, Liu and Berger, 1998). Adaptive quadratures, however, are improvements on the idea of regular quadratures in that they use some sophisticated algorithm for the adequate placement of quadrature nodes for specific integrands. Dumont (1994) proposed a technique for integration of quasi-singular integrals of different shapes, which consists of regularizing the integrand in order to obtain two expressions that can be evaluated by the Gauss-Legendre quadrature and an analytical integral. Lachat and Watson (1976) developed an adaptive element subdivision method using an error estimator for the numerical integration. Telles (1987) used quadratic and cubic variable transformations in order to weaken the near singularity before applying Gauss quadrature. Guigianni and Casalini (1987) introduced a technique that consists of the addition and subtraction of integrand terms to transform a singular integral into a regular one, which can be assessed through a numerical quadrature.

This work investigates numerical integration schemes for the specific case of Green's functions for the axisymmetric vertical displacement of a 3D transversely isotropic homogeneous half-space due to axisymmetric vertical loads. A solution for this problem has been provided by Rajapakse and Wang (1993) in terms of Hankel transforms in cylindrical coordinates and Fourier expansion with respect to the θ-variable (Muki, 1960). The fundamental solution is expressed in terms of Lipschitz-Hankel integrals, which contain a number of singularities corresponding to shear, pressure and Rayleigh wave numbers, and oscillating-decaying terms due to the Bessel functions arising from the Hankel transforms. Rajapakse and Wang (1993) suggested a normalization of the integration interval which causes the singularities to fall within a predictable region, after which only the oscillatory-decaying behavior of the integrand remains. This article brings a study on the localization of the singularities in the integrand. This step allows the singular region to be divided into a number of sections that begin and end in a singularity, which is required by some adaptive quadrature schemes. Despite being focused on a specific case of Green's function, this study brings important insights into the localization of singularities and their relation to wavenumbers in unbound media, and into the selection of appropriate integration schemes for these media.

2 STATEMENT OF THE PROBLEM

This work is invested in the accurate numerical evaluation of definite integrals of continuous, differentiable functions posessing a finite number of singularities within the integration interval. No attention is given at this point to the computational efficiency of the integration scheme. For the present analysis, a representative Green's function is considered, described as follows.

Consider a three-dimensional, transversely isotropic half-space, with a cylindrical coordinate system $O(r, \theta, z)$, defined such that the z-axis is perpendicular to the plane of isotropy (Rajapakse and Wang, 1993). The axisymmetric vertical displacement of a point of coordinates (r, z) due to an axisymmetric unit vertical load uniformly distributed on a disc of unit radius at the surface of the half-space is given by:

$$u_{zz} = \delta^2 \int_0^\infty u^*_{zz}(\zeta)\zeta d\zeta \tag{1}$$

where

$$u^*_{zz} = -(a_7 A e^{-\delta\xi_1 z} + a_8 C e^{-\delta\xi_2 z}), \tag{2}$$

$$\frac{a_7}{\delta\xi_1} = \frac{a_8}{\delta\xi_2} = J_0(\delta\zeta r), \tag{3}$$

$$A = +\frac{b_{52}}{b_{21}b_{52} - b_{51}b_{22}} \frac{J_1(\zeta)}{\zeta\mu}, \tag{4}$$

$$C = -\frac{b_{51}}{b_{21}b_{52} - b_{51}b_{22}} \frac{J_1(\zeta)}{\zeta\mu}, \tag{5}$$

$$b_{2i} = [\alpha\delta^2\xi_i^2 - (\kappa - 1)\delta^2\zeta^2\vartheta_i] J_0(\delta\zeta r), \tag{6}$$

$$b_{5i} = -(1 + \vartheta_i)\delta^2\xi_i J_1(\delta\zeta r). \tag{7}$$

in which J_m is the Bessel function of the first kind and m^{th} order, and μ is Lamé's constant. The other variables are presented in Appendix.

In Eq. (1), δ is a normalized frequency of excitation, and $\zeta = \lambda/\delta$, in which λ is the Hankel space variable. Because of the normalization of the Hankel integration interval from λ to ζ, which encapsulates all excitation frequencies into δ (Rajapakse and Wang, 1993), all the singularities in $u^*_{zz}(\zeta)$ fall within a predictable interval, namely $0 \leq \zeta \leq \zeta'$. ζ' is found empirically to be slightly under 1.2.

3 INTEGRATION SCHEME

This work addresses the integration of Eq. (1) within its singular interval ($0 \leq \zeta \leq \zeta' = 1.2$). The proposed integration scheme is divided into two parts: the localization of the singularities and an analysis of their physical meaning in the present case, and the integration of the singular interval by special methods in the subintervals bound by the singularities.

3.1 Localization of singularities for u^*_z

An analysis of the integrand shows that $\xi_1 = 0$ and $\xi_2 = 0$ correspond to two singularities in $u^*_{zz}(\zeta)$. The substitution of these values into (2) results in

$$\zeta_P = \pm\sqrt{\frac{1}{\beta}} \quad \text{and} \tag{8}$$

$$\zeta_S = \pm 1. \tag{9}$$

These singularities, arising from $\xi_1 = 0$ and $\xi_2 = 0$ correspond respectively to the pressure and shear wave numbers of the half-space (Barros, 1996). The third singularity in the integrand is found when the denominator of A and C, Eqs. (4) and (5), equals zero, that is, $b_{21}b_{52} = b_{22}b_{51}$:

$$d^4 f^2 y^2 + \alpha(-1 + (1 + \beta f)y + d^2 y(2 + y(-4 - 2\beta f^2 + 2y))) + \alpha^2(1 + y(-2 + y+ \beta(-2 + (4 + \beta f^2 - 2y)y))) = 0 \tag{10}$$

where $d = (-1 + \kappa)$, $f = (1 - y)$, and $\sqrt{y} = \zeta_R$. Equation (10) can be solved by numerical methods. ζ_R, the singularity resulting from the solution of (10), corresponds to the Rayleigh wave number in the present half-space (Barros, 1996). Figure 1 shows the singularities in $u^*_{zz}(\zeta)$ for a set of material parameters in which $\zeta_P = 0.577$, $\zeta_S = 1$ and $\zeta_R = 1.088$.

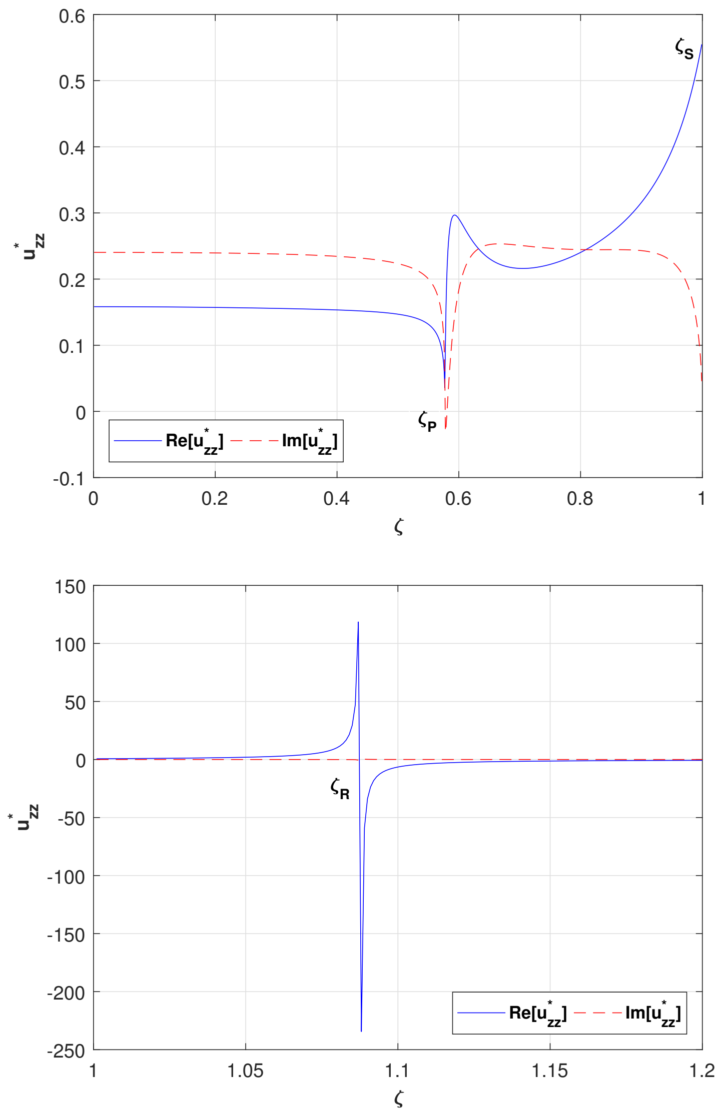

Figure 1: Singularities in the expression of $u^*_{zz}(\zeta)$.

3.2 Integration Methods

In the present work, an adaptive Gaussian quadrature (AGQ) and a special quadrature proposed by Dumont (1994) have been used to integrate Eq. (1) within $0 \leq \zeta \leq \zeta' = 1.2$. The goal of both AGQ and Dumont's methods is to find an approximation to the definite integral of a function $f(x)$,

$$I = \int_0^1 f(x)dx. \tag{11}$$

AGQ approximates I through

$$I \approx \sum_{i=0}^{n-1} w_i f(\xi_i), \tag{12}$$

where ξ_i are the roots of the Legendre polynomial, w_i are corresponding weights and $f(\xi_i)$ is the integrand of I evaluated at the point ξ_i. The AGQ differs from regular Gaussian quadratures in that the placement of ξ_i are adaptively selected by special algorithms to concentrate more points where the integral is more difficult to be obtained. Since implementations of AGQ are so classical and overly studied, this work simply utilizes a widely available implementation provided by Molenberghs and Verbeke (2005) as benchmark.

On the other hand, Dumont (1994) proposed a technique for the approximation of I based on the synthetic division of two polynomials for regularizing the integrand given by:

$$I = \int_0^1 f(\xi)d\xi = \int_0^1 \frac{g(\xi)}{w(\xi)}d\xi \approx GL\int_0^1 \frac{g(\xi)}{w(\xi)}d\xi + R_1C_1 + R_2C_2, \tag{13}$$

where $g(\xi)$ and $w(\xi)$ are regular and singular functions comprised in $f(\xi)$, respectively. The first term of right-hand side can be evaluated numerically by ordinary Gaussian quadrature, whereas R_1C_1 and R_2C_2 are additional correction terms.

In order to illustrate Dumont's method, consider the following integral, with singularities at $x = 1.002$ and $x = 1.5$:

$$I = \int_0^1 f(x)dx = \int_0^1 \frac{cos(\omega x)}{(x-1.002)(x-1.5)}dx, \tag{14}$$

In this case, the regular and singular functions required by Dumont's method are:

$$g_1(\xi) = cos(\omega\xi) \quad \text{and} \tag{15}$$
$$w_1(\xi) = (\xi - 1.002)(\xi - 1.5). \tag{16}$$

Applying Dumont's technique yields:

$$I = GL\int_0^1 \frac{g_1(\xi)}{w_1(\xi)}d\xi + R_1C_1 + R_2C_2, \tag{17}$$

Table 1 presents the errors in the approximation of I in Eq. (14) by AGQ and Dumont's technique for six different values of the parameter ω. It can be seen that Dumont's technique produces consistently better approximations to I than AGQ, regardless of ω, and that AGQ cannot provide accurate approximations for large values of ω.

Table 1: Approximations to I by AGQ and Dumont's methods.

ω	Exact - I	AGQ	Relative error	Dumont	Relative error
0.01	10.27666753622319	10.275241697360935	1.3874E-04	10.276667536223107	8.1241E-15
0.1	10.234280729940446	10.232861971609912	1.3862E-04	10.234280729940426	1.9092E-15
1	6.305681855006313	6.3049138335704722	1.2179E-04	6.305681855001178	8.1427E-13
10	-7.03860689689728	-7.0374262087954262	1.6774E-04	-7.038606896889339	1.1281E-12
100	1.103959757332552	1.1026112321488046	0.0012	1.103959781367154	-2.1771E-08
500	-1.1893735202493794	0.4897605625302468	1.5210	-1.189373520197007	4.7440E-11

As a second illustration, we consider the following integral:

$$I_2 = \int_0^1 Y_0(\alpha x)dx, \tag{18}$$

where $Y_0(x)$ is the Bessel function of the second kind and order zero, which is singular at $x = 0$ for all values of α (Fig. 2). For this integrand, the regular and singular functions are given by:

$$g_2(\xi) = 1 \quad \text{and} \tag{19}$$

$$w_2(\xi) = \frac{1}{Y_0(\alpha x)}. \tag{20}$$

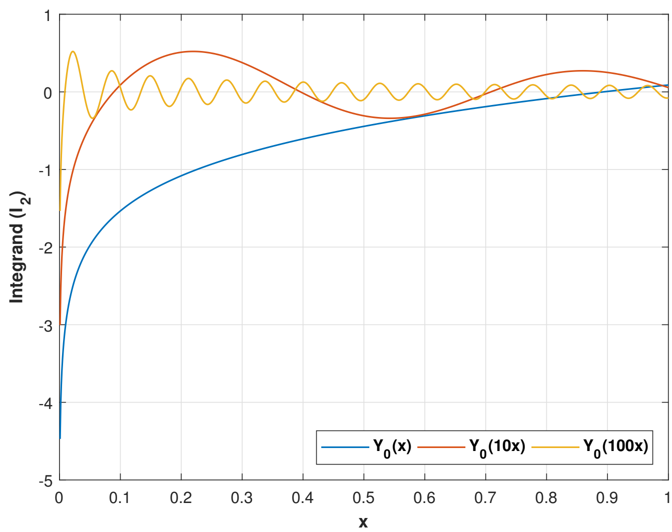

Figure 2: Bessel function of second kind.

Table 2 compares the integration errors for Eq. (18) by AGQ and Dumont's technique, for three values of α. Notice that AGQ becomes inaccute for higher values of α, whereas Dumont's technique presents good agreement throughout the present analysis.

Table 2: Errors related for integral Eq. (12).

α	Exact - I_2	AGQ	Error	Dumont	Error
1	-0.6370693766074229	-0.63691175319250881	2.4741E-04	0.637069376607423	1.7427E-16
10	0.02412903183228272	0.024286654932335852	0.0065	0.024129031832267	6.5149E-13
100	-0.0001959806485341	-0.00003838899537912	0.8041	-0.000195980648534	2.5862E-13

3.3 Integration of $u^*_{zz}(\zeta)$

In this section, the present integration scheme has been applied to integrate Eq. (1). The integration interval is defined as $0 \leq \zeta \leq \zeta' = 1.2$, which contains three singularities (see Section 3.1). The integration interval is divided into four subintervals, namely $0 < \zeta < \zeta_P$, $\zeta_P < \zeta < \zeta_S$, $\zeta_S < \zeta < \zeta_R$, and $\zeta_R < \zeta < \zeta' = 1.2$. Each subinterval is re-scaled into $0 < \zeta < 1$, in order to match the form of Eq. (13). The integration of the oscillatory-decay region, $u^*_{zz}(\zeta > \zeta' = 1.2)$, has been discussed by Cavalcante, Azevedo and Labaki (2017) and is not shown here.

The regular and singular functions for the integrand of u_{zz} are given by:

$$g_{u^*_{zz}} = (-a_7 b_{52} J_1(\zeta) e^{-\delta\xi_1 z} - a_8 b_{51} J_1(\zeta) e^{-\delta\xi_2 z})\zeta\delta^2 \quad \text{and} \tag{21}$$

$$w_{u^*_{zz}} = (b_{21} b_{52} - b_{51} b_{22})\zeta c_{44}. \tag{22}$$

The results shown here consider a half-space with Lamé constants $\mu = \lambda = 1$, mass density $\rho = 1$, and measuring point $(r, z) = (0, 1)$ (consistent units).

Figure 3 shows a comparison of the integration of Eq. (1) with the present technique and with a classical AGQ. The AGQ implementation is not capable of integrating the elastic case; a small damping is necessary in order for the algorithm to be able to deal with the singularities. A damping $\eta = 0.01$, introduced according to Christensen's elastic-viscoelastic principle, is considered in this comparison (Christensen, 2010). Fig. 3 shows that the present implementation agrees with the AGQ algorithm, and that it is capable of considering viscoelastic cases as well.

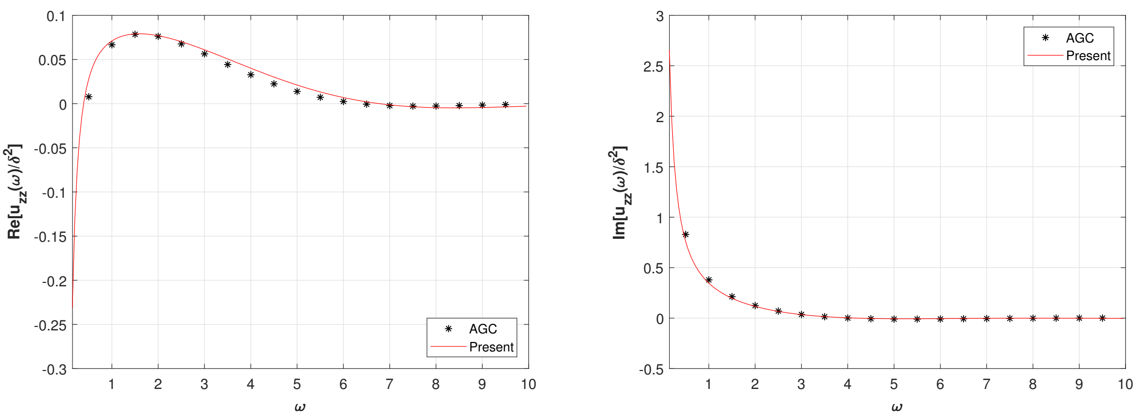

Figure 3: Real and imaginary parts of $u_{zz}(\omega)/\delta^2$ obtained by AGQ and present technique.

On the other hand, Fig. 4 shows the integration of Eq. (1) for the elastic case ($\eta = 0$). These results cannot be reproduced by the AGQ algorithm.

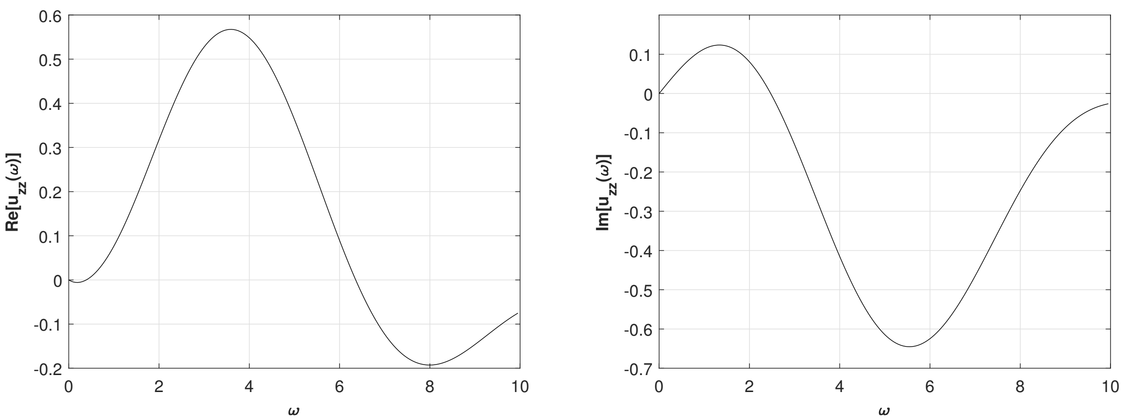

Figure 4: Real and imaginary parts of $u_{zz}(\omega)$, elastic case.

4 CONCLUSIONS

This article dealt with the numerical evaluation of singular integrals. The method was specifically tailored for the case of Green's functions that commonly come up in both direct and indirect formulations of the boundary element method. The article showed that in the case of a homogeneous half-space, the integrals by which the displacement field is described contain a finite number of singularities corresponding to shear, pressure and Rayleigh wave numbers of the medium. These singularities were located by analytical and numerical analysis of the integrand, and used as bounds for subdomains of integration. The integral in each subdomain was evaluated according to Dumont's method. The result from the singular integration showed good agreement with a classical adaptive quadrature algorithm.

5 APPENDIX

This appendix lists the remaining parameters appearing in Eq. (2).

$$\vartheta_{1,2} = \frac{\alpha\xi_{1,2}^2 - \zeta^2 + 1}{\kappa\zeta^2},$$

$$\xi_{1,2}(\zeta) = \frac{1}{\sqrt{2\alpha}}(\gamma\zeta^2 - 1 - \alpha \pm \sqrt{\Phi})^{\frac{1}{2}},$$

$$\Phi(\zeta) = (\gamma\zeta^2 - 1 - \alpha)^2 - 4\alpha(\beta\zeta^4 - \beta\zeta^2 - \zeta^2 + 1),$$

$$\alpha = \beta = 2 + \frac{\lambda}{\mu}, \quad \kappa = 1 + \frac{\lambda}{\mu}, \quad \delta^2 = \frac{\rho\omega^2}{\mu} \quad \text{and} \quad \gamma = 1 + \alpha\beta - \kappa^2,$$

where μ and γ are Lamé constants, ρ is the mass density and ω is the oscillatory frequency.

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