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On a Hermite boundary integral approximation

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Abstract

A cubic Hermite approximation for two-dimensional boundary integral analysis is presented. The method differs from previous Hermite interpolation algorithms in that the gradient equations are sparse, significantly reducing the computational cost, and in that information about the surface normals is incorporated to effect a cubic interpolation of the geometry. A motivation for the development of this approximation is in the solution of moving boundary problems, as high accuracy and surface gradients are required for these simulations.
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1. Introduction

Cubic Hermite interpolation for boundary integral analysis, first introduced by Watson [18], has two primary attractions. First, it yields a differentiable ($\mathscr{C}^1$) interpolation for the primary surface function, e.g., potential for the Laplace equation, displacement for elasticity. This smoothness can be useful for the treatment of hypersingular equations, and indeed a primary motivation in [18] was fracture analysis. The second noteworthy aspect of the Hermite approach is that the higher order interpolation is achieved without the addition of element nodes; in two dimensions for example, the cubic interpolation is based upon the two-noded element more commonly employed for the standard linear element.

Although further development and application of the Hermite approach has been carried out [2,7,17], and most notably by Rudolphi, Muci-Küchler and co-workers [9,10,13] (see [8] for additional references), nevertheless it is fair to say that Hermite elements have not been widely adopted. The higher order interpolation is achieved by incorporating nodal tangential derivatives into the approximation, and the computational cost of setting up and solving the additional boundary integral equations for these derivatives is obviously quite high. Three-dimensional elasticity, for example, at a minimum requires two tangential derivative values for each displacement component, resulting in an *additional* six equations per node. It is, however, convenient to obtain the tangential derivatives by first computing the complete gradient, and this requires an even more expensive nine additional nodal equations.

The motivation for the present work is two-fold. First, it has recently been demonstrated [6] that boundary integral equations for the surface gradient (and hence tangential derivatives) can be written quite

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inexpensively. In brief, the usual complete boundary integration is avoided, it is only necessary to compute 'local' singular integrals to formulate the equations. The Hermite interpolation still requires the solution of a larger system of equations, but to a large extent these fast gradient equations remove the principal drawback of this method. Thus, the general application of Hermite elements is much more attractive.

The second impetus for reconsidering this topic is its potential utility for an important class of applications, the solution of moving boundary problems. A boundary integral approach can be attractive for these simulations, as it is clearly easier to remesh the evolving boundary, rather than the entire volume. Moreover, the primary goal in solving the governing partial differential equation is the determination of the *surface* velocity, which usually depends upon the surface gradient of the solution. In an integral equation formulation, this gradient can be obtained (in particular, by using the gradient algorithm mentioned above) without a numerical differentiation, and can therefore yield an accurate velocity function.

The Hermite approximation is attractive for a boundary integral solution of a moving boundary problem, for a number of reasons. The first is that, as just noted, the surface gradient is generally required for the velocity evaluation. Thus, the computational cost of computing the gradient, the main drawback of the Hermite approximation, is therefore no longer a significant issue. Moreover, as the Hermite method *directly* couples the gradient evaluation with the solution of the PDE, this could provide an advantage in accuracy. Second, our interest is in using the Level Set method [11,14,15] to track the evolving geometry, a combination which has proven to be very effective [3,12,16]. The Hermite element builds a higher order (and therefore, more accurate) interpolation on a relatively simple element; this should be convenient for coupling the two calculations, as the boundary integral calculation is constrained to work with the nodes provided by the Level Set analysis. Moreover, as will be discussed further below, the Hermite approach can exploit the additional information available from the Level Set representation of the surface, namely normal vectors, and this too should improve accuracy.

The algorithm presented below therefore differs from previous methods in two principal ways. The extra equations required to obtain the needed nodal tangential derivatives are the 'sparse' fast equations presented in [6]. In [6] the gradient equations were employed to 'post-process' the gradient after the basic boundary integral equations were solved. A purpose of the present work is to test the direct coupling of the gradient and standard boundary integral equations. Moreover [6] discussed the singular integrations in the gradient equation in terms of a three-dimensional linear element; herein the modifications needed for a two-dimensional *curved* element will be discussed.

The second main difference is that the boundary interpolation in previous algorithms was standard, $\mathscr{C}^0$, (e.g., linear). In this work a cubic $\mathscr{C}^1$ boundary approximation is constructed, based upon assumed knowledge of the normal vector at each node. Finally, and of lesser significance, a Galerkin approximation is employed herein, whereas collocation has been used in previous implementations.

2. Hermite approximation

For simplicity, the two-dimensional algorithm is presented in the context of the Laplace equation $\nabla^2\phi = 0$, $\phi = \phi(x, y)$. The standard boundary integral equation for surface potential [1] is considered first, and then the equation for the potential gradient is discussed. The fast gradient equation is based upon a boundary limit definition of the singular integrals, and thus this approach is employed for the surface potential equation as well. Further details concerning this somewhat nonstandard definition and implementation can be found in [4,5].

2.1. Potential equation

The *exterior limit* boundary integral equation for surface potential can be written as [4]

$$P_E(P) \equiv \lim_{P_E \to P} \int_\Gamma \phi(Q) \frac{\partial G}{\partial \mathbf{n}}(P_E, Q)\, \mathrm{d}Q - \int_\Gamma G(P_E, Q) \frac{\partial \phi}{\partial \mathbf{n}}(Q)\, \mathrm{d}Q = 0, \tag{2.1}$$

where the Green's function is

$$G(P,Q) = -\frac{1}{2\pi} \log(\|Q - P\|) = -\frac{1}{2\pi} \log(r). \tag{2.2}$$

The 'Cauchy Principal Value' (CPV) singular integral is defined as a limit, P_E being *exterior* points converging to P. As a consequence, the $\phi(P)$ term that usually appears in this equation is missing. This term does appear with an interior limit definition, and thus an exterior limit is slightly more convenient. For the gradient equations discussed below, both limit processes will be invoked. Note that the integral involving the Green's function is only weakly singular, it is finite with P on the boundary, and thus a limit process is not needed.

The boundary conditions supply partial data about the boundary values of the potential and flux, and the integral equations can be solved to complete this information. Following standard practice [1], a finite system of linear equations is obtained by approximating the boundary and the boundary functions. As an example, for a simple linear interpolation, the approximate boundary curve connecting two surface nodes

$Q_1 = (x_1, y_1)$ and $Q_2 = (x_2, y_2)$ can be defined parametrically as

$$Q(t) = \sum_{j=1}^{2} (x_j, y_j)\psi_j^l(t), \tag{2.3}$$

where $0 < t < 1$ and the shape (basis) functions are

$$\psi_1^l(t) = 1 - t \quad \psi_2^l(t) = t. \tag{2.4}$$

The corresponding interpolation of the boundary flux is then

$$\frac{\partial \phi}{\partial \mathbf{n}}(Q(t)) = \sum_{j=1}^{2} \frac{\partial \phi}{\partial \mathbf{n}}(Q_j)\psi_j^l(t), \tag{2.5}$$

and similarly for the potential.

For the Hermite interpolation, the shape functions employed to define the boundary and the potential are cubic instead of linear, and the approximations are $\mathscr{C}^1$ continuous at the nodes. To achieve a smooth approximation of the boundary, it is assumed that the normal is known at the nodes, for example from a CAD file, or from the Level Set method in a moving boundary problem. The interpolation of the given nodal positions and normals is accomplished by setting

$$\begin{aligned} Q(t) &= (x(t), y(t)) \\ &= \sum_{j=1}^{2} (x_j, y_j)\psi_j(t) + \sum_{j=3}^{4} (a_j, b_j)\psi_j(t) \end{aligned} \tag{2.6}$$

with the shape functions $\psi_j(t)$, $0 < t < 1$,

$$\begin{aligned} \psi_1(t) &= -(1+2t)(1-t), \\ \psi_2(t) &= -t^2(3-2t), \\ \psi_3(t) &= -t(1-t)^2, \\ \psi_4(t) &= -t^2(1-t). \end{aligned} \tag{2.7}$$

These functions satisfy $\psi_1(0) = \psi_2(1) = 1$, $\psi_3'(0) = \psi_4'(1) = 1$, and all other values of ψ_j and ψ_j' at $t = 0$ and $t = 1$ are zero (the prime indicating differentiation with respect to t). The coefficients (a_3, b_3) and (a_4, b_4) are not uniquely defined, as specifying the unit normal leaves open the value of the Jacobian at the nodes. Herein we have made what appears to be a reasonable choice, choosing the Jacobian to be the value that it would be for linear interpolation, $j_h = \|Q_2 - Q_1\|$. Thus the additional coefficients in (2.6) are given by

$$\begin{aligned} (b_3, -a_3) &= j_h \mathbf{N}(Q_1), \\ (b_4, -a_4) &= j_h \mathbf{N}(Q_2), \end{aligned} \tag{2.8}$$

where $\mathbf{N}(Q_k)$ is the specified outward unit normal at Q_k. Note that if Q_1 is a node on a smooth part of the boundary, then

$$Q'(Q_1) = (a_3, b_3) \tag{2.9}$$

for either of the two elements containing Q_1. Thus the interpolation provides a unique unit tangent at each node.

To approximate the potential, note that

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) = \frac{\mathrm{d}}{\mathrm{d}t}\phi(x(t), y(t)) = \frac{\partial \phi}{\partial x}x'(t) + \frac{\partial \phi}{\partial y}y'(t) \tag{2.10}$$

and thus from Eqs. (2.6) and (2.8)

$$\begin{aligned} \frac{\mathrm{d}\phi}{\mathrm{d}t}(Q_1) &= a_3 \frac{\partial \phi}{\partial x}(Q_1) + b_3 \frac{\partial \phi}{\partial y}(Q_1), \\ \frac{\mathrm{d}\phi}{\mathrm{d}t}(Q_2) &= a_4 \frac{\partial \phi}{\partial x}(Q_2) + b_4 \frac{\partial \phi}{\partial y}(Q_2). \end{aligned} \tag{2.11}$$

The approximation for the surface potential is then given by

$$\phi(Q(t)) = \sum_{j=1}^{2} \phi(Q_j)\psi_j(Q) + \sum_{j=3}^{4} \frac{\mathrm{d}\phi}{\mathrm{d}t}(Q_{j-2})\psi_j(Q). \tag{2.12}$$

As noted above, $\{a_j, b_j\}$ depend only on the node (through the normal vector), not the particular element being considered, and the same will be true for the values of the gradient. Thus, the Hermite interpolation produces a unique tangential derivative of ϕ at the nodes. The needed values of $\nabla\phi(Q_j)$ to complete this approximation are of course unknown, and the additional equations constructed to determine them will be discussed below.

In a complete Hermite formulation, the approximation of the surface flux would follow along the same lines as the potential. However, this would require nodal values for the gradient of the flux, i.e., second order derivatives of ϕ. The boundary integral expressions for these derivatives would involve *third* order derivatives of the Green's function, one degree beyond hypersingular, and this clearly poses significant problems for the singular integration. The possibility of constructing a complete Hermite algorithm will be discussed further in Section 5, but for this initial work, the approximation for the surface flux will utilize the simple linear shape functions ψ^l, Eq. (2.5).

2.2. Gradient equations

As discussed in detail (for three dimensions) in [6], a fast algorithm for evaluating the gradient of the potential is obtained by exploiting the boundary limit formulation of the integral equations. The interior limit equation corresponding to Eq. (2.1) is

$$\begin{aligned} P_I(P) \equiv \phi(P) &+ \lim_{P_I \to P} \int_\Gamma \phi(Q) \frac{\partial G}{\partial \mathbf{n}}(P_I, Q)\,\mathrm{d}Q \\ &- \int_\Gamma G(P_I, Q) \frac{\partial \phi}{\partial \mathbf{n}}(Q)\,\mathrm{d}Q = 0, \end{aligned} \tag{2.13}$$

where now P_I are interior points converging to P. The CPV integral is discontinuous crossing the boundary, and this ensures that the interior and exterior limit processes eventually result in the same equation for surface potential. Differentiating with respect to P, the two limit equations for the gradient (with respect to P) take the form

$$\nabla\mathscr{P}_I(P) \equiv \nabla\phi(P) + \lim_{P_I\to P}\int_\Gamma \left\{\phi(Q)\nabla\frac{\partial G}{\partial \mathbf{n}}(P_I,Q) - \nabla G(P_I,Q)\frac{\partial\phi}{\partial\mathbf{n}}(Q)\right\}\mathrm{d}Q = 0,$$

$$\nabla\mathscr{P}_E(P) \equiv \lim_{P_E\to P}\int_\Gamma \left\{\phi(Q)\nabla\frac{\partial G}{\partial \mathbf{n}}(P_E,Q) - \nabla G(P_E,Q)\frac{\partial\phi}{\partial\mathbf{n}}(Q)\right\}\mathrm{d}Q = 0. \tag{2.14}$$

Unlike for the potential equations these are distinct equations, and it is convenient to take the difference

$$\begin{aligned}\mathscr{G}(P) &\equiv \nabla\mathscr{P}_I(P) - \nabla\mathscr{P}_E(P)\\ &= \nabla\phi(P) + \left[\lim_{P_I\to P} - \lim_{P_E\to P}\right]\\ &\quad\times\int_\Gamma\left\{\phi(Q)\nabla\frac{\partial G}{\partial\mathbf{n}}(P,Q) - \nabla G(P,Q)\frac{\partial\phi}{\partial\mathbf{n}}(Q)\right\}\mathrm{d}Q\\ &= 0.\end{aligned} \tag{2.15}$$

The advantage of this form is that only the integrations that are discontinuous crossing the boundary survive the difference of the limits. In particular, all nonsingular integrations vanish, and thus compared to the complete boundary integration required for the potential equation, the construction of these equations is quite inexpensive. Before discussing the evaluation of the singular integrals that do contribute, the Galerkin form of Eqs. (2.1) and (2.15) will first be discussed.

2.3. Galerkin approximation

In a Galerkin approximation, the integral equations are enforced in a weak sense, multiplying the integral equations by weighting functions and integrating with respect to P. Usually the weight functions are associated with a node and comprised of the basic shape functions. Specifically, the Galerkin form of Eq. (2.1) is

$$\int_\Gamma \hat{\psi}_k(P)\mathscr{P}_E(P)\,\mathrm{d}P = 0, \tag{2.16}$$

where the weight function $\hat{\psi}_k(P)$ consists of all shape functions $\psi_l(P)$ that are nonzero at P_k. Thus, $\hat{\psi}_k(P)$ consists of ψ_j, $j = 1,2$ and has limited support, being nonzero only on the elements containing P_k.

For the gradient equations, there is some discretion in the choice of the weight function. One could reasonably decide to make use of the two shape functions, ψ_3 and ψ_4, that were not employed for the potential equation. However, herein we have elected to use the same weight functions $\hat{\psi}_k(P)$ as for the potential equation

$$\int_\Gamma \hat{\psi}_k(P)\mathscr{G}(P)\,\mathrm{d}P = 0. \tag{2.17}$$

3. Singular integration

As noted above, the evaluation of Eq. (2.15) only requires examining the singular integrals, all nonsingular terms vanish in the difference of the limits. The most singular term in the Galerkin form of this equation is the coincident hypersingular integral

$$\sum_{j=1}^{2}\phi(Q_j)\left[\lim_{P_I\to P} - \lim_{P_E\to P}\right]\int_{E_P}\psi_k(t)j_p(t) \times\int_{E_Q}\psi_j(s)\nabla\frac{\partial G}{\partial\mathbf{n}}(P,Q)j_q(s)\,\mathrm{d}s\,\mathrm{d}t, \tag{3.1}$$

where $E_P = E_Q = E$ is a particular boundary element, $j_p(t)$ and $j_q(s)$ the Jacobians for the parametric representations, and t and s are the parameters for the P and Q integrations, respectively. The evaluation of this integral is considered in this section; the adjacent singular integral, when E_P and E_Q share a node, is simpler and follows the discussion below and in [4]. In addition, it suffices to consider the x component of the gradient, for which the integral kernel is

$$\begin{aligned}\frac{\partial}{\partial x_P}\frac{\partial G}{\partial\mathbf{n}} &= -\frac{1}{2\pi}\frac{\partial}{\partial x_P}\frac{\mathbf{n}\cdot\mathbf{R}}{r^2}\\ &= \frac{1}{2\pi}\left(\frac{n_x}{r^2} - 2\frac{\mathbf{R}_x(\mathbf{n}\cdot\mathbf{R})}{r^4}\right),\end{aligned} \tag{3.2}$$

where $\mathbf{n} = \mathbf{n}(Q) = (n_x, n_y)$ and $R(t,s) = (R_x(t,s), R_y(t,s)) = Q(s) - P(t)$.

To implement the interior limit analysis, the point P is shifted off the boundary, $P(t) - \epsilon\mathbf{N}$ where $\mathbf{N} = \mathbf{N}(P)$ is the unit outward normal at $P(t)$. The change for the exterior limit is simply that P is $P(t) + \epsilon\mathbf{N}$. As the singularity is at $s = t$ it is convenient to change variables from s to $u = s - t$, and the distance function $r^2 = \|\mathbf{R}\|^2$ takes the form

$$r^2 = \epsilon^2 + (a_2 + \beta\epsilon)u^2 + \cdots + a_6u^6, \tag{3.3}$$

where the coefficients a_m are functions of the element nodal coordinates $Q_j = (x_j, y_j)$, $j = 1,2$. The higher order coefficients are also functions of ϵ but the limiting value of the integral is unaffected by setting $\epsilon = 0$. Unlike for the linear element analysis, there is an ϵ dependence in the u^2 term that must be taken into account, β again a function of the node coordinates. The goal is to integrate u analytically, which is clearly not possible with this sixth degree polynomial in the denominator. This is remedied through the expansions [4]

$$\frac{1}{r^2} \approx \frac{1}{\hat{r}^2} - \frac{\beta u^2 \epsilon}{\hat{r}^4}, \qquad \frac{1}{r^4} \approx \frac{1}{\hat{r}^4} - 2\frac{\gamma u^3 - \beta u^2 \epsilon}{\hat{r}^6}, \tag{3.4}$$

where $\hat{r}^2 = \epsilon^2 + a_2 u^2$. Another simplifying aspect of Eq. (2.15) is that the remainder terms from Eq. (3.4) can be ignored: they produce integrals that are continuous crossing the boundary, and thus disappear in the difference of the limits.

With the Jacobians included, the numerators in Eq. (3.2) are polynomial in u, and thus substituting Eq. (3.4) into Eq. (3.2), the integrations with respect to u can be evaluated analytically. The important result of this integration is that it is seen that the limit $\epsilon \to 0$ exists. This is in contrast to the standard hypersingular equation for surface flux, where the coincident and adjacent singular integrals are not separately finite [4]. Finally, the integration with respect to u results in a well behave function of t that can be safely evaluated numerically.

4. Test calculations

The Hermite Laplace algorithm has been tested on two simple problems, an interior and an exterior problem with the boundary being the unit circle. For the problem posed inside the unit disk, Dirichlet data

$$\phi(x,y) = x^2 - y^2 \tag{4.1}$$

is specified, and thus the exact solution for the boundary flux is $2(x^2 - y^2)$. The Neumann data for the exterior problem

$$\frac{\partial \phi}{\partial \mathbf{n}}(x,y) = x \tag{4.2}$$

is the flux on the unit circle that corresponds to the potential

$$\phi(x,y) = \frac{x}{x^2 + y^2} = \frac{\partial}{\partial x}\log(r), \tag{4.3}$$

which is harmonic in any domain not containing the origin. The exact solution for the potential on the circle is therefore simply $\phi(x,y) = x$.

Table 1 lists the L^2 errors in the computed flux (interior problem) and the computed potential (exterior problem) as a function of the number of elements discretizing the circle. In both cases, the convergence is roughly quadratic. This is somewhat disappointing, as this is no better than a linear approximation, but not surprising. The interpolation of the flux is still only linear, and the convergence is controlled by this least accurate aspect of the calculation.

The fact that the exterior solution is more accurate is also to be expected. In this calculation the flux interpolation only contributes to the right hand side, whereas the coefficient matrix for the system of equations is constructed using the cubic interpolation. The reverse is true for the Dirichlet problem, and it is clearly more important to have the higher order interpolation involved in the coefficient matrix.

Table 1
L^2 errors for problems interior and exterior to the unit disk

Elements	Interior Dirichlet	Exterior Neumann
25	2.6285 (−2)	3.1941 (−3)
50	6.2872 (−3)	7.6903 (−4)
100	9.9486 (−4)	1.8992 (−4)
150	4.4088 (−4)	8.3560 (−5)
200	2.4774 (−4)	4.6880 (−5)
250	1.5845 (−4)	2.9957 (−5)

5. Conclusions

This initial work has demonstrated that the sparse gradient boundary integral equations can be employed to construct a Hermite interpolation of the basic function, e.g., potential. This significantly reduces the computational cost of this cubic interpolation, and should make this approximation more attractive for general application. For moving boundary problems, there is the added advantage of exploiting knowledge of the surface normals to obtain a smooth interpolation of the boundary.

However, for this approach to be effective, further development is required. The results for two simple test problems indicate that the linear interpolation of the flux controls the rate of convergence of the algorithm. Quadratic, the convergence rate for a linear approximation, is the best that can be expected. A complete Hermite interpolation, staying within the nodal framework employed herein, would require nodal values of the gradient of the flux,

$$\nabla \frac{\partial \phi}{\partial \mathbf{N}}(P) = -\lim_{P_I \to P} \int_\Gamma \left\{ \phi(Q) \nabla \frac{\partial^2 G}{\partial \mathbf{N} \partial \mathbf{n}}(P,Q) - \nabla \frac{\partial G}{\partial \mathbf{N}}(P,Q) \frac{\partial \phi}{\partial \mathbf{n}}(Q) \right\} \mathrm{d}Q. \tag{5.1}$$

Even with a Galerkin approximation, computing the integral involving three derivatives of the Green's function, appears to be hopeless. However, in the form of the difference of interior and exterior limits,

$$\nabla \frac{\partial \phi}{\partial \mathbf{N}}(P) = -\left[\lim_{P_I \to P} - \lim_{P_E \to P} \right] \times \int_\Gamma \left\{ \phi(Q) \nabla \frac{\partial^2 G}{\partial \mathbf{N} \partial \mathbf{n}} - \nabla \frac{\partial G}{\partial \mathbf{N}} \frac{\partial \phi}{\partial \mathbf{n}}(Q) \right\} \mathrm{d}Q. \tag{5.2}$$

This calculation may be possible. As noted in Section 3, the behavior of the hypersingular integral in the limit difference gradient equation, Eq. (2.15), is not hypersingular, in the sense that the coincident integral is finite. Thus, in effect, the worst singularity in Eq. (5.2) may turn out to be no worse than a manageable hypersingular—the coincident and adjacent integrals are not finite, but the sum of the integrals is finite [5]. This is currently being investigated.

Finally, for applications it will obviously be necessary to extend these methods to three dimensions. While the evaluation of the gradient is not a problem, the definition of an element that incorporates the normal vector information is not obvious. This too is currently under investigation.

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