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A new study of the Burton and Miller method for the solution of a 3D Helmholtz problem

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The exterior Helmholtz problem can be efficiently solved by reformulating the differential equation as an integral equation over the surface of the radiating and/or scattering object. One popular approach for overcoming either non-unique or non-existent problems which occur at certain values of the wave number is the so-called Burton and Miller method which modifies the usual integral equation into one which can be shown to have a unique solution for all real and positive wave numbers. This formulation contains an integral operator with a hypersingular kernel function and for many years, a commonly used method for overcoming this hypersingularity problem has been the collocation method with piecewise-constant polynomials. Viable high-order methods only exist for the more expensive Galerkin method. This paper proposes a new reformulation of the Burton–Miller approach and enables the more practical collocation method to be applied with any high-order piecewise polynomials. This work is expected to lead to much progress in subsequent development of fast solvers. Numerical experiments on 3D domains are included to support the proposed high-order collocation method.

Keywords: exterior Helmholtz; boundary integral equation; Burton–Miller; Green theorem; hypersingular operators; collocation method.

1. Introduction

This paper is concerned with using the boundary integral method (BIM) to solve the exterior Helmholtz problem. Such problems arise in the mathematical modelling of the steady-state single-frequency acoustic field outside an object immersed in a fluid; see Amini *et al.* (1992) and Colton & Kress (1983).

It is advantageous to reformulate the underlying partial differential equation (PDE) as an integral equation because the domain problem is reduced to one on its finite boundary. However, it is well known that for certain frequencies, the solution to integral equation formulations either does not exist

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or is non-unique (when the original PDE has a unique solution). Over the years, a number of methods have been proposed for overcoming these problems, as surveyed in Amini *et al.* (1992). This paper will study the particular unique formulation of the problem devised by Burton & Miller (1971) which we shall refer to as the Burton and Miller method. Although the Burton and Miller method is widely used, due to the presence of a hypersingular operator, the usage is so far limited to the piecewise-constant collocation framework, where it is relatively easy to overcome the hypersingularity (Amini *et al.*, 1992; Chen & Harris, 2001). For the theoretically appealing Galerkin method, methods exist for transforming the hypersingular integral into one which is at worst weakly singular (see Giroire & Nedelec, 1978; Hackbusch, 1995; Harris & Chen, 2003).

This paper proposes a new and high-order collocation method that overcomes this hypersingular nature of operator without using finite-part integration (refer the latter to Harris, 1992; Salvadori, 2001; Schwab & Wendlend, 1998; Aimi & Diligenti, 2002). In what follows, we shall first introduce the exterior Helmholtz problem and the direct method for reformulating it as a simple boundary integral equation which suffers from the non-uniqueness problems outlined above. We then discuss an alternative BIM which possess a unique solution for all wave numbers, but which includes the hypersingular integral operator. The main part of the paper is dedicated to describing a method for evaluating hypersingular operator with polynomial basis functions for any order. Our new idea is to remove the hypersingularity by using domain integrals and then to avoid domain integrals by using singularity subtraction. Finally, we present some numerical results for some typical test problems to show that the method proposed here can be used to obtain a very accurate solution.

We remark in passing that the methods presented in this paper are mainly for solving wave problems with Neumann boundary conditions on the surface of the structure (which is quite common in practice). However, for Dirichlet boundary conditions, while this work still applies, it is possible to avoid the hypersingular operator completely by using an indirect layer potential integral equation formulation (Amini *et al.*, 1992) if the values of the normal derivative on the surface are not specifically required. We also note that the methods presented here are intended for use in solving practical problems, such as the acoustic radiation from a sonar transducer or a loudspeaker, where it is a physical requirement that the acoustic pressure is continuous throughout the fluid-filled domain. This allows us to compute the required domain gradient of the pressure at all points in the fluid domain and on its boundaries.

2. The boundary integral equation formulation of the exterior Helmholtz problem

We first introduce the basic problem formulation and discuss the associated and known problems. Consider the problem of solving the Helmholtz equation

$$\nabla^2\phi(\mathbf{p}) + k^2\phi(\mathbf{p}) = 0, \quad \mathbf{p} \in \Omega_+ \cup S, \tag{2.1}$$

in some unbounded 3D region Ω_+ exterior to a closed surface S, where $k > 0$ is the wave number, subject to a Neumann boundary condition on S and the Sommerfeld radiation condition

$$\lim_{r\to\infty} r\left(\frac{\partial\phi}{\partial r} - \mathrm{i}k\phi\right) = 0. \tag{2.2}$$

Since the above exterior problem cannot be easily solved by discretizing the infinite domain using finite differences or finite elements, we choose to reformulate the problem as an integral equation over the surface S; see Amini *et al.* (1992), Colton & Kress (1983) and Chen & Harris (2001). However, domain methods based on infinite elements or coupled finite and infinite elements have been devised; see Gerdes & Demkowicz (1996) and Gerdes (1998), e.g.

There are essentially two methods for reformulating the exterior Helmholtz problem as an boundary integral equation, the direct method which is used here and the indirect method. The direct method of reformulation as an integral equation is obtained by applying Green's theorem to get a relationship between the acoustic pressure and its normal derivative in the form (Burton, 1973; Hackbusch, 1995)

$$\int_S \phi(\mathbf{q}) \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_q}} - G_k(\mathbf{p},\mathbf{q}) \frac{\partial \phi(\mathbf{q})}{\partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} = \begin{cases} \frac{1}{2}\phi(\mathbf{p}), & \mathbf{p} \in S, \\ \phi(\mathbf{p}), & \mathbf{p} \in \Omega_+, \end{cases} \tag{2.3}$$

where

$$G_k(\mathbf{p},\mathbf{q}) = \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{p}-\mathbf{q}|}}{4\pi\,|\mathbf{p}-\mathbf{q}|} \tag{2.4}$$

is the free-space Green's function, or the fundamental solution, for Helmholtz equation and $\mathbf{n_q}$ is the unit outward normal to S at $\mathbf{q}$. If the normal derivative of the acoustic field is given on the surface S, then (2.3) for $\mathbf{p} \in S$ gives a Fredholm integral equation of the second kind which can be solved for the surface pressure ϕ. The acoustic pressure can then be computed at any point in Ω_+ using (2.3). However, the solution of (2.3) does not posses a unique solution for certain discrete values of the wave number (called characteristic or irregular or resonance wave numbers), although it can be shown that the underlying differential equation has a unique solution for all real and positive wave numbers (Burton, 1973). A number of different methods have been proposed for overcoming this non-uniqueness problem and a survey of these is given in Amini *et al.* (1992). One of the most robust is the so-called Burton and Miller method and for this reason, it is the method we shall use here. It is worth noting at this point that had we used an indirect integral equation formulation, then similar problems with the existence of the solution would have occurred at the characteristic wave numbers.

The Burton & Miller (1971) method proposed using the alternative integral equation formulation

$$\begin{aligned} -\frac{1}{2}\phi(\mathbf{p}) + \int_S \phi(\mathbf{q}) \left(\frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_q}} + \alpha \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right) \mathrm{d}S_\mathbf{q} \\ = \frac{\alpha}{2} \frac{\partial \phi(\mathbf{p})}{\partial \mathbf{n_p}} + \int_S \frac{\partial \phi(\mathbf{q})}{\partial \mathbf{n_q}} \left(G_k(\mathbf{p},\mathbf{q}) + \alpha \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} \right) \mathrm{d}S_\mathbf{q}, \end{aligned} \tag{2.5}$$

where α is a non-zero constant. It can be shown that provided that the imaginary part of α is non-zero, then (2.5) has a unique solution for all real and positive k (Burton & Miller, 1971). However, this formulation has introduced an integral operator with the kernel function $\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}}$ which has a $1/|\mathbf{p}-\mathbf{q}|^3$ singularity. For brevity, we note that (2.5) can be written as

$$-\frac{1}{2}\phi(\mathbf{p}) + \int_S \phi(\mathbf{q}) \left(\frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} + \alpha \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right) \mathrm{d}S_\mathbf{q} = g(\mathbf{p}), \quad \mathbf{p} \in S, \tag{2.6}$$

where $g(\mathbf{p})$ denotes the right-hand side associated with the Neumann's boundary condition.

Two ways which can be used to overcome the problems associated with the hypersingularity are to use a simple piecewise-constant collocation method (which is widely used in practise) or a higher-order Galerkin method. The collocation method has the advantages of being relatively simple to implement and cheap to use in computational terms (see Chen & Harris, 2001, e.g.). However, for any given boundary element mesh, it is not very accurate if only a low-order method, such as piecewise constant, is

used. The Galerkin method has the advantage that it is much more accurate than a low-order collocation method since high-order methods are available, but it is a lot more expensive in computational terms (and less used in engineering practice). An efficient high-order Galerkin method is discussed in Harris & Chen (2003). In Section 3, we present a method which can be used to reformulate the integral involving the second derivative of the Green's function as integrals which are at worst weakly singular for any order of basis functions. This reformulation will allow the use of the simpler collocation method with high-order basis functions, giving a level of accuracy which is comparable to the more expensive Galerkin method.

3. The weakly singular formulation

We now introduce our reformulation of the above (2.5) with a view to remove the hypersingular term. Without loss of generality, we shall assume that the unknown function ϕ lies in the space of $H^{1/2}(S)$, which is a weak assumption as we aim for high-order methods in Section 4. In order to obtain a weakly singular formulation, we need to apply a transformation to the hypersingular term

$$\int_S \phi(\mathbf{p}) \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q}. \tag{3.1}$$

In order to do, this we make use of the following lemma.

LEMMA 1 Let vector $\mathbf{a} \in \mathbb{R}^3$ and S be a piecewise C_2-closed surface enclosing some interior region Ω in $\mathbb{R}^3$. Assume that $\mathbf{p}$ is a point such that $\mathbf{n_p}$ is unique and well defined. Then,

$$\begin{aligned}\int_S \mathbf{a}\cdot(\mathbf{q}-\mathbf{p}) \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} = \int_S \mathbf{a}\cdot\mathbf{n_q} \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}S_\mathbf{q} \\ -k^2 \mathbf{a}\cdot\int_\Omega (\mathbf{q}-\mathbf{p}) \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}V_\mathbf{q} \\ -\frac{\mathbf{a}\cdot\mathbf{n_p}}{2}.\end{aligned} \tag{3.2}$$

(The proof is shown in Appendix A.)

We now consider how to utilize Lemma 1 to express (3.1) in terms of weakly singular integrals (and involving domain integrals). First, we rewrite the hypersingular integral as

$$\begin{aligned}\int_S \phi(\mathbf{q}) \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} = \int_S [\phi(\mathbf{q}) - \phi(\mathbf{p}) - \nabla\phi(\mathbf{p})(\mathbf{q}-\mathbf{p})] \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} \\ +\phi(\mathbf{p}) \int_S \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} \\ +\int_S \nabla\phi(\mathbf{p})\cdot(\mathbf{q}-\mathbf{p}) \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q},\end{aligned} \tag{3.3}$$

where $\nabla\phi(\mathbf{p})$ denotes the domain gradient of ϕ at the point $\mathbf{p}$. The first term on the right-hand side of (3.3) contains what is essentially the difference between $\phi(\mathbf{q})$ and the terms up to and including the first derivative terms of its Taylor's series. Hence, the remainder term in (3.3) is of order $|\mathbf{q}-\mathbf{p}|^2$ and so the

whole first integral behaves as $|\mathbf{q}-\mathbf{p}|^{-1}$ which means it is weakly singular. Clearly, for this to work, we require that ϕ is at least two times differentiable at the point $\mathbf{p}$, but this is not a major restriction as in most physical problems, the acoustic pressure will satisfy this condition. In addition, it is a requirement of Lemma 1 that the point $\mathbf{p}$ be such that S has a well-defined normal, and a consequence of this is that $\nabla\phi$ will be well defined at such points. Hence, the first term on the right-hand side of (3.3) can be evaluated using an appropriate quadrature rule.

The second term can be evaluated using (Meyer *et al.*, 1978)

$$\int_S \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} = k^2 \int_S \mathbf{n_p}\cdot\mathbf{n_q} G_k(\mathbf{p},\mathbf{q})\mathrm{d}S_\mathbf{q} \tag{3.4}$$

to yield that

$$\begin{aligned}\int_S \phi(\mathbf{q})\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}}\mathrm{d}S_\mathbf{q} = &\int_S [\phi(\mathbf{q})-\phi(\mathbf{p})-\nabla\phi(\mathbf{p})\cdot(\mathbf{q}-\mathbf{p})]\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}}\mathrm{d}S_\mathbf{q}\\ &+ k^2\phi(\mathbf{p})\int_S \mathbf{n_p}\cdot\mathbf{n_q}G_k(\mathbf{p},\mathbf{q})\mathrm{d}S_\mathbf{q}\\ &+ \int_S \nabla\phi(\mathbf{p})\cdot(\mathbf{q}-\mathbf{p})\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}}\mathrm{d}S_\mathbf{q},\end{aligned} \tag{3.5}$$

where the first two integrals on the right-hand side are now weakly singular. It now remains to address the singularity in the final integral on the right-hand side.

In order to overcome this singularity, set $\mathbf{a} = \nabla\phi(\mathbf{p})$ (remembering that $\mathbf{p} \in S$ must be a point at which the normal is well defined) and use Lemma 1 to obtain that

$$\begin{aligned}\int_S \nabla\phi(\mathbf{p})\cdot(\mathbf{q}-\mathbf{p})\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}}\mathrm{d}S_\mathbf{q} = &\int_S \nabla\phi(\mathbf{p})\cdot\mathbf{n_q}\frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}}\mathrm{d}S_\mathbf{q}\\ &-k^2\int_\Omega \nabla\phi(\mathbf{p})\cdot(\mathbf{q}-\mathbf{p})\frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}}\mathrm{d}V_\mathbf{q}\\ &-\frac{1}{2}\nabla\phi(\mathbf{p})\cdot\mathbf{n_p}.\end{aligned} \tag{3.6}$$

Substituting (3.6) into (3.5) yields that

$$\begin{aligned}\int_S \phi(\mathbf{q})\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}}\mathrm{d}S_\mathbf{q} = &\int_S [\phi(\mathbf{q})-\phi(\mathbf{p})-\nabla\phi(\mathbf{p})\cdot(\mathbf{q}-\mathbf{p})]\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}\partial \mathbf{n_q}}\mathrm{d}S_\mathbf{q}\\ &+k^2\phi(\mathbf{p})\int_S \mathbf{n_p}\cdot\mathbf{n_q}G_k(\mathbf{p},\mathbf{q})\mathrm{d}S_\mathbf{q}\\ &+\int_S \nabla\phi(\mathbf{p})\cdot\mathbf{n_q}\frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}}\mathrm{d}S_\mathbf{q}\end{aligned}$$

$$-k^2 \int_\Omega \nabla\phi(\mathbf{p}) \cdot (\mathbf{q}-\mathbf{p}) \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}V_\mathbf{q}$$

$$-\frac{1}{2}\nabla\phi(\mathbf{p}) \cdot \mathbf{n_p}, \tag{3.7}$$

where every integral on the right-hand side is now weakly singular.

Theoretically, we have thus completed the task of reformulating (3.1). However, this new formulation has introduced a volume integral over the domain Ω interior to S, although ϕ is only required on S and there is no hypersingularity. This integral can be expensive and difficult to evaluate, so we apply further reformulation.

Clearly, this problem can be avoided by setting $k = 0$ as this will cause the volume integral to disappear along with the second integral on the right-hand side of (3.7). In order to make use of this, we shall use the singularity subtraction technique by rewriting the integral involving the second derivative of the Green's function as

$$\int_S \phi(\mathbf{q}) \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} = \int_S \phi(\mathbf{q}) \left[\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \frac{\partial^2 G_0(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right] \mathrm{d}S_\mathbf{q}$$

$$+ \int_S \phi(\mathbf{q}) \frac{\partial^2 G_0(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q}. \tag{3.8}$$

By using (3.7) with $k = 0$ to evaluate the final integral on the right-hand side of (3.8), we obtain that

$$\int_S \phi(\mathbf{q}) \frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_\mathbf{q} = \int_S \phi(\mathbf{q}) \left[\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \frac{\partial^2 G_0(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right] \mathrm{d}S_\mathbf{q}$$

$$+ \int_S \left(\{\phi(\mathbf{q}) - \phi(\mathbf{p}) - \nabla\phi(\mathbf{p}) \cdot (\mathbf{q}-\mathbf{p})\} \frac{\partial^2 G_0(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right) \mathrm{d}S_\mathbf{q}$$

$$+ \int_S \nabla\phi(\mathbf{p}) \cdot \mathbf{n_q} \frac{\partial G_0(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}S_\mathbf{q}$$

$$-\frac{1}{2}\nabla\phi(\mathbf{p}) \cdot \mathbf{n_p}, \tag{3.9}$$

where every integral on the right-hand side is at worst weakly singular. Hence, we have reformulated (3.1) into a form which only involves boundary or surface integrals which are at worst weakly singular. Substituting (3.9) into (2.6) yields our reformulated Burton–Miller method for (2.1):

$$-\frac{1}{2}\phi(\mathbf{p}) + \int_S \phi(\mathbf{q}) \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}S_\mathbf{q}$$

$$+ \alpha \left\{ \int_S \phi(\mathbf{q}) \left[\frac{\partial^2 G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \frac{\partial^2 G_0(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right] \mathrm{d}S_\mathbf{q} \right.$$

$$+\int_S \left(\{\phi(\mathbf{q}) - \phi(\mathbf{p}) - \nabla\phi(\mathbf{p}) \cdot (\mathbf{q} - \mathbf{p})\} \frac{\partial^2 G_0(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right) \mathrm{d}S_{\mathbf{q}}$$

$$+\int_S \nabla\phi(\mathbf{p}) \cdot \mathbf{n_q} \frac{\partial G_0(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}S_{\mathbf{q}} - \frac{1}{2} \nabla\phi(\mathbf{p}) \cdot \mathbf{n_p} \Bigg\}$$

$$= g(\mathbf{p}), \quad \mathbf{p} \in S, \tag{3.10}$$

which has not only an unique solution (like the well-known Burton–Miller formulation) but also no strong singularises (unlike the well-known Burton–Miller formulation). Hence, subsequent solution of (3.10) by any standard method can be considered (note that, in contrast, most standard methods cannot be applied to solve the well-known Burton–Miller formulation).

Finally, we consider the technical point of computing the gradient of the surface function ϕ without involving interior values. Let the surface be parameterized locally in terms of the two variables u and v so that we can make use of the chain rule to give

$$\begin{cases} \dfrac{\partial\phi}{\partial x}\dfrac{\partial x}{\partial u} + \dfrac{\partial\phi}{\partial y}\dfrac{\partial y}{\partial u} + \dfrac{\partial\phi}{\partial z}\dfrac{\partial z}{\partial u} = \dfrac{\partial\phi}{\partial u}, \\ \dfrac{\partial\phi}{\partial x}\dfrac{\partial x}{\partial v} + \dfrac{\partial\phi}{\partial y}\dfrac{\partial y}{\partial v} + \dfrac{\partial\phi}{\partial z}\dfrac{\partial z}{\partial v} = \dfrac{\partial\phi}{\partial v}, \\ \dfrac{\partial\phi}{\partial x} n_x + \dfrac{\partial\phi}{\partial y} n_y + \dfrac{\partial\phi}{\partial z} n_z = \dfrac{\partial\phi}{\partial \mathbf{n}}. \end{cases} \tag{3.11}$$

Thus, at any surface point (x, y, z), corresponding to local coordinates (u, v) in the reference space, a translation of reference space gradients to physical space gradients can be made.

4. Application to the collocation method

In general, (3.10) cannot be solved analytically. One effective numerical method is the collocation method. It solves (3.10) by approximating the solution by a function of the form

$$\phi(\mathbf{q}) = \sum_{j=1}^{m} \phi_j \psi_j(\mathbf{q}) \tag{4.1}$$

in the subspace of piecewise polynomials, where $\{\psi_1, \psi_2, \ldots, \psi_m\}$ are a set of linearly independent basis functions which are assumed to be polynomials of 'any order', and then picking m collocation points $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_m$ at which the residual due to the use of the approximated solution is forced to be zero. Further, as in many similar applications, we assume that the surface S is approximated by M boundary elements which are interpolated using a parametric mapping to a reference element in the (u, v)-plane. The parametric mapping is used to calculate surface-related quantities such as the Jacobian and unit normal vector at points which are interior to the elements.

However, the use of the collocation method means that we are also required to work out the normal at the collocation points. This presents a problem if the usual continuous approximation based on the

element vertices and mid-side points is used as the unit normal is usually not well defined at such points due to the jump in the derivatives of the interpolating functions at the element boundaries. Further, our new method for evaluating the hypersingular operator requires that the collocation point lies on a smooth part of S which has a well-defined normal vector. For smooth surfaces S, it is possible to use the unit normal to the underlying exact surface (assuming that it is simple to calculate) and ignore the fact that the node lies on a vertex of the approximate surface. However, for surfaces which are not smooth (i.e. they contain edges and/or vertices), it is not possible to compute a unit normal to the surface at any node which lies on an edge or vertex. To overcome this problem, we propose using discontinuous interpolation where the collocation points are chosen to lie inside any given element, corresponding to prescribed points (u, v) in the reference element. As these points will lie on a smooth part of the approximate surface, there are no problems with computing the unit normal at these points. The exact choice of the interior points will be discussed in the Section 5 on numerical results. Here, we will assume that there are L basis functions and collocation points associated with each element. The exact choice of basis functions and collocation points used in this work will be discussed later.

A further problem encountered when attempting to discretize (3.10) using (3.11) to find the gradient of the solution is the complexity of keeping track of the various contributions to the system matrix and right-hand side vector. For example, if there are L basis functions associated with the element, then each integral involving $\nabla\phi(\mathbf{p})$ appearing in (3.10) will give a contribution to L^2 entries in the system coefficient matrix and make L contributions to the right-hand side vector.

A simpler alternative is to substitute (4.1) into (2.6) to give

$$\sum_{j=1}^{m}\phi_j\left[-\frac{1}{2}\psi_j(\mathbf{p}_i)+\int_S\left(\psi_j(\mathbf{q})\frac{\partial G_k(\mathbf{p}_i,\mathbf{q})}{\partial\mathbf{n}_\mathbf{p}}+\alpha\frac{\partial^2 G_k(\mathbf{p}_i,\mathbf{q})}{\partial\mathbf{n}_\mathbf{p}\partial\mathbf{n}_\mathbf{q}}\right)\mathrm{d}S_\mathbf{q}\right]=g(\mathbf{p}_i). \tag{4.2}$$

We now use (3.7) with ϕ replaced by ψ_j to evaluate the hypersingular integral to give

$$\begin{aligned}\sum_{j=1}^{m}\phi_j\Bigg[&-\frac{1}{2}\psi_j(\mathbf{p}_i)+\int_S\psi_j(\mathbf{q})\frac{\partial G_k(\mathbf{p}_i,\mathbf{q})}{\partial\mathbf{n}_\mathbf{p}}\mathrm{d}S_\mathbf{q}\\&+\alpha\int_S\psi_j(\mathbf{q})\left(\frac{\partial^2 G_k(\mathbf{p}_i,\mathbf{q})}{\partial\mathbf{n}_\mathbf{p}\partial\mathbf{n}_\mathbf{q}}-\frac{\partial^2 G_0(\mathbf{p}_i,\mathbf{q})}{\partial\mathbf{n}_\mathbf{p}\partial\mathbf{n}_\mathbf{q}}\right)\mathrm{d}S_\mathbf{q}\\&+\int_S\{\psi_j(\mathbf{q})-\psi_j(\mathbf{p}_i)-\nabla\psi_j(\mathbf{p}_i)\}\frac{\partial^2 G_0(\mathbf{p}_i,\mathbf{q})}{\partial\mathbf{n}_{\mathbf{p}_i}\partial\mathbf{n}_\mathbf{q}}\mathrm{d}S_\mathbf{q}\\&\int_S\nabla\psi_j(\mathbf{p}_i)\cdot\mathbf{n}_\mathbf{q}\frac{\partial G_0}{\partial\mathbf{n}_\mathbf{p}}\mathrm{d}S_\mathbf{q}-\frac{1}{2}\nabla\psi_j(\mathbf{p})\cdot\mathbf{n}_\mathbf{p}\Bigg]=g(\mathbf{p}_i).\end{aligned} \tag{4.3}$$

At this point, it is worth noting that by choosing the basis functions to be piecewise-constant functions, at any point $\mathbf{p}_i$ that is in the interior of one of the surface elements (and recall that this a requirement on the points $\mathbf{p}_i$), $\nabla\psi_j(\mathbf{p}_i)=\mathbf{0}$ and (4.3) reduces to a variation of the standard piecewise-constant approximation.

The gradient of each basis function can be computed from

$$\begin{cases} \dfrac{\partial \psi_j}{\partial x}\dfrac{\partial x}{\partial u} + \dfrac{\partial \psi_j}{\partial y}\dfrac{\partial y}{\partial u} + \dfrac{\partial \psi_j}{\partial z}\dfrac{\partial z}{\partial u} = \dfrac{\partial \psi_j}{\partial u}, \\ \dfrac{\partial \psi_j}{\partial x}\dfrac{\partial x}{\partial v} + \dfrac{\partial \psi_j}{\partial y}\dfrac{\partial y}{\partial v} + \dfrac{\partial \psi_j}{\partial z}\dfrac{\partial z}{\partial v} = \dfrac{\partial \psi_j}{\partial v}, \\ \dfrac{\partial \psi_j}{\partial x}n_x + \dfrac{\partial \psi_j}{\partial y}n_y + \dfrac{\partial \psi_j}{\partial z}n_z = 0, \end{cases} \tag{4.4}$$

where the last equation in (4.4) is due to the fact that the basis functions do not vary in the direction perpendicular to the surface element.

Using the discontinuous basis functions discussed above, assume that the solution over each element is interpolated using L basis functions and hence we will require L collocation points within each element. Hence, the total number of basis functions and collocation points is given by $m = ML$. The approximation to the integral equation (4.3) can be written in terms of matrix notation as

$$(A + \alpha C)\underline{\phi} = \underline{f}, \tag{4.5}$$

where $\underline{\phi} = [\phi_1, \phi_2, \ldots, \phi_{ML}]$ is the vector of the coefficients appearing in (4.1). In general, A will be block matrix consisting of $M \times M$ blocks each of size $L \times L$ and $\underline{f}$ will be a block vector consisting of M blocks of size L. Denote the L collocation points in element i by $\mathbf{p}_l^{[i]}$, $l = 1, \ldots, L$, and let $\psi_l^{[i]}$, $l = 1, \ldots, L$, be the L basis functions for element i. Then, the (i, j) blocks of A and C which we shall denote $A^{[i,j]}$ and $C^{[i,j]}$, respectively, are given by

$$\begin{aligned} A_{l,m}^{[i,j]} &= -\frac{1}{2}\psi_m^{[j]}(\mathbf{p}_l^{[i]}) + \int_{S_j} \frac{\partial G_k(\mathbf{p}_l^{[i]}, \mathbf{q})}{\partial \mathbf{n_q}} \psi_m^{[j]}(\mathbf{q}) \mathrm{d}S_q, \\ C_{l,m}^{[i,j]} &= \int_{S_j} \frac{\partial^2 G_k(\mathbf{p}_l^{[i]}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \psi_m^{[j]}(\mathbf{q}) \mathrm{d}S_q \end{aligned} \tag{4.6}$$

for $1 \leqslant l, m \leqslant L$. Clearly, if $i \neq j$, then the integrals appearing in (4.6) are non-singular and can be evaluated using an appropriate quadrature rule. In the case $i = j$, the integrals for $A^{[i,j]}$ are weakly singular about the point $\mathbf{p}_l^{[i]}$, but this is not a problem provided that special quadrature rules for dealing with this weak singularity are used (see Amini *et al.*, 1992, for a discussion of appropriate quadrature rules). To evaluate the blocks on the diagonal of C, we make use of (3.9) to give

$$\begin{aligned} C_{l,m}^{[i,i]} = &\int_{S_i} \left(\frac{\partial^2 G_k(\mathbf{p}_l^{[i]}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \frac{\partial^2 G_0(\mathbf{p}_l^{[i]}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \right) \psi_m^{[i]}(\mathbf{q}) \mathrm{d}S_{\mathbf{q}} \\ &+ \int_{S_i} (\psi_m^{[i]}(\mathbf{q}) - \psi_m^{[i]}(\mathbf{p}_l^{[i]}) - \nabla \psi_m^{[i]}(\mathbf{p}_l^{[i]}) \cdot (\mathbf{q} - \mathbf{p}_l^{[i]})) \frac{\partial^2 G_0(\mathbf{p}_l^{[i]}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_q \\ &+ \sum_{j=1, j\neq i}^{M} \int_{S_j} (-\psi_m^{[i]}(\mathbf{p}_l^{[i]}) - \nabla \psi_m^{[i]}(\mathbf{p}_l^{[i]}) \cdot (\mathbf{q} - \mathbf{p}_l^{[i]})) \frac{\partial^2 G_0(\mathbf{p}_l^{[i]}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} \mathrm{d}S_q \end{aligned}$$

$$\sum_{j=1}^{M}\int_{S_j}\nabla\psi_m^{[i]}(\mathbf{p}_l^{[i]})\cdot\mathbf{n}_\mathbf{q}\frac{\partial G_0(\mathbf{p}_l^{[i]})}{\partial\mathbf{n}_\mathbf{p}}\mathrm{d}S_\mathbf{q} \tag{4.7}$$

for $1 \leqslant l, m \leqslant L$. All the integrals appearing in (4.7) are at worst weakly singular and so can be evaluated using the same quadrature rules as for the diagonal block of A.

The entries in the right-hand side vector are given by

$$\underline{f}_l^{[i]} = \sum_{j=1}^{M}\int_{S_j}\left(G_k(\mathbf{p}_l^{[i]},\mathbf{q}) + \alpha\frac{\partial G_k(\mathbf{p}_l^{[i]})}{\partial\mathbf{n}_\mathbf{p}}\right)\frac{\partial\phi(\mathbf{q})}{\partial\mathbf{n}_\mathbf{q}}\mathrm{d}S_\mathbf{q} + \frac{\alpha}{2}\frac{\partial\phi(\mathbf{p}_l^{[i]})}{\partial\mathbf{n}_\mathbf{p}}, \tag{4.8}$$

in which all the integrals are at worst weakly singular and provided we take the same care over the choice of quadrature rule as for the matrices, there should not be any problems with evaluating them.

All the integrals in the current formulation are at worst weakly singular and so can be evaluated using appropriate quadrature rules. The change of variables given in Duffy (1982), as used in Amini *et al.* (1992), along with a product Gauss rule has been used here to evaluate the weakly singular integrals. The non-singular integrals have been evaluated using a product Gauss rule mapped onto the reference triangle. As recommended in Amini *et al.* (1992), we have used a higher-order product Gauss rule for the weakly singular integrals than the one used for the non-singular integrals.

The choice of coupling parameter α is crucial to the accuracy of the Burton and Miller method. In Amini (1989) and Amini *et al.* (1992), it was suggested that the almost optimal choice of α which minimizes the condition number of the integral operators is $\alpha = \frac{i}{k}$, and this is the value that we shall use here.

We remark that our new reformulation (3.9) of the second derivative of the Green's function opens up many new possibilities of solving the final linear system by efficient iterative solvers, e.g. by the fast multipole methods (Rokhlin, 1990) or the conjugate-gradient-type methods, using types of sparse preconditioners as developed by Chen & Harris (2001) and Chen (2001). Also related is an application of this work to solving the Helmholtz equation for the case of high wave numbers; see Chandler-Wilde *et al.* (2004) and the references therein. We intend to investigate such methods in the near future.

5. Numerical results

We now demonstrate that the high-order collocation method for solving the exterior Helmholtz equation in three dimensions, proposed in this paper, can yield much higher degree of precision than the piecewise-constant collocation method that is widely used in practice (see Amini *et al.*, 1992; Chen & Harris, 2001, and the references therein, e.g.). The individual test problems considered here are outlined below, where the point sources are used to calculate both the Neumann boundary data and the corresponding exact solution:

1. A unit sphere with point sources at (0, 0, 0.5) and (0.25, 0.25, 0.25) with strengths $2+3\mathrm{i}$ and $4-\mathrm{i}$, respectively.
2. A cylinder of length 0.537 and radius 0.2685 with point sources at (0, 0, 0.15) and (0.25, 0.25, 0.25) with strengths $2+3\mathrm{i}$ and $4-\mathrm{i}$, respectively.
3. A 'peanut'-shaped surface defined by

$$x = \sqrt{\cos 2\theta + \sqrt{1.5 - \sin^2 2\theta}}\,\sin\theta\cos\gamma\,,$$
$$y = \sqrt{\cos 2\theta + \sqrt{1.5 - \sin^2 2\theta}}\,\sin\theta\sin\gamma\,, \qquad 0 \leqslant \theta \leqslant \pi\,, \quad 0 \leqslant \gamma < 2\pi\,,$$
$$z = \sqrt{\cos 2\theta + \sqrt{1.5 - \sin^2 2\theta}}\,\cos\theta,$$

with point sources at (0.2, 0 , 1) and (0, 0.2, -0.75) with strength $2 + 3\mathrm{i}$ and $4 - \mathrm{i}$, respectively.

We note that the second test problem is for a non-smooth surface in the sense that it does not possess a unique normal at every point and that the third test problem is for a surface which is not convex. For each of these, a test mesh with 576 quadratically curved triangular elements and 1154 nodes was used. These are the same test problems as used for the Galerkin method in Harris & Chen (2003).

The basis functions used here are the complete linear and quadratic polynomial basis functions, giving three or six basis functions and collocation points per element, respectively. For the discontinuous linear basis functions, the collocation points are located at $(\delta/3, \delta/3)$, $(1-2\delta/3, \delta/3)$ and $(\delta/3, 1-2\delta/3)$, where $0 < \delta < 1$ is a location parameter. If $\delta = 1$, then the collocation points would all be located at the element centroid, while if $\delta = 0$, the collocation points would be located at the three vertices of the element. Clearly, there would be problems with either of these cases as the resulting linear system of equations would not be linearly independent due to two or more collocation points being coincident. For the discontinuous quadratic basis functions, the collocation points are the three collocation points used for the linear case and the three points which are midway between each of these. The equivalent results that would be obtained using the usual piecewise-constant approximation are also given to illustrate the improvement that can be obtained in the accuracy by using the higher-order basis functions. We remark that while the results presented in this paper are for the usual quadratically curved triangular boundary elements (see Amini *et al.*, 1992, for further details), the methods used can be easily adapted for other types of element.

The relative L_2-error, defined by

$$E = \frac{\|\phi - \tilde{\phi}\|_2}{\|\phi\|_2}, \tag{5.1}$$

where $\|\phi\|_2 = \sqrt{\int_S |\phi(q)|^2\,\mathrm{d}S_q}$ and ϕ and $\tilde{\phi}$ denote the exact (point-source) and approximate solutions, respectively, is the measure of the error used here. All errors are given as a percentage. We note that the integrals appearing in (5.1) have to be evaluated numerically, and here we have used a quadrature rule of sufficient accuracy so that the errors in evaluating these integrals is minute compared to the error in the approximate solution.

Figure 1 shows how the L_2-error varies with δ using linear basis functions. The values of k used for the sphere, cylinder and peanut are 3.142, 3.8 and 6.3, respectively, which are the approximate value of the first characteristic wave number for each surface. The corresponding results for the quadratic basis functions are given in Fig. 2. It is clear that the choice of δ has a significant effect on the overall accuracy of the scheme. The choice $\delta = 0.4$ seems to give the best results for the linear basis functions, while the choice $\delta = 0.25$ gives the best results for the quadratic basis functions, although the appropriate value to use is not so clear in this case. Similar results can be obtained for other values of k and for brevity these are not shown here.

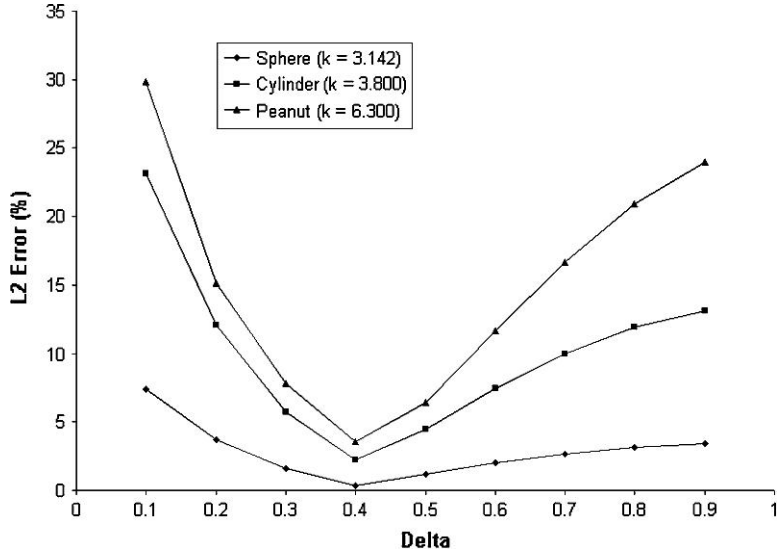

FIG. 1. The original (top) and modified surface (bottom) used to prove Lemma 1.

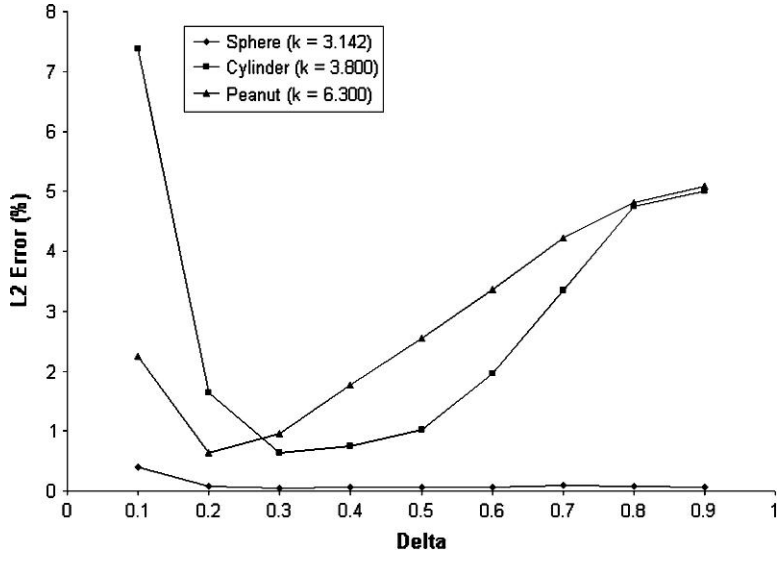

FIG. 2. L_2-relative error on each test surface for different values of δ using the linear basis functions.

Table 1 gives the L_2-relative error in the computed solution for each surface with a piecewise-constant approximation, a discontinuous piecewise-linear approximation and a discontinuous piecewise-quadratic approximation.

These results show that the discontinuous linear and quadratic approximations proposed here are considerably more accurate than the usual piecewise-constant approximation which has been widely used in previous work.

TABLE 1 *L_2-relative error in the computed solution using constant, linear and quadratic approximations for each surface*

	Sphere			Cylinder			Peanut		
k	Constant	Linear	Quadratic	Constant	Linear	Quadratic	Constant	Linear	Quadratic
1	2.63	0.11	0.01	7.18	0.88	0.36	3.77	0.45	0.08
2	3.98	0.2	0.03	10.38	1.08	0.45	5.69	0.67	0.12
3	5.54	0.32	0.04	14.15	1.55	0.57	9.34	1.32	0.17
4	7.21	0.47	0.06	17.84	2.42	0.68	12.29	1.89	0.22
5	8.94	0.66	0.08	22.15	3.64	0.84	14.17	2.52	0.31
6	10.77	0.98	0.21	27.67	5.21	1.08	17.37	3.27	0.54
7	12.65	1.27	0.18	31.32	7.15	1.45	21.78	4.68	0.92
8	14.6	1.6	0.19	35.66	9.1	1.78	24	6.15	1.05
9	16.65	2.09	0.25	45.41	12.13	2.45	27.3	10.18	1.49
10	18.78	3.11	0.38	50.78	15.81	3.52	34.36	12.68	1.9

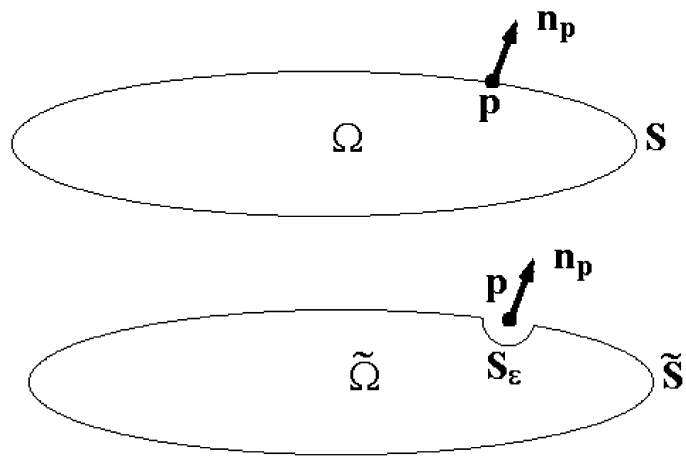

FIG. 3. L_2-relative error on each test surface for different values of δ using the quadratic basis functions.

6. Conclusions

The well-known approach for solving the exterior Helmholtz problem in 3D is the collocation method using piecewise-constant elements. However, until now it has not been possible to use high-order elements with the collocation method, due to the integral operator with a hypersingular kernel function, unless special finite-part quadrature rules are used to evaluate this hypersingular operator. The method proposed here reformulates the hypersingular integral into one which is at worst weakly singular and which can be readily evaluated using well-known techniques.

The numerical results presented in this paper clearly show that there is a considerable improvement in the accuracy of the newly reformulated Burton and Miller method if discontinuous linear or quadratic basis functions are used in place of the more usual piecewise-constant basis functions. Further work on fast solvers' issues is in progress.

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Appendix A. Proof of Lemma 1

Proof. Let S_ε be the surface of a sphere centred on $\mathbf{p}$, $\tilde{\Omega}$ be Ω excluding the interior of S_ε and $\tilde{S}$ denote the surface bounding $\tilde{\Omega}$ (see Fig. 3). We note that for $\mathbf{q} \in \tilde{\Omega}$, it holds that

$$\nabla^2_{\mathbf{q}} \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n}_\mathbf{p}} + k^2 \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n}_\mathbf{p}} = 0. \tag{A.1}$$

Applying Green's second theorem,

$$\int_{\tilde{S}} \left(\phi_1 \frac{\partial \phi_2}{\partial \mathbf{n_q}} - \phi_2 \frac{\partial \phi_1}{\partial \mathbf{n_q}} \right) \mathrm{d}S_{\mathbf{q}} = \int_{\tilde{\Omega}} (\phi_1 \nabla^2_{\mathbf{q}} \phi_2 - \phi_2 \nabla^2_{\mathbf{q}} \phi_1) \mathrm{d}V_{\mathbf{q}} \tag{A.2}$$

with $\phi_1 = \mathbf{a} \cdot (\mathbf{q} - \mathbf{p})$ and $\phi_2 = \frac{\partial G_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{n_p}}$ leads to (taking note of (A.1) in the first integral on the right-hand side of (A.2))

$$\int_{\tilde{S}} \left(\mathbf{a} \cdot (\mathbf{q} - \mathbf{p}) \frac{\partial^2 G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \mathbf{a} \cdot \mathbf{n_q} \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p}} \right) \mathrm{d}S_{\mathbf{q}} = \int_{\tilde{\Omega}} -k^2 \mathbf{a} \cdot (\mathbf{q} - \mathbf{p}) \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}V_{\mathbf{q}}. \tag{A.3}$$

The surface integral in (A.3) can be expressed as the sum of integral over the relevant part of the surface S_ε and the integral over the remaining part of $\tilde{S}$, say $\tilde{S}_\varepsilon$. As $\varepsilon \to 0$, then $\tilde{S}_\varepsilon \to S$, $\tilde{\Omega} \to \Omega$ and

$$\int_{S_\varepsilon} \left(\mathbf{a} \cdot (\mathbf{q} - \mathbf{p}) \frac{\partial^2 G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \mathbf{a} \cdot \mathbf{n_q} \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p}} \right) \mathrm{d}S_{\mathbf{q}} \to \frac{\mathbf{a} \cdot \mathbf{n_p}}{2}. \tag{A.4}$$

Hence, we obtain that

$$\begin{aligned} &\int_S \left(\mathbf{a} \cdot (\mathbf{q} - \mathbf{p}) \frac{\partial^2 G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p} \partial \mathbf{n_q}} - \mathbf{a} \cdot \mathbf{n_q} \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p}} \right) \mathrm{d}S_{\mathbf{q}} \\ &\quad = \int_\Omega -k^2 \mathbf{a} \cdot (\mathbf{q} - \mathbf{p}) \frac{\partial G_k(\mathbf{p}, \mathbf{q})}{\partial \mathbf{n_p}} \mathrm{d}V_{\mathbf{q}} - \frac{\mathbf{a} \cdot \mathbf{n_p}}{2}, \end{aligned} \tag{A.5}$$

which can be rearranged to give the desired result. Hence, the proof is completed. □