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3D Galerkin integration without Stokes' theorem

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Abstract

A direct approach to calculating the hypersingular integral for a three-dimensional Galerkin approximation is presented. The method does not employ either Stokes' theorem or a regularization process to transform the integrand before the evaluation is carried out. Integrating two of the four dimensions analytically, the potentially divergent terms arising from the coincident and adjacent edge integrations are identified and canceled exactly. The method is presented in the simplest possible situation, the hypersingular kernel for the Laplace equation, and linear triangular elements. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Boundary integral method; Singular integrals; Galerkin approximation; Stokes' theorem; Laplace equation

1. Introduction

At the heart of any implementation of the boundary integral method is singular integration. This topic has therefore been studied extensively, and a review of current practices, along with references to the literature, is contained in the volume edited by V. and J. Sladek [37]. Much of the attention in recent years has deservedly focused on the hypersingular equation [5,23], and in this regard it is appropriate to note here that the article by Cruse and Van Buren [7] was one of the first to confront the analysis of this equation. This has proved to be quite an interesting subject, and in particular, the difficulties inherent in *collocating* the hypersingular kernel have now been discussed extensively [6,12,16,21,27–29].

The growing popularity of the Galerkin and symmetric-Galerkin methods is due, at least in part, to the technical problems encountered in marrying collocation and hypersingular integration. An excellent introduction to Galerkin can be found in the text [1], and a recent review with extensive references is Ref. [3]; a few basic references are Refs. [18,19,26,35,36]. The analysis of the two-dimensional Galerkin singular integrals is relatively easy, and both direct and regularization techniques are available [1,4,10,13,20,32,34]. However, methods for the three dimensional integral are less straightforward, relying on manipulating the integrand in some fashion. The most widely used technique is to invoke Stokes' theorem (integration by parts) to reduce the order of the kernel singularity [2,8,9,24]. This results in line integrals over element edges, and the cancellation of pairs of integrals due to reversal of orientation neatly removes the potentially disastrous terms. The thesis by Lutz [25] contains a complete discussion of Stokes vectors and boundary integral equations (see also the related papers [30,31]).

The only drawback of this 'indirect' approach is that, for the particular equation under study, one must be able to implement the integration by parts — for complicated Green's functions, the Stokes vector might not be available. For this reason, it is desirable to have available a more direct approach to evaluating the Galerkin hypersingular integral. For two-dimensional Galerkin boundary integral analysis, a direct method, utilizing analytic integration to explicitly identify and cancel the divergent contributions, was presented in Ref. [13]. The analogous scheme for three-dimensional problems is described herein. A direct approach, also relying on analytic integration, has recently been presented by Salvadori [33,34]. While the methods therefore have much in common, one key difference is that, in this paper, the Hadamard Finite Part [17,22] is not employed to define and evaluate the integrals.

The general situation can be quite involved, so this paper focuses on demonstrating the basic integration procedures for an overly simple situation: the hypersingular kernel for the Laplace equation, employing linear interpolation over triangular elements that coincide with the parameter space domain. Even for this 'simple situation' the computations are somewhat complicated, and symbolic computation is

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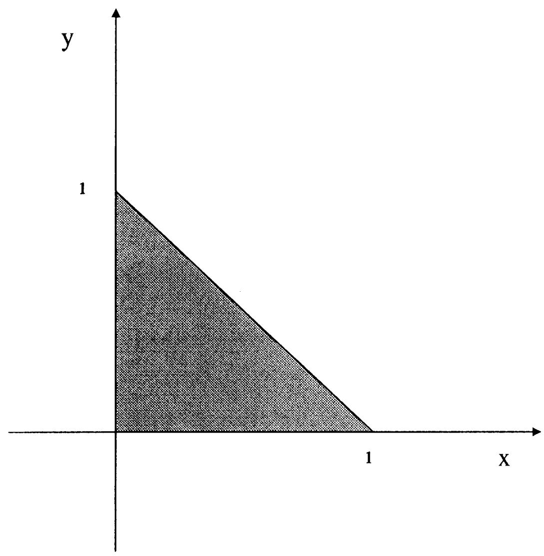

Fig. 1. Right triangle which doubles both as the parameter space and the surface element for the coincident integration.

employed to ease some of the burden of the analytical work. The goal is to explicitly identify the divergences in the coincident and adjacent integrations, and to show that the necessary cancellation occurs. This cancellation is analogous to the behavior seen in the two dimensional case [13], although in three dimensions materializing the divergent terms requires integrating two of the four dimensions analytically. It is hoped that treating this simple situation will provide a clear understanding of the origins of the divergent terms, without all the complications of a general analysis. What follows therefore is *not* a complete discussion of an algorithm: the remaining details needed to implement this approach in a boundary integral approximation will be published elsewhere [14].

2. Hypersingular Galerkin integral

The hypersingular integral for the three-dimensional Laplace equation $\nabla^2\phi = 0$ is

$$\int_\Sigma \phi(Q)\frac{\partial^2 G}{\partial N \partial n}(P,Q)\,\mathrm{d}Q. \tag{1}$$

Here $n = n(Q)$, $N = N(P)$ denote the unit outward normal on the boundary surface Σ, P and Q are points on Σ, and ϕ is the potential function. For the point source fundamental solution $G(P,Q) = 1/(4\pi r)$, the differentiation of the Green's function results in

$$\frac{\partial^2 G}{\partial N \partial n}(P,Q) = \frac{1}{4\pi}\left(\frac{n\cdot N}{r^3} - 3\frac{(n\cdot R)(N\cdot R)}{r^5}\right), \tag{2}$$

where $R = Q - P$ and $r = \|R\|$.

As is standard practice, the boundary potential is approximated in terms of its element nodal values $\{\phi_j\}$ and shape functions $\psi_j(Q)$, i.e.

$$\phi(Q) = \sum_j \phi_j \psi_j(Q). \tag{3}$$

In a Galerkin approximation, the boundary integral equations are enforced by weighting the equation with a particular shape function $\psi_k(P)$, and integrating with respect to P. Thus, Eq. (1) becomes

$$\sum_j \phi_j \int_\Sigma \psi_k(P)\int_\Sigma \psi_j(Q)\frac{\partial^2 G}{\partial N \partial n}(P,Q)\,\mathrm{d}Q\,\mathrm{d}P. \tag{4}$$

As mentioned above, for the purposes of this paper it suffices to employ a simple three-noded linear triangular element, defined by the shape functions

$$\psi_1(\eta,\xi) = 1 - \eta - \xi,$$
$$\psi_2(\eta,\xi) = \eta, \tag{5}$$
$$\psi_3(\eta,\xi) = \xi.$$

The (η,ξ) parameter space is the right triangle $0 \le \eta \le 1$, $0 \le \xi \le 1$, $\eta + \xi \le 1$ (see Fig. 1). As there are two surface integrations, we use (η,ξ) for the outer P integration and (η^*,ξ^*) for Q.

Decomposing the surface Σ into elements creates three types of singular integrals in Eq. (4): *coincident*, when the P and Q elements are the same, and *adjacent edge* and *adjacent vertex*, when the two elements either share a common edge or a common vertex. We define these singular integrals in terms of a 'limit to the boundary' [11,15]: the source point P is replaced by $P + \epsilon N(P)$, and after sufficient integration, the limit $\epsilon \to 0$ is considered. In this paper, we are concerned with potentially divergent terms, of the form $\log(\epsilon)$, that appear in the coincident and adjacent edge integrals. Although the individual integrals are not finite, these log terms do in fact vanish when the integrals are added. Nevertheless, in any implementation the integrals are calculated separately, and clearly the divergent terms cannot be left to cancel numerically. In the Stokes procedure, pairs of line integrals (over the same edge but with opposite orientation) cancel, and this implicitly removes the divergences. The direct evaluation method will explicitly banish the $\log(\epsilon)$ terms, leaving the numerical algorithm to evaluate *finite* integrals.

The coincident and adjacent edge cases are examined in the next two sections. The adjacent vertex case must of course also be integrated appropriately, but since the kernel is only singular at one point, this type of integral is sufficiently innocuous that no divergent terms appear. Thus, the treatment of this integration will not be of concern here.

3. Coincident integration

As in Ref. [13], all the somewhat tedious work required to evaluate the integrals can be automated using a symbolic computation program. For convenience, these scripts are available over the web at http://www.epm.ornl.gov/~gray.

Again for the purposes herein, it is not necessary to treat the entire coincident integral

$$\int_E \psi_k(P) \int_E \phi(Q) \frac{\partial^2 G}{\partial N \partial n}(P,Q)\, dQ\, dP. \tag{6}$$

Rewrite this quantity as

$$\int_E \psi_k(P)\phi(P) \int_E \frac{\partial^2 G}{\partial N \partial n}(P,Q)\, dQ\, dP$$
$$+ \int_E \psi_k(P) \int_E (\phi(Q) - \phi(P)) \frac{\partial^2 G}{\partial N \partial n}(P,Q)\, dQ\, dP \tag{7}$$

and note that the coefficient $\phi(Q) - \phi(P)$ in the second term reduces the order of the singularity at $Q = P$. The divergences are therefore limited to the first integral, and thus terms of the form

$$\int_E \psi_k(P)\psi_j(P) \int_E \frac{\partial^2 G}{\partial N \partial n}(P,Q)\, dQ\, dP \tag{8}$$

must be examined.

The element E is defined by the three nodes $P_1 = (0,0,0)$, $P_2 = (0,1,0)$, and $P_3 = (1,0,0)$,, i.e. the same as the parameter domain (with $\eta = x$, $\xi = y$, see Fig. 1). For the Q-integration we first employ polar coordinates centered at (η,ξ)

$$\eta^* - \eta = \rho\cos(\theta), \qquad \xi^* - \xi = \rho\sin(\theta) \tag{9}$$

as illustrated in Fig. 2. The (ρ,θ) integration must be split into three subtriangles, as the formula for the ρ upper limit (as a function of θ) changes. In the following, we carry out the calculation for the subtriangle associated with $\xi^* = 0$, the remaining two cases are similar. The integration limits in this case are

$$0 \le \rho \le \rho_L, \qquad \rho_L = -\frac{\xi}{\sin(\theta)}, \tag{10}$$

$$\theta_1 \le \theta \le \theta_2, \qquad \theta_1 = -\frac{\pi}{2} - \tan^{-1}\left(\frac{\eta}{\xi}\right),$$
$$\theta_2 = -\frac{\pi}{2} + \tan^{-1}\left(\frac{1-\eta}{\xi}\right). \tag{11}$$

Expressing the kernel function in polar coordinates, and

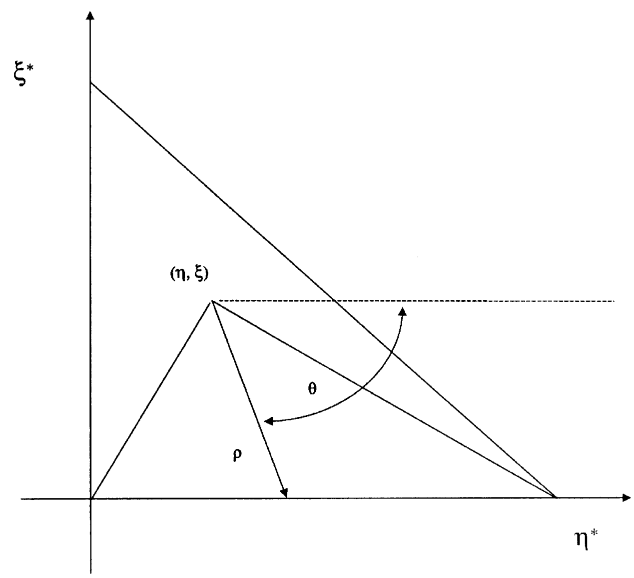

Fig. 2. Polar coordinate system for the coincident integration.

employing the boundary limit procedure, Eq. (8) is

$$\int_0^1 d\eta \int_0^{1-\eta} d\xi \psi_k(\eta,\xi)\psi_j(\eta,\xi)$$
$$\times \int_{\theta_1}^{\theta_2} d\theta \int_0^{\rho_L} \rho\left(\frac{1}{(\rho^2+\epsilon^2)^{3/2}} - 3\frac{\epsilon^2}{(\rho^2+\epsilon^2)^{5/2}}\right) d\rho. \tag{12}$$

The ρ integration is easily evaluated analytically, but this is unfortunately not sufficient to display the divergent terms. As the dependence of the integrand on θ is harmless, an integration with respect to P is necessary. However, the required interchange in the order of integrations is impeded by the fact that θ_1 and θ_2 depend on η and ξ; to get around this, introduce the variable t, $0 \le t \le 1$, via

$$\theta = \frac{\pi}{2} + \tan^{-1}\left(\frac{t-\eta}{\xi}\right). \tag{13}$$

For the change of variables

$$\rho_L = (\xi^2 + (t-\eta)^2)^{1/2}, \qquad \frac{d\theta}{dt} = \frac{\xi}{\xi^2 + (t-\eta)^2}. \tag{14}$$

Moreover, note that the t integration can be considered a line integral, t representing the point $(t,0,0)$ along the edge of the element; thus we have, to an extent, reproduced the integration by parts.

With this change of variable and integrating out ρ, Eq. (12) becomes

$$\int_0^1 d\eta \int_0^1 dt \int_0^{1-\eta} d\xi\, \psi_k(\eta,\xi)\psi_j(\eta,\xi) \frac{-\xi}{(\xi^2 + (t-\eta)^2 + \epsilon^2)^{3/2}}. \tag{15}$$

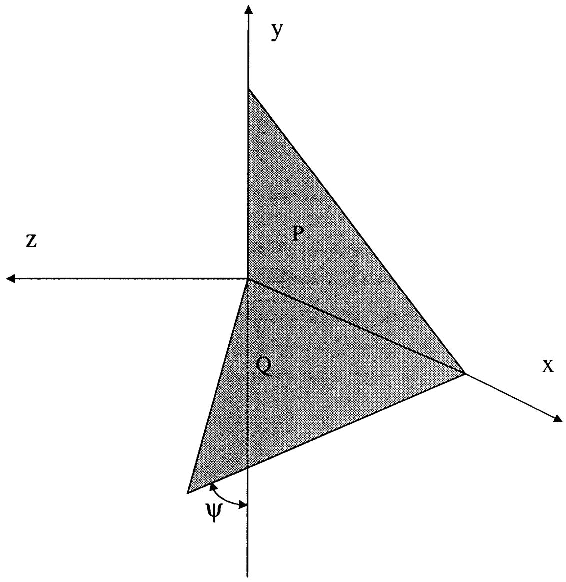

Fig. 3. Geometry for the adjacent edge integration.

The form of the denominator once again suggests polar coordinates (without fear of confusion we recycle ρ and θ) centered at $t = \eta$, $\xi = 0$,

$$t - \eta = \rho\cos(\theta), \qquad \xi = \rho\sin(\theta) \tag{16}$$

with $0 \leq \theta \leq \pi$. (Instead of polar coordinates at this point, it is possible to integrate (ξ,η,t) directly; as $\xi = 0$ is in this case the singular edge, ξ would be integrated first.) Moreover, after $\rho\ \mathrm{d}\rho$ is inserted, the integral in Eq. (15) clearly behaves as $1/\rho$, and thus carrying this computation will give rise to the $\log(\epsilon)$ divergent term. Examining just this term, and completing the integrations over θ and η, we find divergent contributions

$$\begin{aligned} &k=1,\ j=1,\ \frac{2}{3}\log(\epsilon), \qquad k=1,\ j=2,\ \frac{1}{3}\log(\epsilon), \\ &k=2,\ j=1,\ \frac{1}{3}\log(\epsilon), \qquad k=2,\ j=2,\ \frac{2}{3}\log(\epsilon). \end{aligned} \tag{17}$$

There are no $\log(\epsilon)$ terms associated with ψ_3, as this shape function is zero along the $\xi = 0$ edge; this will of course cycle appropriately when the other two subtriangles for the Q integration are considered. The key point is that, having found a procedure to explicitly materialize the divergent terms, a direct evaluation of the coincident integral is feasible. In the integration formulas, the $\log(\epsilon)$ terms can be simply dropped (anticipating that the adjacent edge integration will provide the canceling terms).

One final comment. In a fracture calculation, it appears that full cancellation of the divergent terms will not occur: a crack front element having an edge running along the front is 'missing' a neighboring element. However, the variable on the crack surface, e.g., crack opening displacement for elasticity, jump in potential for Laplace is zero along the front. Thus, no equations are written along the front, and this renders the unmatched divergent terms harmless.

4. Adjacent edge integration

From the Stokes' theorem argument, it is clear that the adjacent edge integrals must produce divergent terms which cancel those in Eq. (17). Nevertheless, it is necessary to explicitly produce the divergent term and verify the cancellation. The method for the edge adjacent integral is similar to that used for the coincident case, relying on two analytical integrations. As with the coincident case, the integral can be split as in Eq. (7), and it is only necessary to treat the first integral.

The geometry for the adjacent edge integration is shown in Fig.3, with $\Psi = 0$. The P element E_P is the same as that for the coincident integration, and E_Q is defined by the three nodes $Q_1 = (0,0,0)$, $Q_2 = (0,-1,0)$, and $Q_3 = (1,0,0)$. Again, the purpose of the additional assumption that $\Psi = 0$ is to simplify the computation as much as possible. The basic procedures for arbitrary Ψ are the same, but the details become quite a bit more laborious. Note that in terms of the parametric mappings, the common edge $y = z = 0$ is $\xi = 0$ for the P element, and $\eta^* = 0$ for Q, and the kernel is singular if $\xi = \eta^* = 0$ and $\xi^* = \eta$.

As with the coincident case, the first step is to employ polar coordinates for the Q integration. For a given point $P = (\eta, \xi)$, the center of the polar coordinates is chosen as the closest Q point on the singular edge, namely $\eta^* = 0$, $\xi^* = \eta$ (see Fig. 4)

$$\xi^* - \eta = \rho\cos(\theta), \qquad \eta^* = \rho\sin(\theta). \tag{18}$$

Thus

$$\begin{aligned} &R = (R_1, R_2, R_3) = (\rho\cos(\theta), -\rho\sin(\theta) - \xi, \rho\sin(\theta) - \epsilon), \\ &r^2 = a_0 + a_1\rho + \rho^2, \\ &a_0 = \epsilon^2 + \xi^2, \qquad a_1 = 2\sin(\theta)\xi. \end{aligned} \tag{19}$$

The Q normal n is $(0,0,1)$, and thus

$$\frac{\partial^2 G}{\partial N \partial n}(P,Q) = \frac{1}{(a_0 + a_1\rho + \rho^2)^{3/2}} - 3\frac{R_3^2}{(a_0 + a_1\rho + \rho^2)^{5/2}}. \tag{20}$$

The program here is to integrate out ρ and ξ, and as the

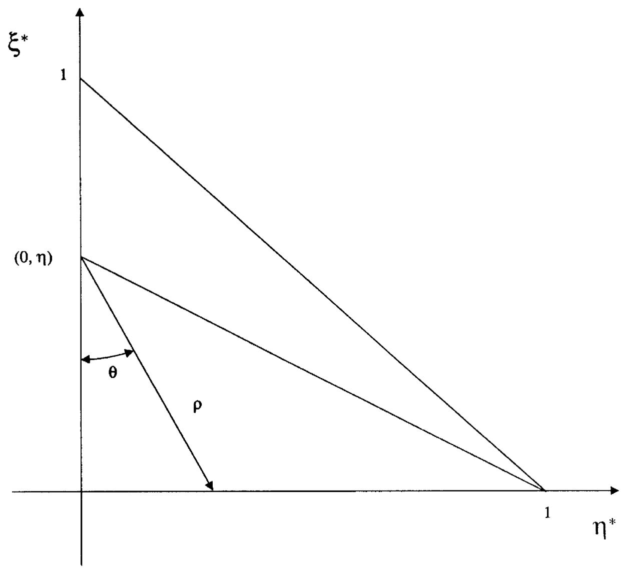

Fig. 4. Polar coordinate system for the adjacent integration.

singularity is located at $\rho = \xi = 0$, this will produce the $\log(\epsilon)$ term. Note that in this case the upper limit on ρ only depends upon η, and thus the ξ integration can be carried out immediately after ρ, without any change of variables.

In the adjacent integrations (and coincident if the second polar coordinate transformation is not employed), Maple will report some results in terms of the inverse hyperbolic tangent. Some of these terms will contribute $\log(\epsilon)$ through the identity

$$\tanh^{-1}\left(\frac{x}{a}\right) = \frac{1}{2}\log\left(\frac{a+x}{a-x}\right)$$
$$= \log((a+x) - \tfrac{1}{2}\log(a^2 - x^2). \tag{21}$$

Thus, the terms of interest in the integration occur when x approaches a as $\epsilon \to 0$, and it is written in this form as in the calculations below a and x involve square roots.

After the $\log(\epsilon)$ term is identified, the integration with respect to θ can once again be carried out by a change of variables t, $0 \le t \le 1$. Referring to Fig. 4, the (ρ,θ) integration in this case forces consideration of two sub-triangles. For the first

$$\theta = \tan^{-1}\left(\frac{t}{\eta}\right), \quad \rho_L = (\eta^2 + t^2)^{1/2}, \quad \frac{\mathrm{d}\theta}{\mathrm{d}t} = \frac{\eta}{\eta^2 + t^2},$$
$$\cos(\theta) = \frac{\eta}{(\eta^2 + t^2)^{1/2}}, \qquad \sin(\theta) = \frac{t}{(\eta^2 + t^2)^{1/2}}, \tag{22}$$

where again $0 \le \rho \le \rho_L$, and for the second

$$\theta = \frac{\pi}{2} + \tan^{-1}\left(\frac{t-\eta}{1-t}\right), \qquad \rho_L = ((t-\eta)^2 + (1-t)^2)^{1/2},$$
$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \frac{1-\eta}{(t-\eta)^2 + (1-t)^2},$$
$$\cos(\theta) = \frac{\eta - t}{((\eta - t)^2 + (1-t)^2)^{1/2}}, \tag{23}$$
$$\sin(\theta) = \frac{1-t}{((\eta - t)^2 + (1-t)^2)^{1/2}}.$$

Carrying out the integrations, it is seen that the adjacent edge integral produces terms identical to the coincident, Eq. (17), only with a negative sign.

5. Conclusions

The framework for an algorithm to directly evaluate three-dimensional Galerkin hypersingular integrals, without the use of Stokes' theorem or regularization, has been presented. The main motivation has been to develop the ability to handle this integral in situations for which Stokes' theorem is unavailable, e.g. three-dimensional anisotropic elasticity. For the very simple specific element treated herein, it was shown that the coincident and adjacent singular integrals over a single element do not exist, but the sum over all elements does. This is analogous to what is seen in two-dimensions (with a lot less work), and is consistent with the Stokes' theorem approach. For a general element, it is to be expected that the analysis to make the divergences appear will be the same, but verifying the cancellation is likely to be more complicated. Nevertheless, the ability to identify the divergent $\log(\epsilon)$ terms from individual integrals will permit a direct calculation.

Although described in a simple setting, linear interpolation and the Green's function for the Laplace equation, the techniques are generally applicable. For higher order interpolation, the kernel can be split into singular and non-singular components; the singular component will resemble a linear element approximation, and thus the analytic integration can be executed. Details concerning this decomposition for two dimensions can be found in Ref. [13].

A potential benefit of the techniques presented herein is that two analytic integrations are executed. The remaining numerical quadrature is therefore over a smaller dimension, and as the singularity has been fully integrated out, the integrand is well behaved. This should not only improve accuracy, but should also help with computational efficiency.

The focus of this paper has been on the divergent terms, and therefore on the most singular component of the hypersingular integral. However, the methods are also needed for a direct treatment of the less singular terms in this integral, and for the non-hypersingular integrals. Applied to some of these integrals, the procedures described above will show that included in the integration are terms of the form

$$\int_0^1 f(t) \log(t)\, dt. \tag{24}$$

If not identified and treated appropriately, either by special quadrature formulas or preferably by analytic integration, significant errors can result. The complete algorithms for three dimensional Galerkin analysis, including consideration of this issue, will be presented elsewhere.

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