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QUADRATURE OF SINGULAR INTEGRANDS OVER SURFACES*

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Abstract. Consider integration over a simple closed smooth surface in $\mathbb{R}^3$, one that is homeomorphic to the unit sphere, and suppose the integrand has a point singularity. We propose a numerical integration method based on using transformations that lead to an integration problem over the unit sphere with an integrand that is much smoother. At this point, the trapezoidal rule is applied to the spherical coordinate representation of the problem. The method is simple to apply and it results in rapid convergence. The intended application is to the evaluation of boundary integrals arising in boundary integral equation methods in potential theory and the radiosity equation.

Key words. spherical integration, singular integrand, boundary integral, trapezoidal rule.

AMS subject classifications. 65D32, 65B15.

1. Introduction.

Consider the approximation of a surface integral

$$I(\rho) = \int_S \rho(Q)dS_Q \tag{1.1}$$

in which $\rho(Q)$ is singular at a point $Q = P$. This is a common integration problem when implementing boundary integral equation methods. Examples are the single layer integral

$$\int_S \frac{\psi(Q)}{|Q-P|}dS_Q \tag{1.2}$$

and the double layer integral

$$\int_S \frac{\partial}{\partial \mathbf{n}_Q}\left[\frac{1}{|Q-P|}\right]\psi(Q)dS_Q \tag{1.3}$$

in which $P \in S$. In this paper we introduce an efficient numerical integration method for such integrals.

We limit the surfaces S to be the boundary of a bounded simply-connected region Ω, and we assume that S is a 'smooth surface'. In addition, we assume that a mapping

$$\mathcal{M} : U \underset{onto}{\xrightarrow{1-1}} S \tag{1.4}$$

is given with U the unit sphere in $\mathbb{R}^3$. For example, with the ellipsoidal surface S defined implicitly by

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 + \left(\frac{z}{c}\right)^2 = 1, \tag{1.5}$$

we can write

$$\mathcal{M} : (\xi,\eta,\zeta) \in U \mapsto (x,y,z) = (a\xi, b\eta, c\zeta) \in S. \tag{1.6}$$

Throughout this paper, we assume that the surface S and the mapping $\mathcal{M}$ are as differentiable as needed. To simplify the later error analysis, we also assume that there is an open

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$\varepsilon-$neighborhood of U, for some $\varepsilon > 0$, on which $\mathcal{M}$ is defined, one-to-one, and differentiable, with a non-zero Jacobian when considered as a three-dimensional mapping. This can be weakened, and we discuss this at the conclusion of the paper.

With such transformations (1.4), the integral (1.1) becomes

$$I(\rho) = \int_U \rho\left(\mathcal{M}(\widehat{Q})\right) J_{\mathcal{M}}(\widehat{Q})\, dS_{\widehat{Q}}, \tag{1.7}$$

with $J_{\mathcal{M}}(\widehat{Q})$ the Jacobian of the mapping $\mathcal{M}$ considered as a two-dimensional mapping of the surface U onto the surface S. For example, with the ellipsoidal surface (1.6),

$$J_{\mathcal{M}}(\widehat{Q}) = \sqrt{(bc\xi)^2 + (ac\eta)^2 + (ab\zeta)^2}, \qquad \widehat{Q} = (\xi, \eta, \zeta) \in U.$$

In the appendix to this paper we give a way to calculate $J_{\mathcal{M}}(\widehat{Q})$ for general transformations $\mathcal{M}$. Based on being able to perform this transformation of variables, we often restrict our interest in this paper to the unit sphere U. The numerical examples, however, will illustrate the use of more general surfaces.

Boundary integral equation methods are of two general types: (*i*) boundary element methods in which S is decomposed into small elements and ρ is approximated by a low degree polynomial over each element; and (*ii*) using approximations to ρ of a global type over the entire surface S, for example, using spherical polynomials. The methods of this paper are intended for integrals arising in the latter second type of boundary integral method. For example, see [1], [3], [6]; and for an earlier discussion of the numerical approximation of surface integrals with a point singularity, see [2]. For a more general introduction to quadrature methods for the sphere, see Stroud [12].

In §2, we introduce and analyze the numerical method, doing so for ρ a smooth function, and we illustrate it numerically in §3. In §4 the numerical method is extended to ρ having a point-singularity, and numerical examples are given in §5.

2. The numerical method. We begin with the problem of approximating

$$I(f) = \int_U f(Q) dS_Q \tag{2.1}$$

in which f is several times continuously differentiable over the unit sphere U. In spherical coordinates, this integral can be written as

$$I(f) = \int_0^{\pi} \int_0^{2\pi} f\left(\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta\right) \sin\theta \, d\phi\, d\theta.$$

Rather than approximating this integral directly, we begin by introducing a transformation $\mathcal{L} : U \xrightarrow[onto]{1-1} U$. With respect to spherical coordinates on U,

$$\mathcal{L} : Q = (\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta) \mapsto \widetilde{Q} = \frac{(\cos\phi \sin^q\theta, \sin\phi \sin^q\theta, \cos\theta)}{\sqrt{\cos^2\theta + \sin^{2q}\theta}} \equiv L(\phi, \theta). \tag{2.2}$$

In this transformation, $q \geq 1$ is a 'grading parameter'. The north and south poles of U remain fixed, while the region around them is distorted by the mapping.

The integral $I(f)$ becomes

$$I(f) = \int_U f\left(\mathcal{L}(\widetilde{Q})\right) J_{\mathcal{L}}\left(\widetilde{Q}\right) dS_{\widetilde{Q}}, \tag{2.3}$$

with $J_{\mathcal{L}}\left(\widetilde{Q}\right)$ the Jacobian of the mapping $\mathcal{L}$,

$$J_{\mathcal{L}}\left(\widetilde{Q}\right) = |D_\phi L(\phi,\theta) \times D_\theta L(\phi,\theta)| = \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}}. \tag{2.4}$$

In spherical coordinates,

$$\begin{aligned} I(f) &= \int_0^\pi \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} \int_0^{2\pi} f\left(\xi,\eta,\zeta\right)\,d\phi\,d\theta, \\ (\xi,\eta,\zeta) &= \frac{\left(\cos\phi\sin^q\theta, \sin\phi\sin^q\theta, \cos\theta\right)}{\sqrt{\sin^{2q}\theta + \cos^2\theta}}. \end{aligned} \tag{2.5}$$

For the example ellipsoidal surface of (1.5),

$$\begin{aligned} I(\rho) = \int_S \rho(Q) dS_Q = \int_0^\pi & \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} \\ & \times \int_0^{2\pi} \rho\left(\xi,\eta,\zeta\right)\sqrt{\left(bc\xi\right)^2 + \left(ac\eta\right)^2 + \left(ab\zeta\right)^2}\,d\phi\,d\theta. \end{aligned} \tag{2.6}$$

For $n \geq 1$, let $h = \pi/n$, and

$$\phi_j = \theta_j = jh.$$

For a generic function g, introduce the bivariate trapezoidal approximation

$$\int_0^\pi \int_0^{2\pi} g(\sin\theta, \cos\theta, \sin\phi, \cos\phi)\,d\phi\,d\theta \approx h^2 \sum_{k=0}^{n}{}'' \sum_{j=0}^{2n}{}'' g(\sin\theta_k, \cos\theta_k, \sin\phi_j, \cos\phi_j),$$

in which the superscript notation $''$ means to multiply the first and last terms by $\frac{1}{2}$ before summing. Apply this to (2.5). Note that the integrand is zero for $\theta = 0, \pi$ and that the integrand has period 2π in ϕ. Therefore

$$\begin{aligned} & \int_0^\pi \int_0^{2\pi} g(\sin\theta, \cos\theta, \sin\phi, \cos\phi)\,d\phi\,d\theta \\ & \qquad \approx h^2 \sum_{k=1}^{n-1} \sum_{j=1}^{2n} g(\sin\theta_k, \cos\theta_k, \sin\phi_j, \cos\phi_j) \equiv \mathcal{T}_n, \\ & g = \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} f\left(\xi,\eta,\zeta\right), \end{aligned} \tag{2.7}$$

with (ξ, η, ζ) as in (2.5).

We note that closely related transformations for single integrals have been used often over the past several decades, with the trapezoidal rule applied to the transformed integral (e.g. see Sidi [9], [10], [11]). A very readable overview and analysis of such transformations and the associated trapezoidal rule is given in Elliott [5].

2.1. Error analysis. Apply the trapezoidal rule

$$I \equiv \int_0^\pi d(\theta)\, d\theta \approx T_n \equiv h \sum_{j=0}^{n}{}'' d\,(jh)\,, \qquad h = \frac{\pi}{n}$$

to the integral

$$\int_0^\pi t(\theta) \sin^m \theta \, d\theta,$$

with $t(\theta)$ a sufficiently differentiable function and $m \geq 0$ an integer. More precisely, assume $t^{(p)} \in L\,(0, \pi)$ with

$$p = \begin{cases} m+2, & m \text{ even}, \\ m+1, & m \text{ odd}. \end{cases}$$

Then

$$I - T_n = O\,(h^p)\,. \tag{2.8}$$

The proof is an immediate corollary of the Euler-MacLaurin expansion [4, p. 285]. For later reference, we state the Euler-MacLaurin expansion.

The Euler-MacLaurin formula. Let $m \geq 0$, $n \geq 1$, and define $h = (b-a)/n$, $x_j = a + jh$ for $j = 0, 1, \ldots, n$. Further assume $\psi(x)$ is $2m+2$ times differentiable on $[a, b]$ with $\psi^{(2m+2)} \in L\,(a, b)$. Then

$$\begin{aligned} \int_a^b \psi(x)\, dx - h \sum_{j=0}^{n}{}'' \psi(x_j) &= \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} h^{2i} \left[\psi^{(2i-1)}(b) - \psi^{(2i-1)}(a)\right] \\ &\quad + \frac{h^{2m+2}}{(2m+2)!} \int_a^b \overline{B}_{2m+2} \left(\frac{x-a}{h}\right) \psi^{(2m+2)}(x)\, dx. \end{aligned} \tag{2.9}$$

In this formula, $\{B_k\}$ are the Bernoulli constants, $B_k(x)$ is the Bernoulli polynomial of degree k, and $\overline{B}_k(x)$ is the periodic extension of $B_k(x)$ on $[0, 1]$.

Using this result, we have the following convergence theorem.

THEOREM 2.1. *In the integral (2.5), assume that $q \geq 1$ and that $2q$ is a positive integer. Introduce*

$$p = \begin{cases} 2q, & 2q \text{ even}, \\ 2q+1, & 2q \text{ odd}. \end{cases}$$

Assume that f is p-times differentiable with $f^{(p)} \in L\,(U)$. Then the error in approximating (2.1) by (2.7) satisfies

$$I - \mathcal{T}_n = O\,(h^p)\,. \tag{2.10}$$

Proof. In order to prove this, we use the Euler-MacLaurin expansion, applying it to both the integration in ϕ and in θ. More precisely, we write

$$
\begin{aligned}
I(f)-\mathcal{T}_n &= \int_0^{\pi} \frac{\sin^{2q-1}\theta\left(q\cos^2\theta+\sin^2\theta\right)}{\left(\sin^{2q}\theta+\cos^2\theta\right)^{\frac{3}{2}}} \int_0^{2\pi} f\left(\xi,\eta,\zeta\right)\,d\phi\,d\theta \\
&\quad - h\sum_{k=1}^{n-1} \frac{\sin^{2q-1}\theta_k\left(q\cos^2\theta_k+\sin^2\theta_k\right)}{\left(\sin^{2q}\theta_k+\cos^2\theta_k\right)^{\frac{3}{2}}} \int_0^{2\pi} f\left(\xi_k,\eta_k,\zeta_k\right)\,d\phi \\
&\quad + h\sum_{k=1}^{n-1} \frac{\sin^{2q-1}\theta_k\left(q\cos^2\theta_k+\sin^2\theta_k\right)}{\left(\sin^{2q}\theta_k+\cos^2\theta_k\right)^{\frac{3}{2}}} \\
&\qquad \times \left[\int_0^{2\pi} f\left(\xi_k,\eta_k,\zeta_k\right)\,d\phi - h\sum_{j=1}^{2n} f\left(\xi_{k,j},\eta_{k,j},\zeta_{k,j}\right)\right],
\end{aligned}
\tag{2.11}
$$

with

$$
\begin{aligned}
\left(\xi_k,\eta_k,\zeta_k\right) &= \frac{\left(\cos\phi\sin^q\theta_k, \sin\phi\sin^q\theta_k, \cos\theta_k\right)}{\sqrt{\sin^{2q}\theta_k+\cos^2\theta_k}}, \\
\left(\xi_{k,j},\eta_{k,j},\zeta_{k,j}\right) &= \frac{\left(\cos\phi_j\sin^q\theta_k, \sin\phi_j\sin^q\theta_k, \cos\theta_k\right)}{\sqrt{\sin^{2q}\theta_k+\cos^2\theta_k}}.
\end{aligned}
$$

The integration in ϕ is that of a periodic function over $[0,2\pi]$, and we need only show that the p^{th}-order derivative with respect to ϕ is absolutely integrable over $0\le\phi\le 2\pi$. This is straightforward, as all such derivatives are well-defined and continuous.

When considering the integration in (2.5) with respect to θ, write the integrand as $F(\theta)G(\theta)$ with

$$
\begin{aligned}
F(\theta) &= \frac{q\cos^2\theta+\sin^2\theta}{\left(\sin^{2q}\theta+\cos^2\theta\right)^{\frac{3}{2}}}\sin^{2q-1}\theta, \\
G(\theta) &= \int_0^{2\pi} f\left(\xi,\eta,\zeta\right)\,d\phi.
\end{aligned}
$$

For the integration in θ, we need to look at the derivatives of $F(\theta)G(\theta)$ with respect to θ for $0\le\theta\le\pi$. In particular, we must show that

$$
\left.\frac{d^k}{d\theta^k}\left[F(\theta)G(\theta)\right]\right|_{\theta=0}^{\pi} = 0, \qquad k=1:2:p-3, \tag{2.12}
$$

$$
\frac{d^p}{d\theta^p}\left[F(\theta)G(\theta)\right] \in L^p\left(0,\pi\right). \tag{2.13}
$$

We show (2.12) by instead showing

$$
\frac{d^k}{d\theta^k}\left[F(\theta)G(\theta)\right] = 0, \qquad k=1:2:p-3, \qquad \theta=0,\pi. \tag{2.14}
$$

For the derivatives of $F(\theta)G(\theta)$, we write

$$
\frac{d^k}{d\theta^k}\left[F(\theta)G(\theta)\right] = \sum_{j=0}^{k}\binom{k}{j}F^{(j)}(\theta)G^{(k-j)}(\theta), \tag{2.15}
$$

and then look at the individual derivatives of F and G.

As a part of differentiating $F(\theta)$, we introduce the following expressions. Let

$$\begin{aligned} R(\theta) &= \sin^{2q}\theta + \cos^2\theta \\ &= \sin^{2q}\theta - \sin^2\theta + 1, \qquad 0 \le \theta \le \pi. \end{aligned}$$

Then

$$\begin{aligned} R'(\theta) &= 2\cos\theta\left[q\sin^{2q-1}\theta - \sin\theta\right] \\ &\equiv c_1(\theta)\sin^{2q-1}\theta - c_2(\theta)\sin\theta, \end{aligned} \tag{2.16}$$

with $c_1(\theta)$ and $c_2(\theta)$ infinitely differentiable functions of θ. It will be important to keep track of powers of $\sin\theta$ in the various derivatives. We will use the notation $c_k(\theta)$, $k \ge 1$, to denote generic smooth functions of θ. Next,

$$\frac{d}{d\theta}\left[q\cos^2\theta + \sin^2\theta\right] = 2(1-q)\sin\theta\cos\theta \equiv (1-q)\sin(2\theta). \tag{2.17}$$

For the derivatives of G, we need the derivatives of (ξ, η, ζ) considered as a function of θ. The first derivatives are given by

$$\begin{aligned} \begin{bmatrix} \dfrac{d\xi}{d\theta} \\ \dfrac{d\eta}{d\theta} \end{bmatrix} &= \sin^{q-1}\theta \left[\underbrace{\frac{q\cos\theta}{\sqrt{R(\theta)}} - \frac{c_1(\theta)\sin^2\theta}{2R(\theta)^{\frac{3}{2}}}}_{\equiv c_5(\theta)}\right] \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \\ &= c_5(\theta)\sin^{q-1}\theta \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix}, \end{aligned} \tag{2.18}$$

$$\frac{d\zeta}{d\theta} = \sin\theta\left[\frac{-1}{\sqrt{R(\theta)}} - \frac{c_1(\theta)\cos\theta}{2R(\theta)^{\frac{3}{2}}}\right] \equiv c_6(\theta)\sin\theta. \tag{2.19}$$

We discuss later the higher order derivatives of (ξ, η, ζ).

We need to prove both (2.12) and (2.13), and in doing so it is crucial to consider the various powers of $\sin\theta$ that occur in the derivatives of F and G. When $2q$ is an integer, $F(\theta)$ is infinitely differentiable on $[0, \pi]$. When q is an integer, life is simpler in that there are never any negative powers of $\sin\theta$ occurring in the differentiation process, with either F or G, no matter how high the order of the derivative. As a consequence we can show both (2.12) and (2.13) with no difficulty. Using (2.8), the main result (2.10) then follows with no difficulty.

From hereon we consider only the case that $2q$ is an odd integer; $q = r/2$ for some odd integer r. Thus $p = 2q + 1$ is an even integer. The proof of (2.13) requires showing that the integrand $F(\theta)G(\theta)$ is p-times differentiable with

$$\frac{d^p}{d\theta^p}\left[F(\theta)G(\theta)\right] \in L(0, \pi). \tag{2.20}$$

We examine the various derivatives of both F and G to determine the powers of $\sin\theta$ occurring in both.

To better follow what is happening, consider only the case of $2q = 3$ and $p = 4$. We then need to show (2.12) and (2.13) with $p = 4$. We are using the Euler-Maclaurin formula (2.9) with $m = 1$, and the form we need is

$$\begin{aligned}\int_0^\pi F(\theta)G(\theta)\,d\theta - h\sum_{k=1}^{n-1} F(\theta_k)G(\theta_k) &= \sum_{i=1}^{m} \frac{B_2}{2} h^2 \left[F(\theta)G(\theta)\right]_{\theta=0}^{\theta=\pi} \\ &\quad + \frac{h^4}{4!}\int_0^\pi \overline{B}_4\left(\frac{\theta}{h}\right)\frac{d^4}{d\theta^4}\left[F(\theta)G(\theta)\right]\,d\theta.\end{aligned} \tag{2.21}$$

The summation limits are changed because $F(0) = F(\pi) = 0$. We want to show the trapezoidal error is of size $O\left(h^4\right)$.

For this case,

$$F(\theta) = \frac{1.5\cos^2\theta + \sin^2\theta}{\left(\sin^3\theta + \cos^2\theta\right)^{\frac{3}{2}}}\sin^2\theta, \tag{2.22}$$

$$G(\theta) = \int_0^{2\pi} f\left(\xi,\eta,\zeta\right)\,d\phi, \tag{2.23}$$

$$(\xi,\eta,\zeta) = \frac{\left(\cos\phi\sin^{1.5}\theta, \sin\phi\sin^{1.5}\theta, \cos\theta\right)}{\sqrt{\sin^3\theta + \cos^2\theta}}, \tag{2.24}$$

$$\begin{aligned}R(\theta) &= \sin^3\theta + \cos^2\theta, \qquad 0 \le \theta \le \pi, \\ R'(\theta) &= c_1(\theta)\sin^2\theta - c_2(\theta)\sin\theta,\end{aligned}$$

with $c_1(\theta)$ and $c_2(\theta)$ infinitely differentiable. Also,

$$\frac{d}{d\theta}\left[q\cos^2\theta + \sin^2\theta\right] = -\sin\theta\cos\theta = -\frac{1}{2}\sin\left(2\theta\right).$$

For the derivatives of (ξ,η,ζ),

$$\begin{aligned}\begin{bmatrix}\dfrac{d\xi}{d\theta} \\ \dfrac{d\eta}{d\theta}\end{bmatrix} &= \sqrt{\sin\theta}\left[\underbrace{\frac{1.5\cos\theta}{\sqrt{R(\theta)}} - \frac{c_1(\theta)\sin^3\theta - c_2(\theta)\sin^2\theta}{2R(\theta)^{\frac{3}{2}}}}_{\equiv c_3(\theta)}\right]\begin{bmatrix}\cos\phi \\ \sin\phi\end{bmatrix} \\ &= c_3(\theta)\sqrt{\sin\theta}\begin{bmatrix}\cos\phi \\ \sin\phi\end{bmatrix}, \\ \frac{d\zeta}{d\theta} &= \sin\theta\left[\frac{-1}{\sqrt{R(\theta)}} - \frac{\left[c_1(\theta)\sin\theta - c_2(\theta)\right]\cos\theta}{2R(\theta)^{\frac{3}{2}}}\right] \equiv c_4(\theta)\sin\theta,\end{aligned}$$

with $c_3(\theta)$ and $c_4(\theta)$ infinitely differentiable. For the first derivative of $G(\theta)$,

$$G'(\theta) = \int_0^{2\pi}\left[f_1\frac{d\xi}{d\theta} + f_2\frac{d\eta}{d\theta} + f_3\frac{d\zeta}{d\theta}\right]\,d\phi,$$

with f_k denoting the partial derivative of f with respect to the argument k. We note that $G'(\theta)$ is continuous for $0 \le \theta \le \pi$, with $G'(\theta) = 0$ at $\theta = 0, \pi$.

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For the second derivative,

$$G''(\theta) = \int_0^{2\pi} \left[f_{1,1}\left(\frac{d\xi}{d\theta}\right)^2 + f_{2,2}\left(\frac{d\eta}{d\theta}\right)^2 + f_{3,3}\left(\frac{d\zeta}{d\theta}\right)^2 \right. \tag{2.25}$$

$$+ 2f_{1,2}\frac{d\xi}{d\theta}\frac{d\eta}{d\theta} + 2f_{1,3}\frac{d\xi}{d\theta}\frac{d\zeta}{d\theta} + 2f_{2,3}\frac{d\eta}{d\theta}\frac{d\zeta}{d\theta} \tag{2.26}$$

$$\left. + f_1\frac{d^2\xi}{d\theta^2} + f_2\frac{d^2\eta}{d\theta^2} + f_3\frac{d^2\zeta}{d\theta^2} \right] d\phi. \tag{2.27}$$

The terms in (2.25) and (2.26) involve $\sin^k\theta$ for $k = 1, 1.5$, and 2, and thus the corresponding integrals are continuous and are zero at $\theta = 0, \pi$. For the terms in (2.27), we need

$$\begin{bmatrix} \dfrac{d^2\xi}{d\theta^2} \\ \dfrac{d^2\eta}{d\theta^2} \end{bmatrix} = \left[\frac{c_3(\theta)}{2\sqrt{\sin\theta}} + c_3'(\theta)\sqrt{\sin\theta} \right] \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix}, \tag{2.28}$$

$$\frac{d^2\zeta}{d\theta^2} = c_4(\theta)\cos\theta + c_4'(\theta)\sin\theta. \tag{2.29}$$

The general pattern will continue. The higher order derivatives of (ξ, η, ζ) will contain powers of $\sin\theta$ as follows.

$$\begin{bmatrix} \dfrac{d^k\xi}{d\theta^k} \\ \dfrac{d^k\eta}{d\theta^k} \end{bmatrix} = O\left((\sin\theta)^{1.5-k} \right) \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix},$$

$$\frac{d^2\zeta}{d\theta^2} = O(1),$$

for $k = 1, 2, 3, 4$. The same behaviour carries across to the derivatives of $G(\theta)$:

$$G^{(k)}(\theta) = O\left((\sin\theta)^{1.5-k} \right), \qquad k = 1, 2, 3, 4. \tag{2.30}$$

For the derivatives of $F(\theta)$, we have the following.

$$\begin{aligned} F'(\theta) &= 2\sin\theta\cos\theta \frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{3}{2}}} + \sin^2\theta \frac{d}{d\theta}\left[\frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{3}{2}}} \right] \\ &= 2\sin\theta\cos\theta \frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{3}{2}}} - \sin^2\theta \frac{\cos\theta\sin\theta}{R(\theta)^{\frac{3}{2}}} \\ &\quad - \frac{3}{2}\sin^2\theta \frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{5}{2}}} \left[c_1(\theta)\sin^2\theta - c_2(\theta)\sin\theta \right] \\ &\equiv \sin(2\theta)\,\frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{3}{2}}} + c_5(\theta)\sin^3\theta, \end{aligned} \tag{2.31}$$

$$F''(\theta) = 2\cos(2\theta)\,\frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{3}{2}}} + c_6(\theta)\sin^2\theta,$$

$$F'''(\theta) = -4\sin(2\theta)\,\frac{1.5\cos^2\theta + \sin^2\theta}{R(\theta)^{\frac{3}{2}}} + c_7(\theta)\sin\theta,$$

for suitably defined infinitely differentiable functions $c_6(\theta)$ and $c_7(\theta)$. The function $F^{(4)}(\theta)$ is well-defined, but does not contain any obvious factor of $\sin\theta$.

Using (2.15) with $k = 4$,

$$\frac{d^4}{d\theta^4}\left[F(\theta)G(\theta)\right] = F(\theta)G^{(4)}(\theta) + 4F^{(1)}(\theta)G^{(3)}(\theta) + 6F^{(2)}(\theta)G^{(2)}(\theta) + 4F^{(3)}(\theta)G^{(1)}(\theta) + F^{(4)}(\theta)G(\theta).$$

Using the above results, we have

$$F(\theta)G^{(4)}(\theta),\ F^{(1)}(\theta)G^{(3)}(\theta),\ F^{(2)}(\theta)G^{(2)}(\theta) = O\left((\sin\theta)^{-\frac{1}{2}}\right),$$
$$F^{(3)}(\theta)G^{(1)}(\theta) = O\left((\sin\theta)^{\frac{1}{2}}\right),$$
$$F^{(4)}(\theta)G(\theta) = O\left(1\right).$$

This leads to

$$\frac{d^4}{d\theta^4}\left[F(\theta)G(\theta)\right] \in L\left(0,\pi\right).$$

Also,

$$\frac{d}{d\theta}\left[F(\theta)G(\theta)\right] = F'(\theta)G(\theta) + F(\theta)G'(\theta).$$

Using the earlier results on the dependence of F and G on $\sin\theta$, it follows that

$$\frac{d}{d\theta}\left[F(\theta)G(\theta)\right] = 0, \qquad \theta = 0, \pi.$$

Referring to (2.21), this proves (2.10) for the case $q = 1.5$.

For the general case of $q = r/2$ with $r \geq 3$ an odd integer, a similar proof can be given. For example, when we consider $q = 2.5$, we have $p = 6$ and the functions of (2.22)-(2.24) are

$$F(\theta) = \frac{2.5\cos^2\theta + \sin^2\theta}{\left(\sin^5\theta + \cos^2\theta\right)^{\frac{3}{2}}}\sin^4\theta,$$
$$G(\theta) = \int_0^{2\pi} f\left(\xi,\eta,\zeta\right)\, d\phi,$$
$$(\xi,\eta,\zeta) = \frac{\left(\cos\phi\sin^{2.5}\theta, \sin\phi\sin^{2.5}\theta, \cos\theta\right)}{\sqrt{\sin^5\theta + \cos^2\theta}}.$$

Then a similar set of results are true regarding the dependence on powers of $\sin\theta$ for the derivatives of F and G, but with the powers increased by 2 in the derivatives of F. We omit a general treatment as we believe it is clear that such a general analysis follows using the above ideas. $\square$

The rates of (2.10), and even better, are observed in practice. This is illustrated with the numerical examples of the following section. Based on those examples and on other partial theoretical results, we state the following conjecture that extends the above theorem.

CONJECTURE 2.2. *Assume $q \geq 1$. Under suitable assumptions on the function f, the error in approximating (2.1) by (2.7) satisfies*

$$I - \mathcal{T}_n = O\left(h^{2q}\right). \qquad (2.32)$$

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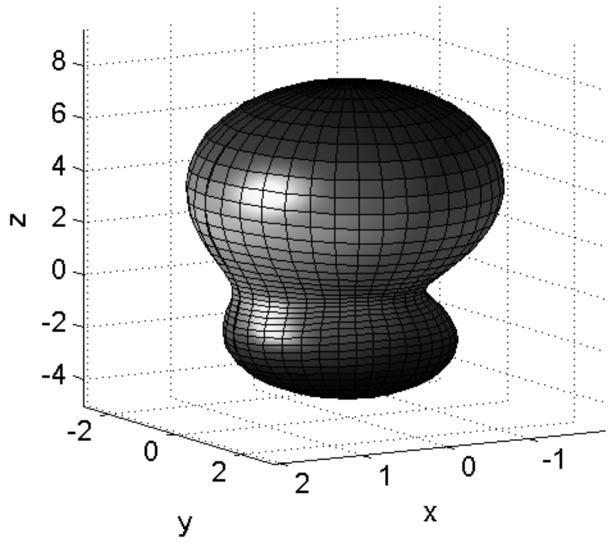

FIG. 3.1. *The nonsymmetric surface of (3.1)*

3. Numerical examples. We give numerical examples based on two surfaces. The first is the ellipsoid of (1.5), and the second is given by

$$\mathcal{M}: \begin{bmatrix} \xi \\ \eta \\ \zeta \end{bmatrix} \in U \quad \longmapsto \quad (x,y,z) = \rho\,(\xi,\eta,\zeta) \begin{bmatrix} a\xi \\ b\eta \\ c\zeta \end{bmatrix} \in S, \tag{3.1}$$
$$\rho\,(\xi,\eta,\zeta) = d\left(\xi^2 + g\xi^3\right) + e\left(\eta^2 + g\eta^3\right) + g\left(\zeta^2 + g\zeta^3\right).$$

For the parameters

$$(a,b,c,d,e,f,g) = (1, 1.5, 2, 1, 0.7, 3, 0.3)$$

a sketch of the surface is given in Figure 3.1 and we refer to it as a 'peanut surface'. The Jacobian $J_{\mathcal{M}}(\widehat{Q})$ was calculated by the method described in the appendix. This surface was designed to demonstrate empirically that the results of the paper do not depend on any symmetry of the surface, as this second surface has no obvious geometric symmetry.

3.1. Numerical results: Ellipsoid. We approximate the integral

$$\int_S e^{x+2y+3z} dS \doteq 18.340419192002230 \tag{3.2}$$

over the ellipsoid (1.5) with $(a,b,c) = (1.0, 0.5, 0.75)$. Numerical results are given in Table 3.1. The differences $\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$ are given for the specific value of $q = 2.25$, along with the ratios of successive differences and the estimated order of convergence (*EOC*). The results are consistent with the conjectured order given in (2.32), as $2q = 4.5$.

For the same integral (3.1), we give in Table 3.2 the estimated order of convergence as q varies. In general the results are consistent with (2.10) and the conjectured convergence result

TABLE 3.1
Numerical integrals for (3.2) over an ellipsoid with $q = 2.25$

n	$\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$	*Ratio*	*EOC*
4	$1.22E+1$		
8	$-2.47E+0$	-4.98	
16	$-3.92E-2$	62.94	5.98
32	$-1.84E-4$	213.14	7.74
64	$-8.36E-6$	21.88	4.45
128	$-3.70E-7$	22.59	4.50
256	$-1.64E-8$	22.62	4.50
512	$-7.23E-10$	22.63	4.50
1024	$-3.20E-11$	22.63	4.50

TABLE 3.2
Numerical integrals for (3.2) over an ellipsoid with varying q

q	1.00	1.25	1.50	1.75	2.00	2.25	2.50
EOC	2.0	2.5	6.0	3.5	4.0	4.5	*large*
q	2.75	3.00	3.25	3.50	3.75	4.00	
EOC	5.5	6.0	6.5	*large*	≈ 7.5	≈ 8.0	

of (2.32). But with the case of $q = 1.5$, 2.5, and 3.5, the estimated order of convergence is much better than that predicted by (2.10). A few additional comments concerning this superconvergence are given in the concluding discussion of this paper.

3.2. Numerical results: Peanut surface. We approximate the integral

$$\int_S e^{0.1(x+2y+3z)} dS \doteq 371.453416333927. \tag{3.3}$$

As before we give results for a fixed value of $q = 2.25$; see Table 3.3. Again the results are consistent with (2.10) and the conjectured convergence result of (2.32). The qualitative results for varying q are the same as earlier in Table 3.2, including the much faster convergence for the cases of $q = 1.5,\ 2.5,\ 3.5$.

4. Treatment of a point singularity. We now consider integrals

$$I(\rho) = \int_S \rho(Q) dS_Q = \int_U \rho\left(\mathcal{M}(\widehat{Q})\right) J_{\mathcal{M}}(\widehat{Q})\, dS_{\widehat{Q}} \tag{4.1}$$

in which ρ is singular at a point $P \in S$; cf. (1.2) and (1.3). As before in (1.7), we transform to an integral over U. Since the subsequent transformation $\mathcal{L}$ of (2.2)-(2.5) is based on smoothing the integrand at the poles of U, we need to have the singularity in ρ correspond to a pole of the sphere U. The original coordinate system of $\mathbb{R}^3$ needs to be rotated to have the north pole (or south pole) of U in the rotated system be the location of the singularity in the integrand.

Let $\mathcal{M}(\widehat{P}) = P$, $\widehat{P} \in U$. We interpose an orthogonal Householder transformation of $\mathbb{R}^3$,

$$\widehat{Q} = \mathcal{H}Q^*, \qquad Q^* \in U \tag{4.2}$$

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TABLE 3.3
Numerical integrals for (3.2) over a peanut with $q = 2.25$

n	$\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$	*Ratio*	*EOC*
4	$5.443E + 2$		
8	$-1.885E + 2$	-2.89	
16	$-8.322E + 0$	22.66	4.50
32	$1.614E - 2$	-515.73	
64	$-4.132E - 4$	-39.05	
128	$-1.842E - 5$	22.44	4.49
256	$-8.143E - 7$	22.62	4.50
512	$-3.599E - 8$	22.62	4.50
1024	$-1.591E - 9$	22.62	4.50

before the final mapping involving $\mathcal{L}$. Choose a Householder matrix $\mathcal{H} = I - 2ww^{\mathrm{T}}$ such that

$$\mathcal{H}\begin{bmatrix} 0 \\ 0 \\ \pm 1 \end{bmatrix} = \widehat{P}, \quad \text{equivalently,} \quad \mathcal{H}\widehat{P} = \begin{bmatrix} 0 \\ 0 \\ \pm 1 \end{bmatrix} \tag{4.3}$$

with the sign chosen later to minimize any loss of significance error. The requirement (4.3) means that $\widehat{P}$ will be mapped to either the North or South Pole of U, or conversely, a pole of U is mapped to $\widehat{P}$.

Finding w is straightforward and inexpensive. In evaluating (4.2), use

$$\begin{aligned} \widehat{Q} &= \mathcal{H}Q^* \\ &= Q^* - w\left(2w^{\mathrm{T}}Q^*\right) \\ &= Q^* - cw, \qquad c = 2w^{\mathrm{T}}Q^*. \end{aligned}$$

Computing $2w^{\mathrm{T}}Q^*$ requires 4 multiplications and 2 additions; and computing $\widehat{Q}$ requires a further 3 multiplications and three subtractions (a total of 12 arithmetic operations for $Q^* \to \widehat{Q}$).

In the integral (4.1), the transformation $\widehat{Q} = \mathcal{H}Q^*$ yields

$$I(\rho) = \int_U \rho\left(\mathcal{M}(\mathcal{H}Q^*)\right) J_{\mathcal{M}}(\mathcal{H}Q^*)\, dS_{Q^*},$$

since the Jacobian of the mapping is 1. Now use the mapping

$$Q^* = \mathcal{L}\left(\widetilde{Q}\right), \qquad \widetilde{Q} \in U$$

as before in (2.2)-(2.5), yielding

$$I(\rho) = \int_U \rho\left(\mathcal{M}(\mathcal{H}\mathcal{L}(\widetilde{Q}))\right) J_{\mathcal{M}}(\mathcal{H}\mathcal{L}(\widetilde{Q}))J_{\mathcal{L}}\left(\widetilde{Q}\right) dS_{\widetilde{Q}}. \tag{4.4}$$

Now apply the scheme of (2.7) as before in (2.7) of §2.

4.1. Error analysis. When considering the earlier convergence results of (2.10)-(2.32), the principal change is that the integrand ρ of the original integral (4.1) is now singular when $Q = P$. To analyze what is happening, we assume that we are dealing with

$$I = \int_U \frac{f\left(\mathcal{M}(\mathcal{HL}(\widetilde{Q}))\right) J_{\mathcal{M}}(\mathcal{HL}(\widetilde{Q})) J_{\mathcal{L}}\left(\widetilde{Q}\right)}{\left|P - \mathcal{M}(\mathcal{HL}(\widetilde{Q}))\right|} \, dS_{\widetilde{Q}}. \tag{4.5}$$

This is an important case of interest when dealing with boundary integral equations. Note that one of the poles of U corresponds to $\widehat{P}$ under the rotation $\mathcal{H}$, say $\mathcal{H} : (0,0,1) \longmapsto \widehat{P}$; and then $\mathcal{M}\left(\widehat{P}\right) = P$, making the denominator of the integrand zero when $\widetilde{Q} = (0,0,1)$.

As assumed earlier, the original smooth mapping $\mathcal{M} : U \xrightarrow[onto]{1-1} S$ can be considered as the restriction of a one-to-one mapping of an open neighborhood of U, call it U_ε, onto an open neighborhood of S:

$$\mathcal{M} : U_\varepsilon \xrightarrow[onto]{1-1} S_\varepsilon \equiv \mathcal{M}\left(U_\varepsilon\right).$$

In addition, this can be done in such a way that the Jacobian of the mapping is nonzero on U_ε when $\mathcal{M}$ is considered as a three-dimensional mapping. We also assume that $f(Q)$ is a smooth differentiable function of Q on S_ε.

We write

$$\mathcal{M}(\mathcal{H}\widehat{Q}) = (x, y, z), \tag{4.6}$$

with x, y, and z functions of (ξ, η, ζ) over U_ε. The functions x, y, and z depend on both $\mathcal{M}$ and $\mathcal{H}$, and thus x, y, and z will vary with P. Nonetheless, the functions x, y, and z will remain differentiable with respect to ξ, η, and ζ, as the differentiability depends on only that of $\mathcal{M}$. In addition,

$$\begin{aligned} x\,(0,0,1) &= P_1, \\ y\,(0,0,1) &= P_2, \\ z\,(0,0,1) &= P_3. \end{aligned}$$

LEMMA 4.1. *Let $F : \mathbb{R}^3 \to \mathbb{R}$ be a continuously differentiable function on a connected convex set $C \subseteq \mathbb{R}^3$. Let $\mathbf{v}, \mathbf{v}_0 \in C$. Then*

$$F(\mathbf{v}) - F(\mathbf{v}_0) = \left(\int_0^1 \nabla F\left(\mathbf{v}_0 + t\left(\mathbf{v} - \mathbf{v}_0\right)\right) dt\right)\left(\mathbf{v} - \mathbf{v}_0\right).$$

For notation, ∇F is a row vector and $\mathbf{v} - \mathbf{v}_0$ is a column vector.

The proof is a straightforward use of the fundamental theorem of the calculus. Apply it to $F\left(\mathbf{v}_0 + t\left(\mathbf{v} - \mathbf{v}_0\right)\right)$ for $0 \le t \le 1$.

With this lemma, we can write

$$(x, y, z) - P = \left(\int_0^1 \begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{bmatrix} dt\right) \begin{bmatrix} \xi \\ \eta \\ \zeta - 1 \end{bmatrix}. \tag{4.7}$$

We are interested in only the case that the point (x, y, z) is being evaluated at points $(\xi, \eta, \zeta) \in U$. In the matrix, $x_1 = \partial x / \partial \xi$, $x_2 = \partial x / \partial \eta$, $x_3 = \partial x / \partial \zeta$, and similarly for the functions y

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and z. The argument of each of these partial derivatives in the matrix is $(t\xi, t\eta, 1 + t(\zeta - 1))$. This formula requires that the line joining (x, y, z) and P be inside the open neighborhood S_ε referenced above, or equivalently, the line joining (ξ, η, ζ) and $(0, 0, 1)$ is inside of U_ε. This will be true if (x, y, z) and P are sufficiently close together, or equivalently, $(\xi, \eta, \zeta) \approx (0, 0, 1)$. Thus we want to deal only with points of U that are sufficiently close to $(0, 0, 1)$. This is sufficient since the integrand in (4.5) is easily nonsingular and differentiable away from $\widetilde{Q} = (0, 0, 1)$.

We apply (4.7) with

$$(\xi, \eta, \zeta) = \frac{(\cos\phi \sin^q\theta, \sin\phi \sin^q\theta, \cos\theta)}{\sqrt{\cos^2\theta + \sin^{2q}\theta}}.$$

Having (ξ, η, ζ) approach $(0, 0, 1)$ is equivalent to letting θ tend to 0. For $(\xi, \eta, \zeta) \approx (0, 0, 1)$, the integral term in (4.7) is approximately

$$J \equiv \left.\begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{bmatrix}\right|_{((\xi,\eta,\zeta)=(0,0,1))}, \tag{4.8}$$

the Jacobian matrix of the three-dimensional mapping $\mathcal{M}$ defined on U_ε and evaluated at $(0, 0, 1)$. The matrix J is nonsingular by our earlier assumption that the Jacobian of $\mathcal{M}$ is nonzero over U_ε. Thus the matrix obtained from the integration in (4.7) is also nonsingular with a determinant bounded away from zero, by continuity.

To introduce some intuition into the present discussion, we give concrete results for the ellipsoidal surface of (1.5) with $P = (0, 0, c)$. Recall that $(x, y, z) = \mathcal{M}(\xi, \eta, \zeta) = (a\xi, b\eta, c\zeta)$. Then

$$\begin{aligned} &|(x, y, z) - (0, 0, c)| = \sqrt{x^2 + y^2 + (z - c)^2} \\ &= \sqrt{\left(\frac{a\cos\phi\sin^q\theta}{\sqrt{\cos^2\theta + \sin^{2q}\theta}}\right)^2 + \left(\frac{b\sin\phi\sin^q\theta}{\sqrt{\cos^2\theta + \sin^{2q}\theta}}\right)^2 + c^2\left(1 - \frac{\cos\theta}{\sqrt{\cos^2\theta + \sin^{2q}\theta}}\right)^2} \\ &\equiv \Omega. \end{aligned}$$

Following some algebraic manipulation, we obtain

$$\Omega = \frac{\sin^q\theta}{\sqrt{\cos^2\theta + \sin^{2q}\theta}} \sqrt{a^2\cos^2\phi + b^2\sin^2\phi + \frac{c^2\sin^{2q}\theta}{\left[\cos\theta + \sqrt{\cos^2\theta + \sin^{2q}\theta}\right]^2}}.$$

Thus the denominator in (4.5) acts like

$$\Omega = O(\sin^q\theta) \tag{4.9}$$

around $\theta = 0$, with the function of proportionality nonzero and differentiable in (θ, ϕ).

For the general case, we write (4.7) in the form

$$(x, y, z) - P = \widehat{\Omega}\left(\int_0^1 \begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{bmatrix} dt\right) \begin{bmatrix} \xi/\widehat{\Omega} \\ \eta/\widehat{\Omega} \\ (\zeta - 1)/\widehat{\Omega} \end{bmatrix}, \tag{4.10}$$

$$\widehat{\Omega} = \frac{\sin^q\theta}{\sqrt{\cos^2\theta + \sin^{2q}\theta}} \sqrt{1 + \frac{\sin^{2q}\theta}{\left[\cos\theta + \sqrt{\cos^2\theta + \sin^{2q}\theta}\right]^2}}. \tag{4.11}$$

The vector that is the last term on the right side of (4.10) is of unit length. The right side of (4.10) is the product of $\widehat{\Omega}$ and a term closely approximated by

$$J\mathbf{v},$$

with $\mathbf{v}$ a unit vector dependent on (θ,ϕ). As $\mathbf{v}$ varies in all possible ways, $J\mathbf{v}$ will be bounded away from zero because J is nonsingular; and $J\mathbf{v}$ will be a smooth differentiable function of (θ,ϕ). We can use this and a continuity argument to show that the term

$$\left(\int_0^1 \begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{bmatrix} dt\right)\begin{bmatrix} \xi/\widehat{\Omega} \\ \eta/\widehat{\Omega} \\ (\zeta-1)/\widehat{\Omega} \end{bmatrix} \tag{4.12}$$

is a continuous and differentiable function of $(\xi,\eta,\zeta)\in U$ in a neigborhood of $(0,0,1)$; and the same is true for (ξ,η,ζ) away from $(0,0,1)$, since the denominator of (4.5) is then nonzero and well-behaved. The main behaviour of interest for $(x,y,z)-P$ is bound up in $\widehat{\Omega}$, and it acts like the product of a smooth function and $\sin^q\theta$. The denominator in (4.5) again behaves as in (4.9).

Summarizing,

$$\left|P-\mathcal{M}(\mathcal{HL}(\widetilde{Q}))\right| = \Psi\left(\theta,\phi\right)\sin^q\theta, \tag{4.13}$$

for some continuously differentiable function $\Psi\left(\theta,\phi\right)$ that is bounded away from zero for $0\le\phi\le 2\pi$ and $0\le\theta\le\pi$.

Return to the discussion of the numerical scheme (2.7) applied to (4.5). The error analysis of (2.7) mimics that given earlier in §2. The principal difference results from combining (4.13) with the Jacobian $J_{\mathcal{L}}\left(\widetilde{Q}\right)$. We now have an integrand of the general form

$$\int_0^\pi [\sin\theta]^{q-1}\int_0^{2\pi}\Psi\left(\sin\theta,\cos\theta,\sin\phi,\cos\phi\right)\,d\phi\,d\theta, \tag{4.14}$$

in which Ψ is a smooth function. Proceeding as in §2, we have the following. The proof is essentially the same as in Theorem 2.1.

THEOREM 4.2. *Let $q\ge 1$ be an integer, and introduce*

$$p=\begin{cases} q, & q \text{ even},\\ q+1, & q \text{ odd}.\end{cases}$$

In the integral (4.5), assume that $f\in L^p(S)$. Assume that the surface S is similarly differentiable, which is equivalent to assuming that the mapping $\mathcal{M}$ is suitably differentiable. Let $\mathcal{T}_n$ be the approximation of (4.5) based on the schema of (2.7). Then

$$I-\mathcal{T}_n = O\left(h^p\right). \tag{4.15}$$

The rates of (4.15), and even better, are observed in practice. This is illustrated with the numerical examples of the following section. Based on those examples and on other partial theoretical results, we state the following conjecture that extends the above theorem.

CONJECTURE 4.3. *Assume $q\ge 1$. Under suitable assumptions on the function f, the error in approximating (4.5) by (2.7) satisfies*

$$I-\mathcal{T}_n = O\left(h^q\right). \tag{4.16}$$

The methods of this section can also be applied to the analysis of the double layer integral of (1.3), but we omit this analysis.

TABLE 4.1
Numerical integrals for (5.1) with $q = 2.5$

	Surface S_1			Surface S_2		
n	$\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$	*Ratio*	*EOC*	$\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$	*Ratio*	*EOC*
4	$1.99E+1$			$1.38E+2$		
8	$-5.93E-1$	-33.65		$-1.53E+1$	-9.01	
16	$1.58E-1$	-3.76		$-1.01E+0$	15.10	
32	$2.56E-2$	6.16	2.62	$6.92E-2$	-14.63	
64	$4.53E-3$	5.64	2.50	$1.83E-2$	3.79	1.92
128	$8.01E-4$	5.66	2.50	$3.24E-3$	5.65	2.50
256	$1.42E-4$	5.66	2.50	$5.72E-4$	5.66	2.50
512	$2.50E-5$	5.66	2.50	$1.01E-4$	5.66	2.50
1024	$4.43E-6$	5.66	2.50	$1.79E-5$	5.66	2.50

TABLE 5.1
Numerical integrals for (5.1) with $q = 3$

	Surface S_1		Surface S_2	
n	$\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$	*Ratio*	$\mathcal{T}_n - \mathcal{T}_{\frac{1}{2}n}$	*Ratio*
4	$2.21E+1$		$1.48E+2$	
8	$-2.46E+0$	-8.96	$-2.42E+1$	-6.12
16	$-7.66E-2$	32.2	$-2.33E+0$	10.4
32	$-1.00E-3$	76.5	$2.45E-2$	-95.12
64	$7.07E-8$	-14168	$-1.76E-5$	-1387
128	$3.22E-10$	219	$5.98E-9$	-2948
256	$5.04E-12$	63.9	$7.53E-12$	794
512	$5.68E-14$	88.8	$1.14E-13$	66.2
1024	0		0	

5. Numerical examples: singular integrand. We begin with numerical results for

$$I = \int_S \frac{e^{0.1(x+2y+3z)}}{|P-Q|} dS_Q, \tag{5.1}$$

with $Q = (x, y, z)$. For the ellipsoidal surface S_1, we use the surface parameters $(a, b, c) = (1, 2, 3)$; and for the peanut surface S_2, we use the surface parameters

$$(a, b, c, d, e, f, g) = (1, 1.5, 2, 1, 0.7, 3, 0.3).$$

Letting I_k denote the integral over S_k, we have

$$I_1 = 38.254918969803924,$$
$$I_2 = 143.25583436283551.$$

The point P was chosen to correspond to the spherical coordinates $(\theta, \phi) = (\pi/4, \pi/4)$ for both surfaces.

In Tables 4.1 and 5.1, we give results for $q = 2.5$ and $q = 3$. In Table 5.2 we give results for varying q. Note that the results agree with (4.15) and the conjectured convergence order of (4.16) except for the case of $q = 3$. For this latter case, the theoretical result of (4.16) predicts

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TABLE 5.2
Estimated order of convergence for the numerical integration (5.1) with varying q

q	1.5	2.0	2.5	3.0	3.5	4.0
Surface S_1	1.5	2.0	2.5	$large$	3.5	4.0
Surface S_2	1.5	2.0	2.5	$large$	3.5	4.0

$I - \mathcal{T}_n = O\left(h^4\right)$. Empirically for $q = 3$, based on both Table 5.1 and other examples, we estimate that $I - \mathcal{T}_n = O\left(h^6\right)$.

CONCLUDING DISCUSSION. The proofs of the conjectures in (2.32) and (4.16) will probably depend on some extension of the asymptotic results of Lyness and Ninham [8]. Also see the recent work of Sidi [10].

As noted in the numerical examples of earlier sections, there are values of q for which the convergence of $\mathcal{T}_n$ to I is extremely rapid, much more so than is predicted by the theoretical convergence results for general q. Consider the special case of

$$I(f) = \int_U f(Q)dS_Q, \tag{5.2}$$

with f nonsingular and $2q = 3$. Using the constructions of the derivatives of $F(\theta)$ and $G(\theta)$ in the proof of Theorem 2.1, it can be shown that

$$\frac{d^k}{d\theta^k}\left[F(\theta)G(\theta)\right] = 0, \qquad k = 1, 3, \qquad \theta = 0, \pi.$$

Thus, we would like to apply the Euler-MacLaurin expansion of (2.9) to conclude that $I - \mathcal{T}_n = O\left(h^6\right)$, which would agree for this case with the observed rate in the examples of §3. Unfortunately, we need to also show that

$$\frac{d^6}{d\theta^6}\left[F(\theta)G(\theta)\right] \in L\left(0, \pi\right),$$

something we have not been able to accomplish to date. Thus, we leave it as a conjecture that superconvergence takes place for (5.2) with f a sufficiently smooth function and $2q$ an odd integer.

Recall the assumptions on the mapping $\mathcal{M}$ given in §1 following (1.6). Smooth mappings $\mathcal{M} : U \xrightarrow[onto]{1-1} S$ defined on surfaces can be extended to meet the earlier assumptions; for example, see Gunter [7, Chap. 1, §3].

There are probably other transformations that can be used to replace (2.2), although ours seems both intuitive and simple to implement. We have implemented our scheme using *Matlab* and will gladly share the codes with others.

APPENDIX. *Defining surface normals and Jacobian for a general surface*. The mapping $\mathcal{M} : U \xrightarrow[onto]{1-1} S$ is given by $(\xi, \eta, \zeta) \mapsto (x, y, z)$. Using spherical coordinates,

$$\begin{aligned} x &= x(\xi, \eta, \zeta), \\ y &= y(\xi, \eta, \zeta), \\ z &= z(\xi, \eta, \zeta). \end{aligned}$$

For derivatives, we use the shorthand notation

$$x_1 = \frac{\partial x(\xi, \eta, \zeta)}{\partial \xi}, \quad x_2 = \frac{\partial x(\xi, \eta, \zeta)}{\partial \eta}, \quad x_3 = \frac{\partial x(\xi, \eta, \zeta)}{\partial \zeta},$$

with similar notation for y and z.

For the surface Jacobian used in the change of variables expression in (1.7),

$$\left[J_{\mathcal{M}}(\widehat{Q})\right]^2 = \begin{vmatrix} \xi & \eta & \zeta \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{vmatrix}^2 + \begin{vmatrix} x_1 & x_2 & x_3 \\ \xi & \eta & \zeta \\ z_1 & z_2 & z_3 \end{vmatrix}^2 + \begin{vmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ \xi & \eta & \zeta \end{vmatrix}^2,$$

with $\widehat{Q} = (\xi, \eta, \zeta)$. For the normal at $(x, y, z) = \mathcal{M}(\xi, \eta, \zeta)$,

$$\mathbf{G} = \begin{bmatrix} (y_1 z_2 - y_2 z_1)\,\zeta + (y_3 z_1 - y_1 z_3)\,\eta + (y_2 z_3 - y_3 z_2)\,\xi \\ (z_1 x_2 - z_2 x_1)\,\zeta + (z_3 x_1 - z_1 x_3)\,\eta + (z_2 x_3 - z_3 x_2)\,\xi \\ (x_1 y_2 - x_2 y_1)\,\zeta + (x_3 y_1 - x_1 y_3)\,\eta + (x_2 y_3 - x_3 y_2)\,\xi \end{bmatrix},$$

$$\mathbf{N} = \frac{\mathbf{G}}{\|\mathbf{G}\|}.$$

REFERENCES

[1] K. ATKINSON, *The numerical solution of Laplace's equation in three dimensions*, SIAM J. Numer. Anal., 19 (1982), pp. 263-274.
[2] K. ATKINSON, *Numerical integration on the sphere*, J. Austral. Math. Soc. Ser. B, 23 (1982), pp. 332-347.
[3] K. ATKINSON, *Algorithm 629: An integral equation program for Laplace's equation in three dimensions*, ACM Trans. Math. Software, 11 (1985), pp. 85-96.
[4] K. ATKINSON, *An Introduction to Numerical Analysis*, 2nd edition, John Wiley, New York, 1989.
[5] D. ELLIOTT, *Sigmoidal transformations and the trapezoidal rule*, J. Austral. Math. Soc. Ser. B (Electronic), 40 (1998), pp. E77–E137.
[6] M. GANESH, I. GRAHAM, AND J. SIVALOGANATHAN, *A pseudospectral 3D boundary integral method applied to a nonlinear model problem from finite elasticity*, SIAM J. Numer. Anal., 31 (1993), pp. 1378-1414.
[7] N. GÜNTER, *Potential Theory*, Ungar Pub., New York, 1967.
[8] J. LYNESS AND B. NINHAM, *Numerical quadrature and asymptotic expansions*, Math. Comp., 21 (1967), pp. 162-178.
[9] A. SIDI, *A new variable transformation for numerical integration*, Numerical Integration IV, H. Brass and G. Hämmerlin, eds., Birkhäuser Verlag, Basel, 1993, pp. 359-373.
[10] A. SIDI, *Class $\mathcal{S}_m$ variable transformations and applications to numerical integration over smooth surfaces in $\mathbb{R}^3$*, preprint, Computer Science Dept., Technion, Haifa, November 2003.
[11] A. SIDI, *Euler-Maclaurin expansions for integrals with endpoint singularities: A new perspective*, *Numer. Math.*, to appear.
[12] A. STROUD, *Approximate Calculation of Multiple Integrals*, Prentice-Hall, New Jersey, 1971.