SOME ERROR ESTIMATES FOR THE NUMERICAL APPROXIMATION OF SURFACE INTEGRALS

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ABSTRACT. Recently, the first author introduced a new approach to the numerical quadrature of surface integrals in the context of boundary element methods. It is assumed that a global parametrization m of the surface is only indirectly given (e.g., via an iterative method) and that m is not accessible analytically. Of particular interest are parametrizations which are based on automatic triangulations of surfaces. In order to avoid an explicit reference to the partial derivatives of m, modified trapezoidal and midpoint rules were introduced. The present paper discusses some error estimates for these methods. The estimates are surprisingly difficult since $\mathcal{O}(h^3)$-terms have to be shown to cancel; this does not occur in the expansion of the standard rules.

1. INTRODUCTION

Efficient numerical approximations of surface integrals are important in boundary element methods; see, e.g., Atkinson [1, 2], Georg and Widmann [4], Hackbusch [5].

Recently, Georg [3] introduced a new approach to the numerical quadrature of surface integrals. It was assumed that the surface $\mathcal{B} \subset \mathbb{R}^3$ was modeled via a piecewise linear approximation (triangulation). Such approximations are typically used in panel methods. Hence, a parametrization m of the surface $\mathcal{B}$ is only indirectly given, e.g., via an iterative method. The main purpose of the new method is to avoid the handling of the partial derivatives of m via finite differences or interpolation.

Throughout this paper, let $\mathcal{S}$ denote a smooth piece of the surface $\mathcal{B}$ and $m : \sigma \to \mathcal{S}$ a smooth (parameter) map. For the purposes of our discussion it is enough to consider the case that $\sigma = \{(s, t) \colon 0 \le s, t, s + t \le 1\}$ is a standard triangle which is isomorphically mapped onto $\mathcal{S}$. We consider the task of numerically approximating

$$(1) \qquad \int_{\mathcal{S}} f \, dS.$$

Here, dS indicates the usual measure on $\mathscr{S}$ (surface element).

The standard approach to this task is to consider the equivalent integral in planar coordinates

$$(2) \qquad \int_{\mathscr{S}} f \, dS = \int_{\sigma} f(m(s,t)) \, \|m_s \times m_t\| \, ds \, dt.$$

Here, m_s denotes the partial derivative of m with respect to the parameter s. In order to numerically approximate (2), a standard approach is to subdivide σ into small triangles σ_i; this corresponds to a subdivision of the surface $\mathscr{S}$ into the pieces $\mathscr{S}_i := m(\sigma_i)$. Then an approximation of the integral can be obtained via one of the composite rules

$$(3) \qquad \begin{aligned} \int_{\mathscr{S}} f \, dS &= \sum_i \int_{\sigma_i} (f \circ m) \, \gamma \, ds \, dt \\ &\approx \sum_i \frac{1}{3} \sum_{j=0}^{2} f(m(x_{i,j})) \, \gamma(x_{i,j}) \, \text{area}(\sigma_i), \end{aligned}$$

$$(4) \qquad \begin{aligned} \int_{\mathscr{S}} f \, dS &= \sum_i \int_{\sigma_i} (f \circ m) \, \gamma \, ds \, dt \\ &\approx \sum_i f(m(x_{i,b})) \, \gamma(x_{i,b}) \, \text{area}(\sigma_i). \end{aligned}$$

Here, the vertices and the barycenter of σ_i are denoted by $x_{i,j}$, $j = 0, 1, 2$, and $x_{i,b}$, respectively, and $\gamma := \|m_s \times m_t\|$.

Methods (3) and (4) are the respective extensions of the trapezoidal and the midpoint rule for a triangle.

The local error, i.e., the error of each summand, is $\mathscr{O}(h^4)$, where $h = \max_i \text{diam}(\sigma_i)$. Under the summation of the composite rule, these local errors lead to a global error $\mathscr{O}(h^2)$. It is also known (in the case of an equidistant subdivision) that the global error can be expanded in terms of h^2, see Lyness [6].

If the partial derivatives of m are not available analytically, a numerical approximation (e.g., via finite differences or interpolation) may be considered; see, e.g., Atkinson [2]. An alternative approach to approximate (1) that does not use the partial derivatives of m was proposed by Georg [3]:

$$(5) \qquad \int_{\mathscr{S}} f \, dS \approx \sum_i \frac{1}{3} \sum_{j=0}^{2} f(v_{i,j}) \, \text{area}[v_{i,0}, v_{i,1}, v_{i,2}],$$

$$(6) \qquad \int_{\mathscr{S}} f \, dS \approx \sum_i f(v_{i,b}) \, \text{area}[v_{i,0}, v_{i,1}, v_{i,2}].$$

Here, $v_{i,j}$ are the images of the vertices $x_{i,j}$ of σ_i under m and $[v_{i,0}, v_{i,1}, v_{i,2}]$ denotes the triangle spanned by $v_{i,0}, v_{i,1}, v_{i,2}$. The point $v_{i,b}$ denotes the barycenter of $[v_{i,0}, v_{i,1}, v_{i,2}]$. Therefore, we need to assume that the integrand f is extended to a smooth function defined on some open neighborhood of $\mathscr{S}$ so that for sufficiently small h the value $f(v_{i,b})$ is defined.

The main result of the present paper is contained in the following

Theorem 1. *The global discretization error of both composite rules* (5) *and* (6) *is* $\mathcal{O}(h^2)$.

Hence, our modified rules have the same global order as the corresponding standard composite rules (3) and (4). In contrast to standard rules, however, it is impossible to prove that the local error is of order four in our modified rules. This is the main difficulty we encounter in our analysis. We will show that the $\mathcal{O}(h^3)$-terms cancel under the summation of the composite rule.

In fact, numerical experiments also suggest that the error of the modified methods (5) and (6) have an h^2-expansion; an analytical demonstration of this observation seems to be difficult, since Lyness's [6] proof for the standard case, which is based on the Euler–Maclaurin sum formula, does not easily carry over to our case.

2. PROOF OF THE ESTIMATE

In this section we will sketch a proof of the above theorem. The argument is somewhat technical, and therefore we will leave some of the more obvious details to the reader.

The subdivision $\{\sigma_i\}$ of σ induces a subdivision $\{\mathscr{S}_i\}$ of $\mathscr{S}$ into curved triangular pieces. The pieces $\mathscr{S}_i$ are approximated by the triangles $T_i :=$ $[v_{0,i}, v_{1,i}, v_{2,i}]$ and the surface area of $\mathscr{S}$ is approximated by the area of the triangulation $\mathscr{T} = \{T_i\}$ of $\mathscr{S}$. We assume that the subdivision $\{\sigma_i\}$ of σ does not produce arbitrarily small angles. More precisely, there are constants α_0 and α_1 independent of h such that

$$(7) \qquad\qquad 0 < \alpha_0 \le \alpha \le \alpha_1 < \pi$$

holds for any interior angle α of each T_i. Thus, the sum in the composite rules (5), (6) is taken over $\mathcal{O}(h^{-2})$ terms. Let P_i denote the plane in which T_i is embedded and n_i its normal vector. We project $\mathscr{S}_i$ in the direction of n_i onto a set $N_i \subset P_i$ and assume that h is chosen to be sufficiently small such that this projection is one to one. It is convenient to introduce a new parametrization of $\mathscr{S}_i$:

Let $g_i(x)$ denote the distance of a point $x \in R^3$ from $\mathscr{S}_i$ in direction of the normal n_i of P_i, and let $m^L \colon R^2 \to P_i$ denote the parametrization of the plane P_i defined by

$$m^L(s, t) = (1 - s - t)v_{0,i} + sv_{1,i} + tv_{2,i}, \qquad (s, t) \in \mathbb{R}^2.$$

Furthermore, we parametrize $\mathscr{S}_i$ via $m^i \colon N_i \to \mathscr{S}_i$ by

$$(8) \qquad\qquad m^i(v) = v + g_i(v)n_i.$$

We will need both parametrizations to prove the first result:

$$(9) \qquad\qquad \int_{\mathscr{S}_i} f\, dS = \int_{N_i} f \circ m^i (1 + \mathcal{O}(h^2))\, dP_i.$$

Here, dP_i denotes the standard measure in the plane P_i.

Proof. For an infinitesimal surface element, we have

(10)
$$
\begin{aligned}
dS &= \|(m^i \circ m^L)_s \times (m^i \circ m^L)_t\| \, ds \, dt \\
&= \|(m^L + g_i(m^L) \, n_i)_s \times (m^L + g_i(m^L) \, n_i)_t\| \, ds \, dt \\
&= \|m_s^L \times m_t^L + (\nabla g_i \cdot m_t^L)(m_s^L \times n_i) - (\nabla g_i \cdot m_s^L)(m_t^L \times n_i)\| \, ds \, dt \\
&= (\|m_s^L \times m_t^L\|^2 + \|(\nabla g_i \cdot m_t^L)(m_s^L \times n_i) - (\nabla g_i \cdot m_s^L)(m_t^L \times n_i)\|^2)^{\frac{1}{2}} \, ds \, dt.
\end{aligned}
$$

Here, the derivative ∇g_i is taken at m^L. The last equality holds since $m_s^L \times n_i$ and $m_t^L \times n_i$ are perpendicular to $m_s^L \times m_t^L$. Furthermore,

(11)
$$
\begin{aligned}
\frac{\|(\nabla g_i \cdot m_t^L)(m_s^L \times n_i) - (\nabla g_i \cdot m_s^L)(m_t^L \times n_i)\|}{\|\nabla g_i\| \, \|m_s^L \times m_t^L\|} &\leq \frac{2\|\nabla g_i\|\|m_s^L\|\|m_t^L\|}{\|\nabla g_i\| \, \|m_s^L \times m_t^L\|} \\
&\leq \frac{2\|m_s^L\|\|m_t^L\|}{\|m_s^L \times m_t^L\|} = \mathscr{O}(1)
\end{aligned}
$$

because the angle α is bounded by (7). We now estimate (10) by making use of (11), and obtain

$$
dS = \|m_s^L \times m_t^L\| \, (1 + \mathscr{O}(1)\|\nabla g_i\|^2)^{\frac{1}{2}} \, ds \, dt.
$$

It is well known that $g_i = \mathscr{O}(h^2)$, and hence $\nabla g_i = \mathscr{O}(h)$, since the triangle T_i is a linear approximation of the surface element $\mathscr{S}_i$. This implies

$$
dS = \|m_s^L \times m_t^L\| \, (1 + \mathscr{O}(h^2))^{\frac{1}{2}} \, ds \, dt = \|m_s^L \times m_t^L\| \, (1 + \mathscr{O}(h^2)) \, ds \, dt.
$$

Since m^L is a linear parametrization of P_i, it follows that

$$
dS = (1 + \mathscr{O}(h^2)) \, dP_i.
$$

From the above equations it is clear that $dS \geq dP_i$, and hence (9) follows. $\square$

The obvious way to proceed from here is to replace the in general irregularly shaped projection N_i by T_i in integral (9). Let us first note that we have only the estimate $|\operatorname{area}(N_i) - \operatorname{area}(T_i)| = \mathscr{O}(h^3)$, and this estimate cannot be improved to order four. Hence, a straightforward replacement of N_i by T_i would yield a local error $\mathscr{O}(h^3)$ and a global error $\mathscr{O}(h)$ which would be insufficient to prove our theorem. We will show, however, that most of the $\mathscr{O}(h^3)$ error terms in the approximation

$$
\int_{N_i} f \circ m^i \, dP_i \approx \int_{T_i} f \circ m^i \, dP_i
$$

cancel under the summation over i.

Recall that N_i and $T_i = [v_{i,0}, v_{i,1}, v_{i,2}]$ lie in the same plane P_i. We consider the boundary of N_i near the edge $[v_{i,j-1}, v_{i,j+1}]$ of T_i which is opposite to the vertex $v_{i,j}$. Note that the index j is taken modulo 2. It is not difficult to see that for sufficiently small h this boundary can be described as a

curve of the form

$$(12) \qquad tv_{i,j-1} + (1-t)v_{i,j+1} + \delta_{i,j}(t)n_{i,j}, \qquad 0 \le t \le 1.$$

Here, $n_{i,j}$ denotes the vector in the plane P_i with unit length which is orthogonal to the edge $[v_{i,j-1}, v_{i,j+1}]$ and points out of T_i, and $\delta_{i,j}$ denotes the distance of the curve from this edge in the direction of $n_{i,j}$. Furthermore, we introduce the orthogonal coordinate system of P_i corresponding to (12):

$$(13) \qquad m_{i,j}(t,s) = tv_{i,j-1} + (1-t)v_{i,j+1} + sn_{i,j}.$$

This is used to introduce a parametrization of $\mathscr{S}_i$:

$$(14) \qquad \tilde{m}_{i,j}(t,s) = m_{i,j}(t,s) + g(m_{i,j}(t,s))n_i.$$

The difference between the integrals over N_i and T_i can now be expressed in the following formula

$$(15) \qquad \int_{N_i} f \circ m^i \, dP_i = \int_{T_i} f \circ m^i \, dP_i + \sum_j I_{i,j},$$

where

$$(16) \qquad I_{i,j} := \int_0^1 \int_0^{\delta_{i,j}(t)} f(\tilde{m}_{i,j}(t,s)) \|v_{i,j-1} - v_{i,j+1}\| \, ds \, dt.$$

Note that

$$(17)$$
$$\delta_{i,j}(t) = \sin\alpha_{i,j}(t) \underbrace{\| m(tx_{i,j-1} + (1-t)x_{i,j+1}) - (tv_{i,j-1} + (1-t)v_{i,j+1}) \|}_{=: \, d_{i,j}(t)},$$

where $\alpha_{i,j}(t)$ describes the angle between $d_{i,j}(t)$ and the normal n_i of T_i. The sign of $\alpha_{i,j}(t)$ is chosen so that $d_{i,j}(t)$ points out of the prism $\{v + \tau n_i : v \in T_i, \tau \in \mathbb{R}\}$ over T_i for positive $\alpha_{i,j}(t)$.

The vector $d_{i,j}(t)$ is the error term of a linear interpolation, and hence $\|d_{i,j}(t)\| = \mathscr{O}(h^2)$. It is not possible to give an $\mathscr{O}(h)$-estimate for the angle $\alpha_{i,j}(t)$; thus a straightforward estimate of (17) only leads to $I_{i,j} = \mathscr{O}(h^3)$. When summing in (15) over i, these terms add up to $\mathscr{O}(h)$ instead of $\mathscr{O}(h^2)$.

To overcome this difficulty, we consider an edge $[v_{i,j-1}, v_{i,j+1}] = [v_{i',j'-1}, v_{i',j'+1}]$ of two adjacent triangles T_i and $T_{i'}$. Since $\alpha_{i,j}(t)$ represents the angle between n_i and $d_{i,j}(t)$, and $\alpha_{i',j'}(t)$ represents the angle between $n_{i'}$ and $d_{i,j}(t) = d_{i',j'}(t)$, it is not too difficult to see that

$$(18) \qquad \alpha_{i,j}(t) + \alpha_{i',j'}(t) = \beta_{i,i'},$$

where $\beta_{i,i'}$ is the angle between the normals of n_i and $n_{i'}$. Since the edges of the triangles have length $\mathscr{O}(h)$, it is well known that $\beta_{i,i'} = \mathscr{O}(h)$. Therefore, (18) and (17) immediately imply that

$$(19) \qquad \delta_{i,j}(t) + \delta_{i',j'}(t) = \mathscr{O}(h^3).$$

Furthermore, the following estimate can be obtained:

$$(20) \qquad \|\tilde{m}_{i,j}(t, s) - \tilde{m}_{i',j'}(t, -s)\| = |s| \mathcal{O}(h).$$

The estimates (19) and (20) imply the following estimates for neighboring edges:

$$(21) \qquad I_{i,j} + I_{i',j'} = \mathcal{O}(h^4).$$

We are now in a position to show the central estimate of this section:

$$(22) \qquad \int_{\mathscr{S}} f \, dS = \left(\sum_i \int_{T_i} f \circ m^i \, dP_i \right) + \mathcal{O}(h^2).$$

Proof. Given formula (9) and the notation, we have

$$\int_{\mathscr{S}} f \, dS = \sum_i \int_{N_i} f \circ m^i (1 + \mathcal{O}(h^2)) \, dP_i$$

$$= \left(\sum_i \int_{T_i} f \circ m^i \, dP_i \right) + \mathcal{O}(h^2) + \sum_{i,j} I_{i,j}.$$

It remains to estimate the last sum $\sum_{i,j} I_{i,j}$ in which the number of terms is $\mathcal{O}(h^{-2})$. Most edges $[v_{i,j-1}, v_{i,j+1}]$ occur in pairs and because of (21) only contribute an error $\mathcal{O}(h^4)$ per pair. The number of edges which are not common to two triangles and which hence belong to the boundary of the triangulation, is only $\mathcal{O}(h^{-1})$. These edges contribute an error $\mathcal{O}(h^3)$ per term. Taking the sum now yields $\sum_{i,j} I_{i,j} = \mathcal{O}(h^2)$, and the proof is complete. □

The conclusion of the proof of Theorem 1 now follows from standard arguments. Note that the integral

$$\int_{T_i} f \circ m^i \, dP_i$$

is taken over a triangle, using planar coordinates. We can hence apply the well-known error estimates for the standard trapezoidal and midpoint rules, see, e.g., Lyness [6]:

$$\int_{T_i} f \circ m^i \, dP_i = \frac{1}{3} \sum_{j=0}^{2} (f \circ m^i)(v_{i,j}) \, \mathrm{area}[v_{i,0}, v_{i,1}, v_{i,2}] + \mathcal{O}(h^4)$$

$$(23)$$

$$= \frac{1}{3} \sum_{j=0}^{2} f(v_{i,j}) \, \mathrm{area}[v_{i,0}, v_{i,1}, v_{i,2}] + \mathcal{O}(h^4)$$

for the trapezoidal rule, and

$$(24) \qquad \int_{T_i} f \circ m^i \, dP_i = (f \circ m^i)(v_{i,b}) \, \mathrm{area}[v_{i,0}, v_{i,1}, v_{i,2}] + \mathcal{O}(h^4)$$

$$= f(v_{i,b}) \, \mathrm{area}[v_{i,0}, v_{i,1}, v_{i,2}] + \mathcal{O}(h^4)$$

for the midpoint rule. In these estimates we made use of the fact that

$$v_{i,j} = m^i(v_{i,j}), \qquad v_{i,b} = m^i(v_{i,b}) + \mathscr{O}(h^2)$$

for the midpoint rule. Incorporating the estimates (23) and (24) into the central estimate (22) finishes the proof of Theorem 1.

3. Numerical experiments

In this section we illustrate the behavior of the composite trapezoidal (3) and midpoint (4) rules and give numerical evidence for the following conjecture (see [3, Conjecture 5.1]):

Conjecture 1. *If $\mathscr{I}(h)$ denotes the approximation (3) or (4) of the integral (1) when σ is uniformly subdivided, then $\mathscr{I}(h)$ can be expanded in terms of h^2, i.e.,*

$$\mathscr{I}(h) = \mathscr{I}_0 + h^2\mathscr{I}_1 + \cdots + h^{2k}\mathscr{I}_k + \mathscr{O}(h^{2k+1}).$$

Note, that the first term in the expansion is the true value of integral (1).

In our example we integrate the function $f(x, y, z) = x^2 + y^2 + z^2$ on the surface

$$\mathscr{S} = \{(x, y, z) : x^2 + y^2 + z^2 = 1, \ x, y, z \geq 0\}.$$

Then we have $\mathscr{I}_0 = \frac{\pi}{2}$ for the integral. The surface $\mathscr{S}$ is parametrized in the following way: First, the standard triangle σ is mapped affinely on the triangle $[a\mathbf{e}_1, b\mathbf{e}_2, c\mathbf{e}_3]$ in $\mathbf{R}^3$; here a, b, c are positive coefficients and $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ denotes the standard basis of $\mathbf{R}^3$. This triangle is mapped via the radial projection $x \mapsto \frac{x}{\|x\|}$ onto $\mathscr{S}$. It is possible to generate very slanted and therefore ill-conditioned projections onto $\mathscr{S}$ by varying the constants a, b, c.

The meshsize of the standard triangle σ is $h_0 = 1$. By subdividing σ uniformly, we generate a sequence of meshsizes $h_i = 2^{-i}$. For each meshsize we calculate the corresponding approximate integral $\mathscr{I}(h_i)$ and generate a Romberg tableau with entries $T_{i,k}$ in the ith row and kth column in a standard manner. Provided that the Conjecture 1 holds, we obtain the following error estimate (see [7, §3.4]):

$$T_{i,k} - \mathscr{I}_0 = (-1)^k h_{i-k}^2 h_{i-k+1}^2 \cdots h_i^2 \left(1 + \mathscr{O}(h_{i-1-k})\right).$$

In order to verify this last estimate, we calculate the logarithmic ratio

$$\Delta_{i,k} = \log_4 \frac{T_{i-1,k} - \mathscr{I}_0}{T_{i,k} - \mathscr{I}_0}$$

and compare the numerical result with the assymptotic behavior

$$(25) \qquad \Delta_{i,k} = k + 1 + \mathscr{O}(h_{i-k-1}).$$

The following Romberg tableaus display the results for two different sets of coefficients a, b, c and for both composite rules (3) and (4).

Trapezoidal Rule: $a = 1$, $b = 1$, $c = 1$

Absolute Errors						Logarithmic Ratio $\Delta_{i,k}$				
2.6e-01										
7.7e-02	1.3e-02					0.897				
2.0e-02	1.2e-03	4.3e-04				0.965	1.721			
5.1e-03	8.5e-05	6.7e-06	5.6e-08			0.991	1.945	3.006		
1.3e-03	5.4e-06	1.1e-07	3.1e-09	3.4e-09		0.998	1.986	2.979	2.079	
3.2e-04	3.4e-07	1.7e-09	4.1e-11	2.9e-11	2.6e-11	0.999	1.997	2.983	3.128	3.433

Midpoint Rule: $a = 1$, $b = 1$, $c = 1$

Absolute Errors						Logarithmic Ratio $\Delta_{i,k}$				
6.2e-01										
2.0e-01	5.3e-02					0.836				
5.3e-02	4.9e-03	1.7e-03				0.947	1.714			
1.3e-02	3.4e-04	3.2e-05	5.7e-06			0.986	1.932	2.864		
3.4e-03	2.2e-05	5.4e-07	3.9e-08	1.6e-08		0.997	1.983	2.948	3.600	
8.4e-04	1.4e-06	8.7e-09	2.3e-10	8.0e-11	6.4e-11	0.999	1.996	2.981	3.693	3.841

Trapezoidal Rule: $a = 0.5$, $b = 1$, $c = 2$

Absolute Errors						Logarithmic Ratio $\Delta_{i,k}$				
3.9e-01										
1.5e-01	7.4e-02					0.678				
4.3e-02	6.9e-03	2.4e-03				0.909	1.711			
1.1e-02	4.7e-04	4.2e-05	4.7e-06			0.977	1.936	2.916		
2.8e-03	3.3e-05	3.6e-06	3.0e-06	3.0e-06		0.994	1.921	1.776	0.326	
7.1e-04	2.1e-06	4.7e-08	9.8e-09	2.1e-08	2.5e-08	0.998	1.985	3.135	4.127	3.556

Midpoint Rule: $a = 0.5$, $b = 1$, $c = 2$

Absolute Errors						Logarithmic Ratio $\Delta_{i,k}$				
8.6e-01										
3.8e-01	2.3e-01					0.577				
1.2e-01	2.8e-02	1.4e-02				0.860	1.527			
3.1e-02	2.1e-03	4.1e-04	1.90e-04			0.962	1.854	2.550		
7.8e-03	1.5e-04	1.5e-05	8.4e-06	7.7e-06		0.990	1.928	2.404	2.265	
2.0e-03	9.3e-06	2.2e-07	9.9e-09	4.3e-08	5.0e-08	0.997	1.984	3.031	4.866	3.742

These tableaus confirm our Conjecture 1, given the finite-precision arithmetic of the computer used and the $\mathcal{O}(h_{i-k-1})$ error of the asymptotic behavior of (25).

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