MULTIDIMENSIONAL NUMERICAL INTEGRATION AND APPLICATIONS TO BOUNDARY INTEGRAL EQUATIONS

by

Yajun Yang

An Abstract

Of a thesis submitted in partial fulfillment of the requirements for the Doctor of Philosophy degree in Mathematics in the Graduate College of The University of Iowa

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ABSTRACT

We consider the numerical solution of boundary integral equations of the second kind, that are reformulations of Laplace's equation $\Delta u = 0$ on connected regions D in $\mathbf{R}^3$ with a smooth boundary S. Symbolically, we write the boundary integral equation as $(\lambda - \mathcal{K})\rho = g$. The numerical method is collocation with piecewise polynomial interpolation in the parametrization variables. We approximate both the surface S and the unknown solution ρ by using such interpolation.

In this thesis, we first deal with the numerical integration of functions with point singularities over a planar wedge S using piecewise polynomial interpolation of the function and the wedge. Such integrals often occur in solving boundary integral equations using the collocation method. In order to obtain the same order of convergence as is true with uniform meshes for smooth functions, we introduce a graded refinement of the triangulation of S. Error analyses and several examples are given for a certain type of graded refinement.

Next, we extend these results to potential integrals over surfaces in $\mathbf{R}^3$. Finally, a numerical integration scheme for collocation integrals is given, which leads to a discrete collocation method. We establish the rate of convergence of this method and give an error analysis for the numerical evaluation of single layer and double layer integrals.

Abstract approved: ____________________
Thesis supervisor

____
Title and department

____
Date

Graduate College
The University of Iowa
Iowa City, Iowa

CERTIFICATE OF APPROVAL

PH.D. THESIS

This is to certify that the Ph.D. thesis of

Yajun Yang

has been approved by the Examining Committee for the thesis requirement for the Doctor of Philosophy degree in Mathematics at the December 1993 graduation.

Thesis committee: ______________________________
Thesis supervisor

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Member

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Member

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Member

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Member

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To my parents

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CHAPTER I

INTRODUCTION

Let D be a bounded and simply connected region in $\mathbf{R}^3$ with its boundary $S = \partial D$ being smooth. We consider the numerical solution of boundary value problems, for example, the interior Dirichlet problem

$$\Delta u(A) = 0, \qquad A \in D \tag{1.1}$$

$$u(P) = f(P), \qquad P \in S \tag{1.2}$$

via a boundary integral equation (BIE) reformulation. Under certain assumptions on the boundary S and the function f, it is well-known that (1.1)-(1.2) has a unique solution which depends continuously on the given boundary data.

The use of integral equation methods in the solution of boundary value problems for partial differential equations plays an important role in many problems of mathematical physics. Questions of existence and uniqueness of solutions are conveniently studied from the point-of-view of integral equations. Also, many mathematical problems, for instance, problems in fluid dynamics, elasticity and heat conduction, can be solved by using integral equations.

The theory of integral equation was initiated over a century ago. Recently, much work has been done for boundary integral equations of second kind over smooth boundaries in two dimensional and three dimensional spaces. In most of these cases, the integral operator involved in the integral equation is compact, or else compact operators are involved in the analysis. The compactness leads to a fairly well developed mathematical analysis, for example, see Günter (1967), Mikhlin (1970) and Pogorzelski (1966). A wide variety of numerical methods have been used to study three dimensional BIE problems (e.g., see Atkinson [11]), and most numerical methods for the problems can be considered to be of collocation or Galerkin type.

The most general convergence results for collocation methods are given by Wendland (1985). He used polynomials of degree k to approximate surfaces and polynomials of degree d to approximate functions, and showed that the error of the numerical solutions is of order n, where n is the minimum of $d+1$ and $k+1$. Later, Atkinson and Chien (1992) obtained superconvergence results for collocation method with piecewise quadratic approximations. A Galerkin method with spherical harmonics as the basis functions was investigated by Atkinson (1980, 1982).

In the past few years, much attention has been given to the case of piecewise smooth boundaries. The analysis of the numerical solution of BIEs for three dimensional domains with only a piecewise smooth boundary is in a rather incomplete stage. There are varied special results by Wendland (1968) and Atkinson (1985a) on the stability and rate of convergence of collocation methods with piecewise polynomials of degree less than or equal to 2, for certain classes of piecewise smooth boundaries. Recently Rathsfeld (1992a) has obtained new results on the stability of the panel method (i.e. piecewise constant collocation) for boundary integral equations over polyhedral boundaries. He also gave the stability of a certain piecewise polynomial collocation over the wedge and the cube. See Rathsfeld [42].

Using Galerkin methods with piecewise polynomials of an arbitrary degree on graded meshes, Elschner (1992b) presented a stability theorem and quasioptimal error estimates in the L^2-norm for problems on polyhedra. The Galerkin method for the first kind integral equations on a Lipschitz boundary was considered by Costabel (1988). In the papers [40], [43], Nyström methods have been considered by Rathsfeld. Some of the work mentioned above is the extension of results for the corresponding equations in the two dimensional case. See Graham and Chandler (1988), Elschner (1990), and Atkinson and de Hoog (1984).

Whatever method is chosen for solving boundary integral equations, we always have to compute integrals

$$\int_S f(Q)k(P,Q)dS_Q, \tag{1.3}$$

usually of several kinds. In most case, an analytical expression for (1.3) cannot be obtained and a numerical approximation is required.

Numerical quadratures along with estimates of the quadrature error for the near field, the far field, and the intermediate field were considered by Guermond and Fortaine (1991) and Guermond (1992). Schwab and Wendland (1992) presented and analyzed methods for the accurate and efficient evaluation of weakly, Cauchy and hypersingular integrals over piecewise smooth surfaces in $\mathbf{R}^3$. The approach of using extrapolation methods based on the asymptotic expansion for the quadrature error was discussed in Lyness [35] and [36]. Rathsfeld (1991, 1992c) proposed numerical integrations associated with graded meshes when numerically solving the integral equation over the boundary of a polyhedron. He also studied the effect of mesh refinement near the corners and edges of the polyhedron.

Atkinson (1989) and Atkinson and Chien (1992) gave numerical schemes for evaluating collocation integrals. A package of programs for solving integral equations using piecewise polynomial collocation methods over surfaces in $\mathbf{R}^3$ was written by Atkinson [13]. It is also used to implement methods developed in this thesis.

In Chapter II, we define some terminology and notation, and state results which will be used in subsequent chapters. Chapter III studies a numerical integration method for singular integrals based on graded meshes. Following that, we extend the results to potential integrals over surfaces in $\mathbf{R}^3$, which is given in Chapter IV. Finally, in Chapter V we investigate the collocation method for BIEs over a smooth boundary in $\mathbf{R}^3$ and propose a discrete collocation method.

CHAPTER II

PRELIMINARIES

2.1 Introduction

This chapter gives terminology, notation, and results that are required in defining and solving problems that are presented in the remaining chapters. The presentation is organized into six sections besides the introduction. Section 2.2 states the boundary integral equation (BIE) method for Laplace's equation in $\mathbf{R}^3$, with two specific problems that motivate our studies. These are

1. The interior Dirichlet problem, using an indirect BIE formulation.

2. The exterior Neumann problem, using a direct BIE formulation.

In Section 2.3 we present some results that are associated with the collocation method for a compact operator. Section 2.4 gives the definitions, notation and assumptions on the triangulation of the surface S. Section 2.5 reviews results on the interpolation of functions on the triangulation of S. The final section of this chapter discusses the Nyström method.

2.2 The two BIE problems

Two problems for Laplace's equation and their associated boundary integral equations were studied. We transform the boundary value problems to integral equations by using surface potentials and Green's identities. We also state some solvability results for each of these problems.

P1. The interior Dirichlet problem. Let D be a bounded, open, simply connected region in $\mathbf{R}^3$, and let its boundary S be smooth, which is defined more precisely in Section 2. Given a continuous function f on S, we wish to find a function $u \in C(\bar{D}) \cap C^2(D)$ such that

$$\begin{aligned} \Delta u(A) &= 0, \qquad A \in D \\ u(P) &= f(P), \qquad P \in S \end{aligned}$$

We seek to solve this problem in terms of a double layer potential. That is, for points $A \in D$, we set

$$u(A) = \int_S \rho(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid A - Q \mid} \right] dS_Q \ , \tag{2.1}$$

where ρ is a density function to be determined from the integral equation

$$2\pi\rho(P) + \int_S \rho(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q = f(P), \ P \in S. \tag{2.2}$$

For notation, ν_Q denotes the unit normal to S at Q (if it exists), pointing into D. Symbolically, we write the integral equation (2.2) as

$$(2\pi + \mathcal{K})\rho = f$$

where

$$\mathcal{K}\rho(P) = \int_S \rho(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q \ , \qquad P \in S.$$

Theorem 2.1 The interior Dirichlet problem has a unique solution that can be expressed as a double layer potential (2.1).

Proof. See Kress [34, Chap. 6]. ∎

P2. The exterior Neumann problem. Let D and S be as above, and let $D_e = \mathbf{R}^3 \backslash \bar{D}$, the region exterior to D and S. The problem is to find $u \in C(\bar{D}_e) \cap C^2(D_e)$

such that

$$\begin{aligned} \Delta u(A) &= 0, \qquad A \in D_e \\ \frac{\partial u(P)}{\partial \nu_P} &= f(P), \qquad P \in S \end{aligned}$$

$$u(P) = O(\mid P \mid^{-1}), \quad \mid \nabla u(P) \mid = O(\mid P \mid^{-2}) \text{ as } \mid P \mid \to \infty \tag{2.3}$$

where f is a given continuous function. This time we seek a solution represented as a combination of single layer and double layer potentials. It can be shown that Green's third identity can be applied to u:

$$4\pi u(A) = \int_S f(Q) \frac{1}{\mid A - Q \mid} dS_Q - \int_S u(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid A - Q \mid} \right] dS_Q, \ A \in D_e \tag{2.4}$$

To find u on S, we solve the integral equation

$$2\pi u(P) + \int_S u(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q = \int_S f(Q) \frac{1}{\mid P - Q \mid} dS_Q, \ P \in S \tag{2.5}$$

Then (2.4) gives u on D_e. Symbolically, we write (2.5) as

$$(2\pi + \mathcal{K})u = \mathcal{S}f$$

with $\mathcal{K}$ as before and $\mathcal{S}$ the single layer potential integral operator.

Theorem 2.2 The exterior Neumann problem has a unique solution that can be expressed as (2.4).

Proof. See Kress [34, Chap. 6]. ■

Theorem 2.3 The solutions to the interior Dirichlet problem and exterior Neumann problem depend continuously in the maximum norm on the given data.

Proof. See Kress [34, Chap. 6]. ■

The integral equations (2.2) and (2.5) are different only in their right-hand inhomogeneous term. In general, we write them as

$$(\lambda + \mathcal{K})\rho = g.$$

2.3 Compact integral operators

In this section we state some of the important results used in this thesis. We describe the collocation method which will be applied to solve problems on a surface S in $\mathbf{R}^3$. This material is based on Atkinson [2, pp. 54–62].

To solve approximately the integral equation

$$\lambda f(P) - \int_S k(P,Q)\, f(Q)\, dS_Q = g(P), \qquad P \in S\,, \tag{2.6}$$

we now turn to the collocation method. We write (2.6) in the operator form

$$(\lambda - \mathcal{K})f = g$$

and the operator $\mathcal{K}$ is assumed to be compact in a Banach space X to X. For our work, X is the space of continuous functions on the surface S equipped with supremum norm. Let $\{Q_1, \ldots, Q_n\}$ be a set of distinct *collocation nodes*, and let $\phi_1(P), \ldots, \phi_n(P)$ be continuous functions on S with

$$\det[\phi_i(Q_j)] \neq 0.$$

Define the collocation method as following: for

$$f_n(P) = \sum_{j=1}^{n} \alpha_j \phi_j(P)\,, \tag{2.7}$$

define the residual as

$$r_n(P) = \lambda f_n(P) - \mathcal{K} f_n(P) - g(P)\,.$$

Determine $\alpha_1, \ldots, \alpha_n$ by making

$$r_n(Q_i) = 0 \qquad i = 1, 2, \ldots, n\,; \tag{2.8}$$

and therefore, hopefully, making $r_n(P)$ also small everywhere else in S and making f_n close to the true solution. The resulting linear system is

$$\sum_{j=1}^{n} \alpha_j \left[\lambda \phi_j(Q_i) - \int_S k(Q_i, Q)\phi_j(Q) dS_Q\right] = g(Q_i) \qquad i = 1, 2, \ldots, n\,.$$

In Atkinson [2, pp. 50–62], it is shown that (2.7) and (2.8) define a projection method. Let X be a Banach space, X_n a finite dimensional subspace, and $\mathcal{P}_n$ a bounded projection operator from X onto X_n. The projection method for solving $(\lambda - \mathcal{K})f = g$ is to solve

$$(\lambda - \mathcal{P}_n\mathcal{K})f_n = \mathcal{P}_n g\,.$$

Theorem 2.4 Let $\mathcal{K} : X \to X$ be a bounded operator, with X a Banach space. Assume $\lambda - \mathcal{K} : X \xrightarrow[\text{onto}]{1-1} X$. Further assume

$$\|\mathcal{K} - \mathcal{P}_n\mathcal{K}\| \to 0 \qquad \text{as } n \to \infty$$

Then, for all sufficiently large n, say $n \geq N$, the operator $(\lambda - \mathcal{P}_n\mathcal{K})^{-1}$ exists as a bounded operator from X to X. Moreover, it is uniformly bounded:

$$\sup_{n \geq N} \|(\lambda - \mathcal{P}_n\mathcal{K})^{-1}\| < \infty$$

For $(\lambda - \mathcal{K})f = g$ and $(\lambda - \mathcal{P}_n\mathcal{K})f_n = \mathcal{P}_n g$,

$$f - f_n = \lambda(\lambda - \mathcal{P}_n\mathcal{K})^{-1}(f - \mathcal{P}_n f)$$

$$\frac{|\,\lambda\,|}{\|\lambda - \mathcal{P}_n\mathcal{K}\|}\,\|f - \mathcal{P}_n f\| \leq \|f - f_n\| \leq |\,\lambda\,|\;\|(\lambda - \mathcal{P}_n\mathcal{K})^{-1}\|\,\|f - \mathcal{P}_n f\|\,.$$

From this theorem, we notice that the rate of convergence of f_n to f is exactly the same as the interpolation error $f - \mathcal{P}_n f$. To apply the above theorem, we need to know whether

$$\|\mathcal{K} - \mathcal{P}_n\mathcal{K}\| \to 0, \qquad \text{as } n \to \infty.$$

The following theorem addresses this question.

Theorem 2.5 let X be a Banach space, X_n a sequence of finite dimensional subspaces. Let $\{\mathcal{P}_n : X \to X_n\}$ be a family of bounded projections with

$$\mathcal{P}_n f \to f \qquad \text{as } n \to \infty, \qquad f \in X.$$

Let $\mathcal{K} : X \to X$ be compact. Then

$$\|\mathcal{K} - \mathcal{P}_n\mathcal{K}\| \to 0 \qquad \text{as } n \to \infty.$$

There are a broad variety of collocation methods corresponding to various choices for the subspace X_n and for the collocation nodes $Q_1, \ldots, Q_n$. The method we use is often referred to as the piecewise polynomial collocation method. The idea of this method is to first decompose the integration region S into elements $\triangle_1, \triangle_2, \ldots, \triangle_n$; and then approximate a function $f \in C(S)$ by a low degree polynomial over each of the elements $\triangle_i$. We describe the decomposition of S and the approximation of f in the next two sections.

2.4 The triangulation and refinement

In this section, we describe the triangulation of the surface S and discuss its refinement to a finer mesh. As discussed in [6], we assume the surface S can be written as

$$S = S_1 \cup S_2 \cup \cdots \cup S_J \tag{2.9}$$

where each S_i is a closed, "smooth" surface in $\mathbf{R}^3$. The only possible intersection of a pair S_i and S_j is to be along a common portion of the edges of these two sub-surfaces. Assume that for each S_j, there is a mapping

$$F_j : R_j \xrightarrow[\text{onto}]{1-1} S_j \,, \qquad 1 \le j \le J \,, \tag{2.10}$$

where R_j is a polygonal domain in the plane and F_j is as smooth as needed. In this case, we say S is *piecewise smooth*. By a *smooth surface*, we mean that for each point $P \in S$, there is a neighborhood on S of P, with the neighborhood having a local parametrization in $\mathbf{R}^2$, with as many continuous derivatives as needed. Most surfaces S of interest can be decomposed as in (2.9), with each S_j representable as in (2.10). Also, the surface S could be smooth, and we would often still want to decompose it as in (2.9).

The surface S of (2.9) is divided into a triangular mesh

$$\tau_n = \{ \ \triangle_{K,n} \mid 1 \le K \le N_n \ \} \tag{2.11}$$

for a sequence $n = 1, 2, \ldots$. Each S_j is to be broken apart into a set of nonoverlapping triangular shaped elements $\triangle_{K,n}$, about which we say more below. In referring to the element $\triangle_{K,n}$, the reference to n is often omitted, but understood implicitly. Define the mesh size of (2.11) by

$$\delta_n = \max_{1 \le K \le N_n} diam(\triangle_K),$$

$$diam(\triangle_K) = \max_{p,q \in \triangle_K} \mid p - q \mid . \tag{2.12}$$

One way of obtaining the triangulation (2.11) is by means of the parametric representation (2.10) for the region S_j of (2.9). Triangulations of R_j map onto triangulations of S_j. Since the R_j's are polygonal domains and can be written as a union of triangles, without loss of generality, we assume in this paper that the R_j's are triangles. We choose τ_1 to be $\{S_j \mid j = 1, \ldots, J\}$.

The sequence of triangulations (2.11) will usually be obtained by successive refinements. We first construct this sequence by a quasi-uniform refinement, which is based on connecting the midpoints of the sides of every element $\widehat{\triangle}_K$ in the triangulation of R_j for $j = 1, \ldots, J$. Let $\widehat{v}_1$, $\widehat{v}_2$, and $\widehat{v}_3$ be the vertices of $\widehat{\triangle}_K$, $\widehat{v}_4$, $\widehat{v}_5$, and $\widehat{v}_6$ be the midpoints of its sides. Connect $\widehat{v}_4, \widehat{v}_5, \widehat{v}_6$ by straight lines, as in Figure 1, producing four new triangular elements. The new elements are all congruent, and they are similar to $\widehat{\triangle}_K$. More importantly, any *symmetric pair of triangles*, as shown in Figure 2, have the following property:

$$\widehat{v}_{2,k} - \widehat{v}_{1,k} = -(\widehat{v}_{2,l} - \widehat{v}_{1,l}) \quad \text{and} \quad \widehat{v}_{3,k} - \widehat{v}_{1,k} = -(\widehat{v}_{3,l} - \widehat{v}_{1,l}) \tag{2.13}$$

For the analysis of the numerical integration, we need to introduce another special refinement, which is called an '$La+u$' refinement about P with L a positive integer and P a vertex of some triangle in τ_1. The sequence τ_n is constructed as follows. We divide each triangle R_j, whose image S_j contains P, into four

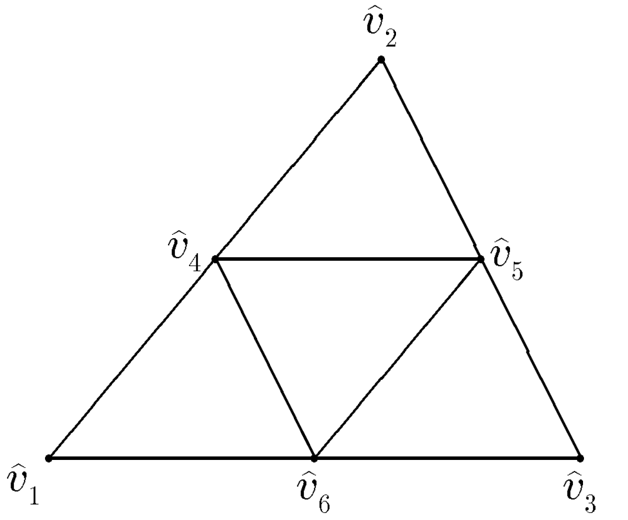


Figure 1: Quasi-uniform refinement

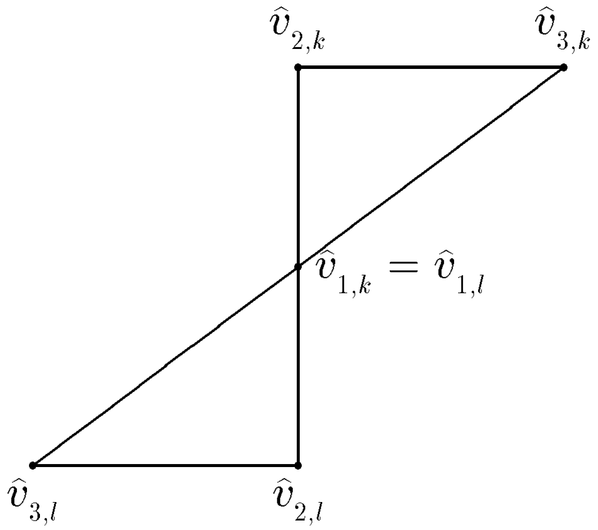


Figure 2: A symmetric pair of triangles

new triangular elements. For the resulting triangulation, divide each triangle whose image contains P into four new triangular elements. After doing this L times, we divide simultaneously every triangle into four new triangles. The final triangulation produces $\tau_2 = \{\triangle_{K,2} \mid 1 \leq K \leq N_2\}$ under the parametric representation (2.10). Repeat the preceding subdivision, we obtain $\tau_3, \tau_4, \ldots$. In other words, at level n, we perform L times an adaptive subdivision on triangles containing P, and then we do one simultaneous subdivision of all triangles. An advantage of this form of graded refinement is that each set of mesh points contains those at the preceding level.

As an example, we choose S to be a polygon and illustrate the '$2a + u$' refinement for $n = 1, 2$ in Figures 3, 4. When $n = 2$, there are three different triangular elements in size. Let B_l be the union of the triangles of the same size in S, and which therefore have been uniformly divided by the triangulation. The diameter of triangles in B_l is $O(2^{-(2+l)})$.

More generally, by examining the structure of the '$La + u$' refinement, we can calculate the total number N_n of triangles at level $n > 1$, namely

$$\left[(L + \frac{1}{4})J^* + J - J^*\right] 2^{2n} - 4LJ = O(2^{2n}).$$

In this, J is the number of S_j's, J^* is the number of S_j's containing P. For each S_j containing P, there are $Ln - L$ different triangular elements in size. The closer the triangle is to the point P, the smaller it is. As the triangles vary in size from large to small, we name the region containing triangles of the same size to be $B_0, B_1, \ldots, B_{Ln-L-1}$, respectively. Let $\widehat{B}_l$ be the pre-image of B_l. The diameter of triangles in $\widehat{B}_l$, denoted by $\widehat{\delta}_l$, is $O(2^{-(n+l)})$. Let N_l be the number of triangles in $\widehat{B}_l$. Then N_l is proportional to 4^{n-i} where $l = iL + i_1$ for $0 \leq i_1 \leq L-1$. The distance from the point $\widehat{P}$, the pre-image of P, to $\widehat{B}_l$, denoted by r_l, is $O(\frac{1}{2^{(L+1)i}})$.

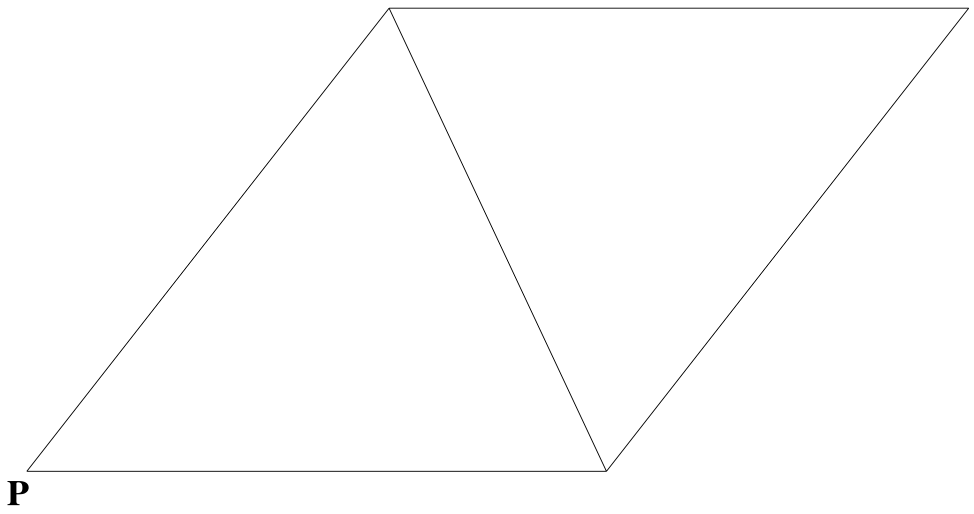


Figure 3: $n = 1$

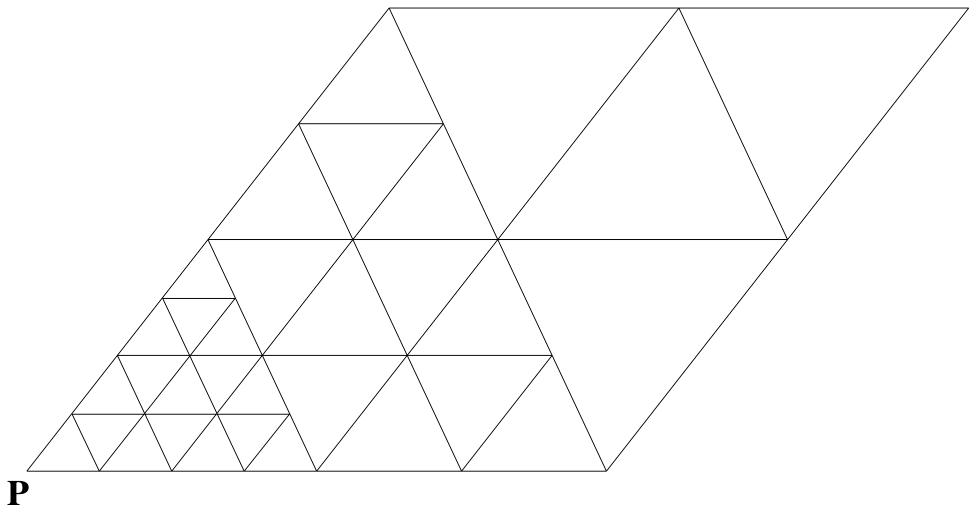


Figure 4: $n = 2$

In each $\widehat{B}_l$ $(l = 0, \ldots, Ln-L-1)$, the triangular elements $\widehat{\triangle}_K$ are true triangles and all are congruent. And any symmetric pair of triangles have the property (2.13). The total number of symmetric pairs of triangles in $\widehat{B}_l$ is $O(N_l)$ and the remaining triangles in $\widehat{B}_l$ is $O(\sqrt{N_l})$.

For S_j not containing P, it is divided by a quasi-uniform refinement. If let $L = 0$, then the '$La+u$' refinement is quasi-uniform. The analysis given in [16] indicates that a quasi-uniform refinement is a better scheme to use with smooth integrands in the numerical integration, while a graded mesh is needed with the singular integrals. See [47] for a paper based on some of the results of this thesis.

2.5 Interpolation

For interpolation, we use piecewise polynomials with a focus on interpolating a given function by a quadratic polynomial over each triangle. Let σ denote the unit simplex in the $st-plane$

$$\sigma = \{(s,t) \mid 0 \le s, t, s+t \le 1\} .$$

Let $\rho_1, \ldots, \rho_6$ denote the three vertices and three midpoints of the sides of σ, numbered according to Figure 5.

To define interpolation, introduce the basis functions for quadratic interpolation on σ. Letting $u = 1-(s+t)$, define

$$\begin{aligned} &l_1(s,t) = u(2u-1), \quad &&l_2(s,t) = t(2t-1), \quad &&l_3(s,t) = s(2s-1), \\ &l_4(s,t) = 4tu, &&l_5(s,t) = 4st, &&l_6(s,t) = 4su. \end{aligned}$$

We give the corresponding set of basis functions $\{l_{j,K}(q)\}$ on $\triangle_K$ by using its parametrization over σ. Let $\widehat{\triangle}_K$ be an element in the triangulation of R_j, corresponding to $\triangle_K$, and let $\widehat{v}_1$, $\widehat{v}_2$, and $\widehat{v}_3$ be its vertices. Define

$$m_K(s,t) = F_j(u\widehat{v}_1 + t\widehat{v}_2 + s\widehat{v}_3), \qquad u = 1-s-t\,, \qquad (s,t) \in \sigma \tag{2.14}$$

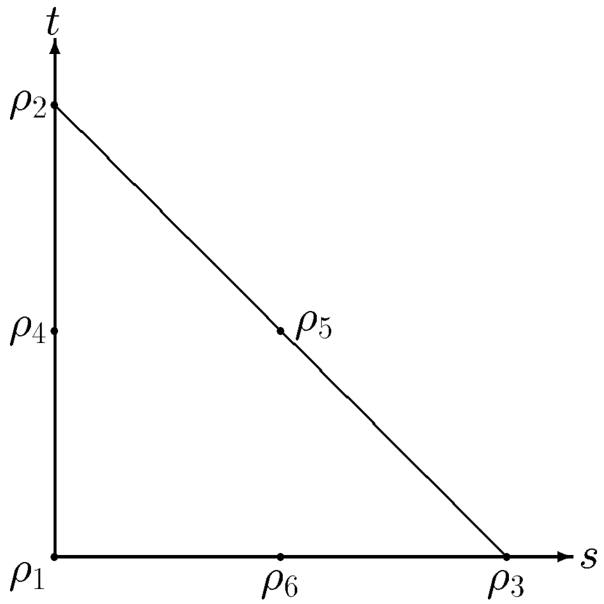


Figure 5: The unit simplex

where $F_j : R_j \xrightarrow[\text{onto}]{1-1} S_j$ is a six-times continuously differentiable function. Then m_K is a bijective mapping from σ to $\triangle_K$ with $m_K \in C^6(\sigma)$. Introduce the node points for $\triangle_K$ by $v_{j,K} = m_K(\rho_j), j = 1, \cdots, 6$. The first three are the vertices and the last three are approximate midpoints of the sides of $\triangle_K$. Define

$$l_{j,K}(m_K(s,t)) = l_j(s,t), \quad 1 \leq j \leq 6, \quad 1 \leq K \leq N.$$

Given a function f, define

$$\mathcal{P}_N f(q) = \sum_{j=1}^{6} f(v_{j,K}) l_{j,K}(q), \quad q \in \triangle_K, \tag{2.15}$$

for $K = 1, \ldots, N$. This is called the *piecewise quadratic function interpolating* f on the nodes of the mesh $\{\triangle_K \mid 1 \leq K \leq N\}$ for S.

Other kinds of interpolation can be used, such as piecewise cubic function interpolation to f, and in this case, we need ten node points, $\rho_1, \ldots, \rho_{10}$, and ten basis functions for this interpolation on σ. In general, suppose that we use interpolation of degree d to approximate the function f. Let $\{\rho_1, \ldots, \rho_v\}$ be the node points in the unit simplex and let $\{l_1, \ldots, l_v\}$ be the basis functions in the Lagrange form, where $v = \frac{(d+1)(d+2)}{2}$. The points $\{\rho_1, \ldots, \rho_v\}$ will be equally spaced over σ and of the form $(\frac{i}{d}, \frac{j}{d})$, $0 \le i + j \le d$. The interpolation of f is defined by

$$\mathcal{P}_N f(s,t) = \sum_{j=1}^{v} f(\rho_j) l_j(s,t).$$

Some of our results will be stated for interpolation of an arbitrarily given degree.

Lemma 2.6 Let $\{\triangle_K\}$ be a sequence of triangulations for S. Then $\mathcal{P}_N$, as in (2.15), defines a bounded projection operator on $C(S)$ with

$$\|\mathcal{P}_N\| = 5/3\,.$$

For any $f \in C(S)$,

$$\|f - \mathcal{P}_N f\|_\infty \le \frac{5}{3}\,\omega(f, \delta_N) \tag{2.16}$$

with ω the modulus of continuity function.

Proof. See Atkinson [6]. ∎

This shows that $\mathcal{P}_N f \to f$ for all $f \in C(S)$. To improve the order of convergence in (2.16), we use the Taylor error formula. Let $g \in C^3(\sigma)$. Then

$$g(s,t) - T_2(s,t) = \frac{1}{2}\int_0^1 [(s\frac{\partial}{\partial x} + t\frac{\partial}{\partial y})^3 g(x,y)]\mid_{(x,y)=\xi(s,t)} d\xi$$

with $T_2(s,t)$ the degree two Taylor polynomial for $g(s,t)$ about $(0,0)$.

Lemma 2.7 Let the triangulation $\{\triangle_{K,N}\}$ be defined by using the mapping (2.14) and a triangulation $\{\widehat{\triangle}_{K,N}\}$ of the polygonal regions R_j in (2.10). Then for $f \in C^3(S)$,

$$\|f - \mathcal{P}_N f\|_\infty \le c\hat{\delta}_N^3\,.$$

$\widehat{\delta}_N$ is the mesh size of the triangulation $\{\widehat{\triangle}_{K,N}\}$. The constant c depends on f and F_j, but not on N or the triangulation.

Proof. See Atkinson [6]. ■

2.6 Some additional results

We describe now the Nyström method, following Atkinson [2, pp. 88–93]. Let

$$\int_S f(Q)\, dS_Q \approx \sum_{j=1}^{n} \omega_{j,n} f(Q_{j,n}) \qquad f \in C(S)\ , \quad n \geq 1 \tag{2.17}$$

denote a numerical method which converges for all continuous functions f on S, and assume that all the node points $Q_{j,n}$ lie in S; generally the second subscript n will be dropped, although implicitly understood. The Nyström method approximates (2.6) by the equation

$$\lambda f_n(P) - \sum_{j=1}^{n} \omega_{j,n} k(P, Q_{j,n}) f_n(Q_{j,n}) = g(P) \qquad P \in S\ . \tag{2.18}$$

By letting $P = Q_1, \ldots, Q_n$, we convert the equation (2.18) into the linear system

$$\lambda z_i - \sum_{j=1}^{n} \omega_j k(Q_i, Q_j) z_j = g(Q_i) \qquad i = 1, \ldots, n\ . \tag{2.19}$$

At this point, Nyström found that to each solution $\{z_1, \ldots, z_n\}$ of (2.19), there corresponds a unique solution $z(P)$ of (2.18) with which it agrees at node points $Q_1, \ldots, Q_n$.

Theorem 2.8 Let f_n be a solution of (2.18). Then the values $f_j^{(n)} = f_n(Q_j)$, $j = 1, \ldots, n$ satisfies the linear system (2.19). Conversely, let z_j, $j = 1, \ldots, n$ be a solution of the system (2.19). Then the function f_n defined by

$$f_n(P) \equiv \frac{1}{\lambda}\left(g(P) + \sum_{j=1}^{n} \omega_j k(P, Q_j) z_j\right) \qquad P \in S$$

solves equation (2.18).

Now, introduce the numerical integration operator $\mathcal{K}_n$,

$$\mathcal{K}_n f(P) = \sum_{j=1}^{n} \omega_j k(P, Q_j) f(Q_j), \qquad P \in S\,, \quad f \in C(S)\,. \tag{2.20}$$

$\mathcal{K}_n$ is a compact operator on $C(S)$ to $C(S)$. Symbolically, we can write equations (2.6), (2.18) and (2.19) as

$$(\lambda - \mathcal{K})f = g\,, \qquad (\lambda - \mathcal{K}_n)f = g\,, \qquad (\lambda I - K_n)Z = G_n\,,$$

respectively.

Lemma 2.9 Let $k(P,Q)$ be continuous and $\mathcal{K}$ be the associated integral operator on $C(S)$. Let the numerical scheme (2.17) converge for all continuous functions, and let $\mathcal{K}_n$ be defined by (2.20) . Then:

1. For any $f \in C(S)$, $\quad \mathcal{K}_n f \to \mathcal{K} f$ as $n \to \infty$;
2. For all $n \geq 1$, $\quad \|\mathcal{K} - \mathcal{K}_n\| \geq \|\mathcal{K}\|$;
3. $\|(\mathcal{K} - \mathcal{K}_n)\mathcal{K}\| \to 0$ as $n \to \infty$; (2.21)
4. $\|(\mathcal{K} - \mathcal{K}_n)\mathcal{K}_n\| \to 0$ as $n \to \infty$. (2.22)

The following set of assumptions are due to P. Anselone and R. Moore (see Anselone [1, pp. 5-8]) and they will imply (2.21) and (2.22).

A1) X is a Banach space and $\mathcal{K}$, $\mathcal{K}_n$, $n \geq 1$, are linear operators on X to X.

A2) $\mathcal{K}_n x \to \mathcal{K} x$, $\quad \forall\, x \in X$.

A3) $\{\mathcal{K}_n\}$ is a collectively compact family of operators, i. e., the set

$$S = \{\ \mathcal{K}_n x \mid n \geq 1 \quad \text{and} \quad \|x\| \leq 1\ \}$$

has compact closure in X.

Lemma 2.10 Assume A1–A3. Then

1. $\mathcal{K}$ is compact;
2. The sequence $\{\mathcal{K}_n\}$ is uniformly bounded;

3. $\|(\mathcal{K}-\mathcal{K}_n)\mathcal{M}\| \to 0$ as $n \to \infty$, for any compact operator $\mathcal{M} : X \longrightarrow X$.

4. $\|(\mathcal{K}-\mathcal{K}_n)\mathcal{K}_n\| \to 0$ as $n \to \infty$.

Now we complete the abstract error analysis.

Theorem 2.11 Assume A1–A3. Assume $\lambda \neq 0$ is not an eigenvalue of $\mathcal{K}$. Then for all sufficiently large n, say $n \geq N(\lambda)$, we have

$$\|(\mathcal{K}-\mathcal{K}_n)\mathcal{K}_n\| \leq \frac{|\lambda|}{\|(\lambda-\mathcal{K})^{-1}\|} \quad .$$

Furthermore, $(\lambda-\mathcal{K}_n)^{-1}$ exists for all $n \geq N(\lambda)$, and

$$\|(\lambda-\mathcal{K}_n)^{-1}\| \leq \frac{1+\|(\lambda-\mathcal{K})^{-1}\|\,\|\mathcal{K}_n\|}{|\lambda| - \|(\lambda-\mathcal{K})^{-1}\|\,\|(\mathcal{K}-\mathcal{K}_n)\mathcal{K}_n\|} \quad ;$$

this means that $(\lambda-\mathcal{K}_n)^{-1}$ is uniformly bounded for all $n \geq N(\lambda)$. For the error in $(\lambda-\mathcal{K}_n)f_n = g$ as an approximation to $(\lambda-\mathcal{K})f = g$, we have

$$\|f - f_n\| \;\leq\; \|(\lambda-\mathcal{K}_n)^{-1}\|\|(\mathcal{K}-\mathcal{K}_n)f\| \,. \tag{2.23}$$

This can be applied to also obtain an asymptotic error formula for the numerical integration error $(\mathcal{K}-\mathcal{K}_n)f(P)$. Also, the hypotheses A1–A3 allow $\mathcal{K}_n$ to have its definition extended to include product integration, which will include $\mathcal{K}_n = \mathcal{K}\mathcal{P}_n$, $\mathcal{P}_n$ an interpolatory projection. Thus, the iterated collocation solution $\hat{f}_n$ of the equation

$$(\lambda - \mathcal{K}\mathcal{P}_n)\hat{f}_n = g$$

is simply a Nyström method. In addition, the collocation method is related to the Nyström method when the quadrature formulas for the matrix elements can be carried out in closed form for the approximating subspace and collocation nodes.

The next theorem states that the Nyström method essentially preserves the stability of the original integral equation.

Theorem 2.12 Assume A1-A3. Then

$$\|(\lambda I - K_n)^{-1}\| \leq \|(\lambda - \mathcal{K}_n)^{-1}\|$$

where the matrix norm is the standard row norm.

CHAPTER III

A NUMERICAL INTEGRATION METHOD FOR SINGULAR INTEGRALS

3.1 Introduction

We consider the problem of approximating an integral of the form

$$\int_S f(x, y)\, dS$$

where S is a closed bounded connected set in $\mathbf{R}^2$. When the integrand has singularities within the integration region, the use of a standard quadrature method may be very inefficient. There are several ways to deal with this problem. One approach is to use a change of variables [44] to transform a singular integrand into a well behaved function over a new region. A second approach is to use 'graded mesh' numerical integration, to place more node points near where the integrand is badly behaved in order to improve the performance of a standard quadrature method. A third approach is to use extrapolation methods to construct new and more accurate integration formulas based on the asymptotic expansion for the quadrature error in the original quadrature rule. The generalization of the classical Euler-Maclaurin expansion to functions having a particular type of singularity, as obtained by Lyness [35], [36], provides a basis for extrapolation methods in the same way as the Euler-Maclaurin expansion is used as a basis for Romberg integration. For the one dimensional case, a standard discussion of these methods and others can be found in Atkinson [9, Chap.5].

In this chapter we discuss numerical integration with a graded mesh for the two dimensional case. The process of placing node points with variable spacing so as to better reflect the integrand is called grading the mesh. We choose the '$La + u$' refinement, as proposed in Section 2.3, for which the order of convergence is the same as for smooth functions, but with the integrand function having a particular type of singularity, specified below.

In the case of smooth integrand functions, Chien [16], [17] and [18] obtained that for integrals over a piecewise smooth surface in $\mathbf{R}^3$, the numerical integration using piecewise interpolation of degree d for both the surface and the integrand leads to the order of convergence $O(\widehat{\delta}^{d^*})$, where $d^* = d + 2$ when d is an even number and $d^* = d + 1$ when d is an odd number. And $\widehat{\delta}$ is the mesh size of a quasi-uniform triangulation of the surface. In terms of the number N of triangles, the order of convergence is $O(1/N^2)$. We extend these results to singular integrands.

To simplify our discussion, we study only the following class of problems. The integration region S is a wedge, i.e.

$$S = \{(x, y) \in \mathbf{R}^2 \mid 0 \leq r \leq 1,\ 0 \leq \theta \leq \Theta\}\,, \quad 0 < \Theta < \pi.$$

The integration function is singular at only the origin, and it is of the form

$$f(x, y) = r^{\alpha}\varphi(\theta)h(r)g(x, y), \quad \alpha > -2 \tag{3.1}$$

or the form

$$f(x, y) = r^{\alpha}\ \ln r\ \varphi(\theta)h(r)g(x, y), \quad \alpha > -2 \tag{3.2}$$

Here (x, y) are the Cartesian coordinates with the corresponding polar coordinates (r, θ). The functions $\varphi(\theta)$, $h(r)$, $g(x, y)$ are assumed to be sufficiently smooth. This is also the class of functions considered in Lyness [35] .

In Section 3.2, the interpolation-based quadrature formulas are given. Section 3.3 contains the error analyses and a discussion of the results. Numerical examples are given in Section 3.4.

This chapter presents detailed results for only the use of quadratic interpolation. The method being used generalizes to other degrees of piecewise polynomial interpolation, and the results are consistent with the kind of results we have obtained for the quadratic case. This generalization for other degrees of interpolation is given in Section 3.5.

Because integrals of non-smooth functions often occur in solving boundary integral equations, we expect that the error analysis of the present numerical integration methods eventually will lead to better numerical methods for the solution of boundary integral equations.

3.2 Numerical integration

Let $\{\triangle_1, \triangle_2, \ldots, \triangle_N\}$ be a triangulation of S. We write

$$\int_S f(q)\, dS = \sum_{K=1}^{N} \int_{\triangle_K} f(q)\, dS$$

For each K, with the mapping $m_K : \sigma \xrightarrow[\text{onto}]{1-1} \triangle_K$, we have

$$\int_{\triangle_K} f(q)\, dS = \int_\sigma f(m_K(s,t)) \mid D_s m_K(s,t) \times D_t m_K(s,t) \mid ds\, dt \tag{3.3}$$

D_s and D_t denote differentiation with respect to s, t, respectively. The quantity $\mid D_s m_K(s,t) \times D_t m_K(s,t) \mid$ is the Jacobian determinant of the mapping $m_K(s,t)$ used in transforming surface integrals over $\triangle_K$ into integrals over σ. When $\triangle_K$ is a triangle, the Jacobian is twice the area of $\triangle_K$.

The numerical integration formula used here is

$$\int_\sigma g(s,t)\, ds\, dt \approx \frac{1}{6} [\, g(\rho_4) + g(\rho_5) + g(\rho_6)\,] \tag{3.4}$$

which is based on integrating the quadratic polynomial interpolating g on σ at

$\rho_1, \ldots, \rho_6$. This integration has degree of precision 2. Applying (3.4) to the right side of (3.3), we have

$$\int_{\triangle_K} f(q)\, dS \approx \frac{1}{6} \sum_{j=4}^{6} f(m_K(\rho_j)) \mid D_s m_K(s,t) \times D_t m_K(s,t) \mid_{\rho_j} \tag{3.5}$$

A major problem with (3.5) is that $D_s m_K$ and $D_t m_K$ are inconvenient to compute for some elements $\triangle_K$ on many surfaces S. Therefore, we approximate $m_K(s,t)$ in terms of only its values at $\rho_1, \ldots, \rho_6$. Define

$$\widetilde{m}_K(s,t) = \sum_{j=1}^{6} m_K(\rho_j) l_j(s,t) = \sum_{j=1}^{6} v_{j,K} l_j(s,t).$$

Then

$$\begin{aligned} \int_{\triangle_K} f(q)\, dS &\approx \frac{1}{6} \sum_{j=4}^{6} f(m_K(\rho_j)) \mid D_s \widetilde{m}_K(s,t) \times D_t \widetilde{m}_K(s,t) \mid_{\rho_j} \\ &= \sum_{j=4}^{6} \widetilde{\omega}_{j,K} f(v_{j,K}) \end{aligned} \tag{3.6}$$

where

$$\widetilde{\omega}_{j,K} = \frac{1}{6} \mid D_s \widetilde{m}_K(s,t) \times D_t \widetilde{m}_K(s,t) \mid_{\rho_j} .$$

For the case of the wedge of a circle, in this chapter, only the outer triangles will be affected by this approximation. It would be more significant for triangular shaped surface elements, where those elements are approximated by the above interpolation formula. We return to a more extended analysis of the use of surface interpolation in a later chapter.

3.3 Error analysis

In this section, let the initial triangulation τ_1 of the planar wedge S be defined by connecting the midpoints of the sides of S using straight lines. The sequence of triangulations $\tau_n = \{\triangle_K\}$ is constructed by the '$La + u$' refinement about the origin. If L is a positive integer, then the refinement is graded. If $L = 0$, it is quasi-uniform. We first analyze numerical integrations with the graded meshes. Let L be a positive integer. Then there are $Ln - (L-1)$ different triangular elements in size. As the triangles vary in size from large to small, we name the region containing triangles of the same size to be $B_0, B_1, \ldots, B_{Ln-L}$, respectively, from largest to smallest. Each B_l is uniformly divided, and additional facts on the '$La + u$' refinement are given in Section 2.4. Write

$$\int_S f(q)\, dS = \int_{B_{Ln-L}} f(q)\, dS + \sum_{l=1}^{Ln-L-1} \int_{B_l} f(q)\, dS + \int_{B_0} f(q)\, dS$$

We study the error of integrating using the following decomposition.

$$\begin{aligned}
&\int_S f(q)\, dS - \sum_{K=1}^{N} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \\
=\ & \int_{B_{Ln-L}} f(q)\, dS - \sum_{\triangle_K \subset B_{Ln-L}} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \\
+\ & \sum_{l=1}^{Ln-L-1} \left(\int_{B_l} f(q)\, dS - \sum_{\triangle_K \subset B_l} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right) \\
+\ & \int_{B_0} f(q)\, dS - \sum_{\triangle_K \subset B_0} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K})
\end{aligned}$$

Lemma 3.1 Assume that f is of form (3.1). Let N be the total number of triangles in the triangulation $\{\triangle_K\}$. Then

$$\left| \int_{B_{Ln-L}} f(q)\, dS \ - \sum_{\triangle_K \subset B_{Ln-L}} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right| \le O(\frac{1}{N^{p_1}}) \tag{3.7}$$

where $p_1 = \frac{(L+1)(\alpha+2)}{2}$.

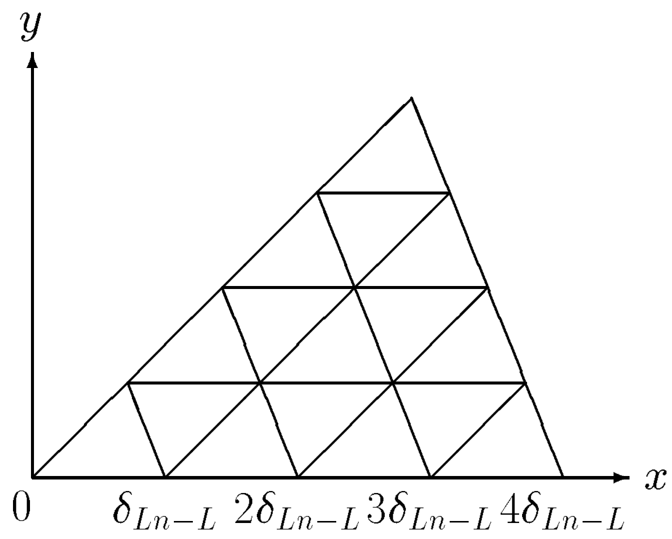


Figure 6: The partition of B_{Ln-L}

Proof. Let

$$\delta_{Ln-L} = \frac{1}{2^{n+(Ln-L)}}.$$

The partition of B_{Ln-L} is shown in Figure 6. Let $\{\triangle_K \mid K = 1, \ldots, 16\}$ denote the sixteen triangles in B_{Ln-L}, and let $\triangle_1$ contain the origin. Then the area of $\triangle_K$ is $\frac{1}{2}\delta_{Ln-L}^2 \sin(\Theta)$.

(a) We first estimate the error of

$$\mid \int_{\triangle_1} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,1} f(v_{j,1}) \mid .$$

Define

$$g_1(x, y) = \varphi(\theta) h(r) g(x, y),$$

and note that $g_1(x, y)$ is integrable over $\triangle_1$. Since $r^\alpha \geq 0$, by the integral mean value theorem we have

$$\int_{\triangle_1} f(q)\, dS = \mu \int_{\triangle_1} r^\alpha\, dS$$

where

$$\inf_{\triangle_1} \; g_1(x, y) \leq \mu \leq \sup_{\triangle_1} \; g_1(x, y).$$

Also,

$$\begin{aligned} \mid \mu \mid &\leq \sup_S \mid g_1(x, y) \mid \\ &\leq \sup_S \mid \varphi(\theta) \mid \sup_S \mid h(r) \mid \sup_S \mid g(x, y) \mid \\ &= \max_{0 \leq \theta \leq \Theta} \mid \varphi(\theta) \mid \max_{0 \leq r \leq 1} \mid h(r) \mid \max_S \mid g(x, y) \mid \\ &\equiv M < \infty \end{aligned}$$

Therefore,

$$\begin{aligned} \mid \int_{\triangle_1} f(q)\, dS \mid &\leq M \int_{\triangle_1} r^\alpha\, dS \\ &\leq M \int_0^{\delta_{Ln-L}} \int_0^\Theta r^{\alpha+1} d\theta dr \\ &= \frac{M\Theta}{\alpha+2}\, \delta_{Ln-L}^{\alpha+2}. \end{aligned}$$

On the other hand,

$$\mid \sum_{j=4}^{6} \widetilde{\omega}_{j,1} f(v_{j,1}) \mid \leq \frac{1}{6}\, \delta_{Ln-L}^{\alpha+2} \sin\Theta\ (2^{1-\alpha} + \mid \cos(\Theta/2) \mid^\alpha)\ M$$

This inequality comes from the following:

$$\widetilde{\omega}_{j,1} \;=\; \frac{1}{6} \mid D_s \widetilde{m}_1(s,t) \times D_t \widetilde{m}_1(s,t) \mid_{\rho_j}\, .$$

$$
\begin{aligned}
&= \frac{1}{6}\, 2 \text{ (Area of } \triangle_1) \\
&= \frac{1}{6}\, \delta_{Ln-L}^{\alpha+2} \sin\Theta, \quad \text{for } j = 4,5,6
\end{aligned}
$$

and

$$
\begin{aligned}
\mid f(v_{j,1}) \mid \;&\le\; \mid v_{j,1} \mid^{\alpha} M \\
&= \begin{cases} (\frac{\delta_{Ln-L}}{2})^{\alpha} M & \text{if } j = 4,6 \\ \delta_{Ln-L}^{\alpha} \mid \cos(\Theta/2) \mid^{\alpha} M & \text{if } j = 5 \end{cases}
\end{aligned}
$$

Hence,

$$
\mid \int_{\triangle_1} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,1} f(v_{j,1}) \mid \le\; O(\delta_{Ln-L}^{\alpha+2}).
$$

Notice that $\delta_{Ln-L} = O(\frac{1}{N^{\frac{L+1}{2}}})$. It follows that the error over $\triangle_1$ is $O(\frac{l}{N^{p_1}})$.

(b) The error over $\triangle_K$ $(K = 2, \ldots, 16)$ can be obtained by using Taylor's error formula. Assume that v_1, v_2 and v_3 are three vertices of $\triangle_K$. Define

$$
m_K(s,t) = uv_1 + tv_2 + sv_3, \qquad u = 1 - s - t
$$

Then m_K is a bijection mapping from σ onto $\triangle_K$. Since f is smooth on $\triangle_K$ and $m_K : \sigma \xrightarrow[\text{onto}]{1\text{–}1} \triangle_K$ is also smooth, we have

$$
f(m_K(s,t)) - \sum_{j=1}^{6} f(m_K(\rho_j)) l_j(s,t) = H_{f,K}(s,t;\zeta,\eta) \tag{3.8}
$$

where

$$
\begin{aligned}
&H_{f,K}(s,t;\zeta,\eta) \\
&= \frac{1}{3!}\left[(s\frac{\partial}{\partial s} + t\frac{\partial}{\partial t})^3 f(m_K(\zeta,\eta)) - \sum_{j=1}^{6} (s_j\frac{\partial}{\partial s} + t_j\frac{\partial}{\partial t})^3 f(m_K(\zeta_j,\eta_j)) l_j(s,t) \right]
\end{aligned}
$$

In this, $\rho_j = (s_j, t_j)$, (ζ, η) is on the line segment from (0,0) to (s,t), and (ζ_j, η_j) is on the line segment from (0,0) to (s_j, t_j). Notice that (ζ, η) and (ζ_j, η_j) belong to σ.

For $(s,t) \in \sigma$, $m_K(s,t) \in \triangle_K$, and

$$0 < \cos(\frac{\Theta}{2})\delta_{Ln-L} \le r(m_K(s,t)) \le 4\delta_{Ln-L}$$

where $r(m_K(s,t)) = \mid m_K(s,t) \mid$, the distance from the point $m_K(s,t)$ to (0,0).

We would like to examine one term in $H_{f,K}$, that associated with s^3, and it will show the general behavior of $H_{f,K}$.

$$\frac{\partial^3}{\partial s^3} f(m_K(\zeta,\eta)) = \frac{\partial^3}{\partial s^3}\left(r^\alpha(m_K(s,t)) \cdot g_1(m_K(s,t))\right)\Big|_{\substack{s=\zeta \\ t=\eta}}$$

$$= g_1(m_K(\zeta,\eta))\frac{\partial^3}{\partial s^3}\left(r^\alpha(m_K(s,t))\right)\Big|_{\substack{s=\zeta \\ t=\eta}} \tag{3.9}$$

$$+ 3\left\{\frac{\partial}{\partial s} g_1(m_K(s,t))\frac{\partial^2}{\partial s^2}\left(r^\alpha(m_K(s,t))\right)\right\}\Big|_{\substack{s=\zeta \\ t=\eta}} \tag{3.10}$$

$$+ 3\left\{\frac{\partial^2}{\partial s^2} g_1(m_K(s,t))\frac{\partial}{\partial s}\left(r^\alpha(m_K(s,t))\right)\right\}\Big|_{\substack{s=\zeta \\ t=\eta}} \tag{3.11}$$

$$+ r^\alpha(m_K(\zeta,\eta))\frac{\partial^3}{\partial s^3} g_1(m_K(s,t))\Big|_{\substack{s=\zeta \\ t=\eta}} \tag{3.12}$$

The magnitudes of (3.9), ..., (3.12) vary from $O(\delta^\alpha_{Ln-L})$ to $O(\delta^{\alpha+3}_{Ln-L})$. and $O(\delta^\alpha_{Ln-L})$ is the dominant term in (3.9), ..., (3.12). As an example, we show that (3.10) is $O(\delta^{\alpha+1}_{Ln-L})$. Let

$$m_K(s,t) = \begin{bmatrix} x(s,\ t) \\ y(s,\ t) \end{bmatrix}$$

Note that the derivatives of x, y with respect to (s,t) give rise to formulas involving $v_2 - v_1$ and $v_3 - v_1$. For example,

$$x_s(s,t) \;=\; \frac{\partial x}{\partial s} = (v_{3,x} - v_{1,x})$$

Then the magnitudes of the derivatives of x and y are $O(\delta_{Ln-L})$. Furthermore, the high-order derivatives of x and y is zero because of the linearity of the function $m_K(s,t)$.

The expression in the brackets of (3.10) becomes

$$\begin{aligned}
&\frac{\partial}{\partial s} g_1(m_K(s,t)) \frac{\partial^2}{\partial s^2}\left(r^\alpha(m_K(s,t))\right) \\
&= \left(\frac{\partial g_1}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial g_1}{\partial y}\frac{\partial y}{\partial s}\right) \cdot \frac{\partial}{\partial s}\left\{\alpha\, r^{\alpha-1}\left(\frac{\partial r}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial r}{\partial y}\frac{\partial y}{\partial s}\right)\right\} \\
&= \left(\frac{\partial g_1}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial g_1}{\partial y}\frac{\partial y}{\partial s}\right) \cdot \left\{\alpha(\alpha-1)\, r^{\alpha-2}\left(\frac{\partial r}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial r}{\partial y}\frac{\partial y}{\partial s}\right)^2 + \right. \\
&\qquad \left. \alpha\, r^{\alpha-1}\left[\left(\frac{\partial^2 r}{\partial x^2}\frac{\partial x}{\partial s} + \frac{\partial^2 r}{\partial x \partial y}\frac{\partial y}{\partial s}\right)\frac{\partial x}{\partial s} + \left(\frac{\partial^2 r}{\partial x \partial y}\frac{\partial x}{\partial s} + \frac{\partial^2 r}{\partial y^2}\frac{\partial y}{\partial s}\right)\frac{\partial y}{\partial s}\right]\right\} \\
&= O(\delta_{Ln-L})\left[O(\delta_{Ln-L}^{\alpha-2})O(\delta_{Ln-L}^2) + O(\delta_{Ln-L}^{\alpha-1})O(\delta_{Ln-L}^2)\right] \\
&= O(\delta_{Ln-L}^{\alpha+1})
\end{aligned}$$

In the above computation, we use that the derivatives of r with respect to x, y are bounded.

The dominant term in (3.9), ..., (3.12) is $O(\delta_{Ln-L}^\alpha)$. It follows that the coefficient of s^3 in $H_{f,K}$ is of $O(\delta_{Ln-L}^\alpha)$. Consequently,

$$\mid H_{f,K}(s,t;\zeta,\eta) \mid \leq\; O(\delta_{Ln-L}^\alpha)$$

for any $(s,t) \in \sigma$.

Therefore,

$$\left|\int_{\triangle_K} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K})\right|$$

$$\begin{aligned}
&\le O(\delta_{Ln-L}^2) \int_\sigma \mid f(m_K(s,t)) - \sum_{j=1}^{6} f(m_K(\rho_j)) l_j(s,t) \mid dS \\
&\le O(\delta_{Ln-L}^2) \int_\sigma \mid H_{f,K}(s,t;\zeta,\eta) \mid dS \\
&\le O(\delta_{Ln-L}^{\alpha+2}).
\end{aligned}$$

Hence, (3.7) holds. ∎

Lemma 3.2 Under the assumptions in Lemma 3.1, let $\beta = \alpha + 2 + \frac{\alpha-2}{L}$. Then

$$\left|\int_{B_l} f(q)\, dS - \sum_{\triangle_K \subset B_l} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K})\right| \le \begin{cases} O(2^{-4n-l\beta}) & \text{if } \alpha < 3 \\ O(2^{-4n-\frac{l}{L}-5l}) & \text{if } \alpha \ge 3 \end{cases} \tag{3.13}$$

for $l = 1, \ldots, Ln - L - 1$.

Proof. There are two types of triangles in B_l. Those triangles that are part of symmetric pairs of triangles (cf. Figure 2) are of the first type and remaining triangles are of the second type. By analysis of the '$La + u$' refinement in Section 2.4, the number of triangles of the first type is $O(N_l)$, where N_l is the number of triangles in B_l, and the number of triangles of the second type is $O(\sqrt{N_l})$. Then N_l is proportional to 4^{n-i}, where l is decomposed as $l = iL + i_1$ for $0 \le i_1 \le L - 1$.

Since f is smooth on B_l , then by Taylor's error formula we have

$$f(m_K(s,t)) - \sum_{j=1}^{6} f(m_K(\rho_j)) l_j(s,t) = H_{f,K}(s,t) + G_{f,K}(s,t;\zeta,\eta) \tag{3.14}$$

where

$H_{f,K}(s,t)$

$$= \frac{1}{3!}\left[(s\frac{\partial}{\partial s}+t\frac{\partial}{\partial t})^3 f(m_K(0,0)) - \sum_{j=1}^{6}(s_j\frac{\partial}{\partial s}+t_j\frac{\partial}{\partial t})^3 f(m_K(0,0))l_j(s,t)\right]$$

$G_{f,K}(s,t;\zeta,\eta)$

$$= \frac{1}{4!}\left[(s\frac{\partial}{\partial s}+t\frac{\partial}{\partial t})^4 f(m_K(\zeta,\eta)) - \sum_{j=1}^{6}(s_j\frac{\partial}{\partial s}+t_j\frac{\partial}{\partial t})^4 f(m_K(\zeta_j,\eta_j))l_j(s,t)\right]$$

We examine (3.14) and we can find the following.

First, $H_{f,K}(s,t)$ is a polynomial of degree three. Second, the coefficients of $H_{f,K}(s,t)$ are combinations of $(v_{2,K}-v_{1,K})$ and $(v_{3,K}-v_{1,K})$. For instance, the coefficient of s^3 is

$$\frac{1}{3!}\frac{\partial^3}{\partial s^3} f(m_K(0,0))$$

$$\begin{aligned}
&= \frac{1}{3!}\left[\frac{\partial^3}{\partial x^3} f(m_K(\rho_1))(v_{3K,x}-v_{1K,x})^3 + \frac{\partial^3}{\partial y^3} f(m_K(\rho_1))(v_{3K,y}-v_{1K,y})^3\right.\\
&+ 3\,\frac{\partial^3}{\partial x^2 \partial y} f(m_K(\rho_1))(v_{3K,x}-v_{1K,x})^2(v_{3K,y}-v_{1K,y})\\
&\left.+ 3\,\frac{\partial^3}{\partial x \partial^2 y} f(m_K(\rho_1))(v_{3K,x}-v_{1K,x})(v_{3K,y}-v_{1K,y})^2\right]
\end{aligned} \tag{3.15}$$

where $v_{j,K} = (v_{jK,x},\ v_{jK,y})$ for $j = 1,2,3$. For every symmetric pair of triangles, say $\triangle_1$ and $\triangle_2$, in B_l (see Figure 2, with $k=1$ and $l=2$), let

$$\begin{aligned}
m_1(s,t) &= (v_{3,1}-v_{1,1})s + (v_{2,1}-v_{1,1})t + v_{1,1}\\
m_2(s,t) &= (v_{3,2}-v_{1,2})s + (v_{2,2}-v_{1,2})t + v_{1,2}
\end{aligned}$$

Then

$$v_{1,1}-v_{2,1} = -(v_{1,2}-v_{2,2})$$

$$v_{1,1} - v_{3,1} \;=\; -(v_{1,2} - v_{3,2})\,.$$

We now have for $H_{f,1}$ and $H_{f,2}$, that the coefficient of s^3 in $H_{f,1}$ is

$$\frac{1}{3!}\left[\frac{\partial^3}{\partial x^3} f(m_1(\rho_1))(v_{31,x} - v_{11,x})^3 + \frac{\partial^3}{\partial y^3} f(m_1(\rho_1))(v_{31,y} - v_{11,y})^3\right.$$

$$+\,3\,\frac{\partial^3}{\partial x^2 \partial y} f(m_1(\rho_1))(v_{31,x} - v_{11,x})^2(v_{31,y} - v_{11,y})$$

$$\left.+\,3\,\frac{\partial^3}{\partial x \partial^2 y} f(m_1(\rho_1))(v_{31,x} - v_{11,x})(v_{31,y} - v_{11,y})^2\right] \tag{3.16}$$

and the coefficient of s^3 in $H_{f,2}$ is

$$\frac{1}{3!}\left[\frac{\partial^3}{\partial x^3} f(m_2(\rho_1))(v_{32,x} - v_{12,x})^3 + \frac{\partial^3}{\partial y^3} f(m_2(\rho_1))(v_{32,y} - v_{12,y})^3\right.$$

$$+\,3\,\frac{\partial^3}{\partial x \partial^2 y} f(m_2(\rho_1))(v_{32,x} - v_{12,x})^2(v_{32,y} - v_{12,y})$$

$$\left.+\,3\,\frac{\partial^3}{\partial x \partial^2 y} f(m_2(\rho_1))(v_{32,x} - v_{12,x})(v_{32,y} - v_{12,y})^2\right] \tag{3.17}$$

Adding (3.16) and (3.17) gives us zero, and an analogous argument holds for the remaining coefficients. This means that cancellation happens on any symmetric pair of triangles. It follows that

$$\left| \int_{\triangle_1 \cup \triangle_2} f(q)\, dS - \sum_{K=1}^{2} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right| \le O(\delta_l^2) \sum_{K=1}^{2} \int_\sigma \mid G_{f,K}(s,t;\zeta,\eta) \mid ds\, dt$$

where δ_l is the diameter of $\triangle_1$ and $\triangle_2$. This argument is based on Chien [16].

We now bound $G_{f,K}(s,t;\zeta,\eta)$ on $\triangle_K \subset B_l$, for $K = 1,2$. Since $1 \ge r(m_K(s,t)) \ge r_l > 0$ for $(s,t) \in \sigma$, and $r_l = O(2^{-(L+1)i})$, we have for $\alpha < 4$,

$$\begin{aligned} \mid G_{f,K}(s,t;\zeta,\eta) \mid & \leq O(\delta_l^4)\{O(r(m_K(\zeta,\eta))^{\alpha-4}) + \sum_{j=1}^{6} O(r(m_K(\zeta_j,\eta_j))^{\alpha-4})\} \\ & \leq O(\delta_l^4)O(r_l^{\alpha-4}) \\ & \leq O(\delta_l^4)O(2^{(4-\alpha)(L+1)i}) \end{aligned}$$

The first inequality arises from bounding the individual terms of $\frac{\partial^4 f}{\partial^a s \partial^b t}, a+b=4$, based on the kind of expansion done in (3.15). Otherwise, for $\alpha \geq 4$,

$$\mid G_{f,K}(s,t;\zeta,\eta) \mid \leq O(\delta_l^4).$$

So,

$$\left| \int_{\triangle_1 \cup \triangle_2} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right| \leq \begin{cases} O(\delta_l^6)O(2^{(4-\alpha)(L+1)i}) & \text{if } \alpha < 4 \\ O(\delta_l^6) & \text{otherwise} \end{cases}$$

The error contributed by triangles of the first type is as follows. If $\alpha < 4$,

$$\begin{aligned} & \left| \sum_{\triangle_K \ of first \ type} \left(\int_{\triangle_K} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right) \right| \\ \leq \ & O(N_l)O(\delta_l^6)O(2^{(4-\alpha)(L+1)i}) \\ \leq \ & O(2^{2n-2i}\frac{1}{2^{6n+6l}})O(2^{(4-\alpha)(L+1)i}) \\ \leq \ & O(2^{-4n-l\beta}) \end{aligned} \tag{3.18}$$

For $\alpha \geq 4$,

$$\begin{aligned} & \left| \sum_{\triangle_K \ of first \ type} \left(\int_{\triangle_K} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right) \right| \\ \leq \ & O(N_l)O(\delta_l^6) \ \leq O(2^{-4n-\frac{2l}{L}-6l}) \end{aligned} \tag{3.19}$$

For the remaining triangles in B_l, those of the second type, use (3.8), the fact that $r_l \leq r(m_K(s,t)) \leq 1$ for $\triangle_K \subset B_l$, and that their number is $O(\sqrt{N_l})$. Then

$$| H_{f,K}(s,t;\zeta,\eta) | \leq \begin{cases} O(\delta_l^3)O(r_l^{\alpha-3}) & \text{if } \alpha < 3 \\ O(\delta_l^3) & \text{otherwise} \end{cases} \tag{3.20}$$

and

$$\left| \sum_{\triangle_K \ of second \ type} \left(\int_{\triangle_K} f(q)\, dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right) \right|$$

$$\leq \begin{cases} O(2^{-4n-l\beta}) & \text{if } \alpha < 3 \\ O(2^{-4n-\frac{l}{L}-5l}) & \text{otherwise} \end{cases} \tag{3.21}$$

The total error over B_l is given by (3.13). ■

Lemma 3.3 Under the assumptions in Lemma 3.1,

$$| \int_{B_0} f(q)\, dS - \sum_{\triangle_K \subset B_0} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) | \leq O(\frac{1}{N^2}). \tag{3.22}$$

Proof. The function f is smooth on B_0, and B_0 is uniformly divided by triangular elements. By the results in [16], (3.22) follows. ■

Combining the above lemmas, we get the following result, which gives the total error of integrating over S.

Theorem 3.4 Let f be of the form (3.1) and let L be a positive integer. Then

$$\left| \int_S f(q)\, dS - \sum_{K=1}^{N} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right| \leq \begin{cases} O(\frac{\ln N}{N^2}) & \text{if } p_1 = 2 \\ O(\frac{1}{N^p}) & \text{otherwise} \end{cases} \tag{3.23}$$

where N is the total number of triangles in the triangulation, $p_1 = \frac{(\alpha+2)(L+1)}{2}$, and $p = \min\{p_1, 2\}$.

Proof. We first add all errors contributed by each $\triangle_K \subset B_1 \cup \cdots \cup B_{Ln-L-1}$. For $\alpha < 3$, if $p_1 \neq 2$ (i.e. $\beta \neq 0$),

$$\sum_{l=1}^{Ln-L-1}\left|\int_{B_l} f(q)\,dS - \sum_{\triangle_K\subset B_l}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K})\right|$$

$$\begin{aligned}
&\leq \sum_{l=1}^{Ln-L-1} O(2^{-4n-l\beta}) \\
&= O\left(2^{-4n}\frac{2^{-\beta}-2^{-\beta(Ln-L)}}{1-2^{-\beta}}\right) \\
&\leq O(2^{-2pn}) = O(\frac{1}{N^p})
\end{aligned}$$

while

$$\sum_{l=1}^{Ln-L-1}\left|\int_{B_l} f(q)\,dS - \sum_{\triangle_K\subset B_l}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K})\right| \leq O(\frac{n}{2^{2n}}) \leq O(\frac{\ln N}{N^2}) \quad \text{for } \beta = 0.$$

When $\alpha \geq 3$, β is nonzero. By a similar argument,

$$\sum_{l=1}^{Ln-L-1}\left|\int_{B_l} f(q)\,dS - \sum_{\triangle_K\subset B_l}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K})\right| \leq O(\frac{1}{N^p}) \ \text{ for } \alpha \geq 3.$$

Combining with Lemma 3.1 and Lemma 3.3, we have

$$\begin{aligned}
&| \int_S f(q)\,dS - \sum_{K=1}^{N}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K}) | \\
&\leq | \int_{B_{Ln-L}} f(q)\,dS - \sum_{\triangle_K\subset B_{Ln-L}}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K}) | \\
&\quad + \sum_{l=1}^{Ln-L-1} | \int_{B_l} f(q)\,dS - \sum_{\triangle_K\subset B_l}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K}) | \\
&\quad + | \int_{B_0} f(q)\,dS - \sum_{\triangle_K\subset B_0}\sum_{j=4}^{6}\tilde{\omega}_{j,K}f(v_{j,K}) | \\
&\leq O(\frac{1}{N^{p_1}}) + O(\frac{1}{N^p}) + O(\frac{1}{N^2})
\end{aligned}$$

$$\leq \quad O(\frac{1}{N^p}) \qquad \text{for } \beta \neq 0.$$

And it is $O(\frac{\ln N}{N^2})$ for $\beta = 0$. The quantity p_1 is defined in Lemma 3.1, and $p = \min\{p_1, 2\}$. ■

Corollary 3.5 Let L be any positive integer greater than $\frac{4}{\alpha+2} - 1$. Then the error for evaluating the integral over S is $O(1/N^2)$. In particular, a '$1a + u$' refinement gives an error of $O(1/N^2)$, for any $\alpha > 0$.

For a uniform mesh of S, the rate of convergence is predicted by the formula (3.23) with $L = 0$, although the preceding proof must be modified.

Theorem 3.6 Let f be of the form (3.1) and $L = 0$. Then

$$\left| \int_S f(q)\, dS - \sum_{K=1}^{N} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \right| \leq \begin{cases} O(\frac{\ln N}{N^2}) & \text{if } \alpha = 2 \\ O(\frac{1}{N^p}) & \text{otherwise} \end{cases} \tag{3.24}$$

where N is the total number of triangles in the triangulation, and $p = \min\{\frac{\alpha+2}{2}, 2\}$.

Proof. Let the triangulation $\tau_n = \{\triangle_K\}$ be constructed by the '$La + u$' refinement with $L = 0$ at level n. The size of the triangles in τ_n is of the same size $O(\frac{1}{2^n})$. The number of triangles in τ_n, N, is 2^{2n}.

We divide the wedge S into $2^{n-2}+1$ subregions according to the triangulation:

$$\begin{aligned} D_i &= \{(x,y) \in S \mid \frac{i}{2^{n-1}}\eta \leq \eta x - y \leq \frac{i+1}{2^{n-1}}\eta\}, \\ & \qquad i = 0, 1, \ldots, 2^{n-2} - 1 \\ D_{2^{n-2}} &= \{(x,y) \in S \mid \eta x - y \geq \frac{1}{2}\eta\}. \end{aligned}$$

where $\eta = \frac{\sin\Theta}{\cos\Theta - 1}$. The distance from the origin to D_i, denoted by r_i, is $O(\frac{i}{2^n})$.

Let N_i be the number of triangles in D_i. Then $N_i = 4(2i+1) = O(i)$. Moreover, the total number of symmetric pairs of triangles in D_i is $O(N_i) = O(i)$, and the remaining triangles in D_i is bounded.

Let E_i denote the error contributed by D_i. Using the argument in the proof of Lemma 3.1, we have that

$$E_0 = O(\delta_n^{\alpha+2}) = O(\frac{1}{N^{\frac{\alpha+2}{2}}}).$$

Also, applying Lemma 3.3 to $E_{2^{n-2}}$, we obtain that

$$E_{2^{n-2}} = O(\frac{1}{N^2}).$$

For E_i $(i = 1, 2 \ldots, 2^{n-2}-1)$, we write $E_i = E_{i1} + E_{i2}$, where

$$E_{i1} = \sum_{\triangle_K \ of first \ type} (\int_{\triangle_K} f(q)\ dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}))$$

$$E_{i2} = \sum_{\triangle_K \ of second \ type} (\int_{\triangle_K} f(q)\ dS - \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}))$$

Then, following the idea given in Lemma 3.2, we have

$$\begin{aligned} E_{i1} &= \begin{cases} O(N_i)O(\delta_i^6)O(r_i^{\alpha-4}) & \text{if } \alpha < 4 \\ O(N_i)O(\delta_i^6) & \text{otherwise} \end{cases} \\ &= \begin{cases} O(i^{\alpha-3})O(\frac{1}{2^{(\alpha+2)n}}) & \text{if } \alpha < 4 \\ O(i\frac{1}{2^{6n}}) & \text{otherwise} \end{cases} \end{aligned}$$

and

$$E_{i2} = \begin{cases} O(1)O(\delta_i^5)O(r_i^{\alpha-3}) & \text{if } \alpha < 3 \\ O(1)O(\delta_i^5) & \text{otherwise} \end{cases}$$

$$= \begin{cases} O(i^{\alpha-3})O(\frac{1}{2^{(\alpha+2)n}}) & \text{if } \alpha < 3 \\ O(\frac{1}{2^{5n}}) & \text{otherwise} \end{cases}$$

Finally, we add all errors E_i together. A straightforward computation leads to (3.24). ■

Theorem 3.7 Let f be of the form (3.2) and let L be a positive integer. Then

$$|\int_S f(q)\,dS - \sum_{K=1}^{N}\sum_{j=4}^{6}\tilde{\omega}_{j,K} f(v_{j,K})\,| \le O(\frac{\ln N}{N^{p_1}}) + O(\frac{1}{N^2})$$

where N is the total number of triangles in the triangulation, $p_1 = \frac{(\alpha+2)(L+1)}{2}$.

Proof. The proof is analogous to that of Theorem 3.4. ■

Corollary 3.8 Let L be any positive integer greater than $\frac{4}{\alpha+2} - 1$. Then the error for evaluating the integral over S is $O(\frac{1}{N^2})$. For $\alpha > 0$, a '$1a + u$' refinement still gives an error of $O(1/N^2)$.

Theorem 3.9 Let f be of the form (3.2) and $L = 0$. Then

$$\left|\int_S f(q)\,dS - \sum_{K=1}^{N}\sum_{j=4}^{6}\tilde{\omega}_{j,K} f(v_{j,K})\right| \le \begin{cases} O(\frac{1}{N^2}) & \text{if } \alpha > 4 \\ O(\frac{\ln N}{N^p}) & \text{otherwise} \end{cases}$$

where N is the total number of triangles in the triangulation, and $p = \min\{\frac{\alpha+2}{2}, 2\}$.

Proof. The proof is analogous to that of Theorem 3.6. ■

3.4 Numerical examples

We give numerical examples using the method analyzed in Section 3.2 and 3.3. The integration region is the wedge of the unit circle with the central angle $\pi/2$, i.e.

$$S = \{(x, y) \in \mathbf{R}^2 \ \mid\ 0 \le r \le 1,\ 0 \le \theta \le \pi/2\}.$$

The method was implemented with a package of programs written by K. Atkinson, which is described in [6], [13]. All examples were computed on a Hewlett-Packard workstation in double precision arithmetic.

For the first example consider the function

$$f_1(x, y) = r^{\alpha}, \quad \alpha > -2. \tag{3.25}$$

The results are given in Table 1 for $\alpha = 0.1,\ 0.5$ with $L = 1$. The column labeled *Order* gives the value

$$p_n = \frac{\ln |E_n/E_{n+1}|}{\ln(N_{n+1}/N_n)}$$

where E_n is the error at level n. Since the theoretical result shows that the error is $O(1/N^2)$, we expect that p_n will converge to 2.

Table 2 gives the results for $\alpha = -1$ with $L = 0$, $L = 1$ and $L = 3$. The empirical orders of convergence p_n approach 0.5, 1 and 2, respectively, as expected. When $L = 0$, the mesh is uniform, the convergence of the numerical integration is very slow. This indicates that the uniform mesh is very inadequate if the integrand is not smooth.

The next example uses the function

$$f_2(x, y) = r^{\alpha}\ \sin(\theta), \quad \alpha > -2. \tag{3.26}$$

It is of the form (3.1). Results for function f_2 are shown in Table 3 and Table 4. Note that the very regular rates of convergence exhibited.

We also consider a function of the form (3.2). Define

$$f_3(x, y) = r^{\alpha}\ \ln r, \quad \alpha > -2. \tag{3.27}$$

In order to compare with the preceding examples, we choose the same parameters in our experiment. The error in this case decreases slowly at the beginning, but eventually it approaches the theoretical rate of convergence. See Table 5 and Table 6.

n	N	$\alpha = .1$		$\alpha = .5$	
		Error	Order	Error	Order
1	4	$-2.36\text{E}{-4}$		$-9.47\text{E}{-4}$	
2	28	$-9.00\text{E}{-6}$	1.68	$2.90\text{E}{-6}$	3.10
3	124	$3.97\text{E}{-7}$	2.10	$3.22\text{E}{-6}$	-0.23
4	508	$7.13\text{E}{-8}$	1.22	$2.91\text{E}{-7}$	1.71
5	2044	$6.95\text{E}{-9}$	1.67	$2.10\text{E}{-8}$	1.89
6	8188	$5.70\text{E}{-10}$	1.81	$1.40\text{E}{-9}$	1.95

Table 1: Evaluation of f_1 with $L = 1$

N	$L = 0$		N	$L = 1$		N	$L = 3$	
	Error	Order		Error	Order		Error	Order
4	$1.49\text{E}{-1}$		4	$1.49\text{E}{-1}$		4	$1.49\text{E}{-1}$	
16	$8.08\text{E}{-2}$	0.10	28	$4.01\text{E}{-2}$	0.68	52	$9.51\text{E}{-3}$	1.08
64	$4.06\text{E}{-2}$	0.50	124	$1.07\text{E}{-2}$	0.93	244	$5.61\text{E}{-4}$	1.83
256	$2.03\text{E}{-2}$	0.50	508	$2.53\text{E}{-3}$	0.98	1012	$3.35\text{E}{-5}$	1.98
1024	$1.02\text{E}{-2}$	0.50	2044	$6.32\text{E}{-4}$	1.00	4084	$2.00\text{E}{-6}$	2.02
4096	$5.08\text{E}{-3}$	0.50	8188	$1.58\text{E}{-4}$	1.00			

Table 2: Evaluation of f_1 with $\alpha = -1$

n	N	$\alpha = .1$		$\alpha = .5$	
		Error	Order	Error	Order
1	4	2.87E−3		7.32E−4	
2	28	2.51E−4	1.25	5.92E−5	1.29
3	124	1.15E−5	2.58	2.35E−6	2.17
4	508	5.46E−7	2.16	1.14E−7	2.15
5	2044	2.49E−8	2.22	6.11E−9	2.11
6	8188	1.06E−9	2.28	3.50E−10	2.06

Table 3: Evaluation of f_2 with $L = 1$

N	$L = 0$		N	$L = 1$		N	$L = 3$	
	Error	Order		Error	Order		Error	Order
4	1.17E−1		4	1.17E−1		4	1.17E−1	
16	6.50E−2	0.42	28	3.26E−2	1.45	52	8.29E−3	1.03
64	3.25E−2	0.50	124	8.11E−3	0.94	244	4.83E−4	1.84
256	1.62E−2	0.50	508	2.03E−3	0.98	1012	2.87E−5	1.98
1024	8.12E−3	0.50	2044	5.07E−4	1.00	4084	1.71E−6	2.02
4096	4.06E−3	0.50	8188	1.27E−4	1.00			

Table 4: Evaluation of f_2 with $\alpha = -1$

n	N	$\alpha = .1$		$\alpha = .5$	
		Error	Order	Error	Order
1	4	−6.30E−3		5.56E−4	
2	28	−2.68E−4	1.62	1.06E−4	0.86
3	124	−5.43E−6	2.62	5.39E−6	2.00
4	508	1.71E−7	2.45	1.81E−7	2.41
5	2044	3.48E−8	1.44	2.69E−9	3.02
6	8188	3.30E−9	1.70	−2.17E−10	1.82

Table 5: Evaluation of f_3 with $L = 1$

N	$L = 0$		N	$L = 1$		N	$L = 3$	
	Error	Order		Error	Order		Error	Order
4	−5.60E−1		4	−5.60E−1		4	−5.60E−1	
16	−3.50E−1	0.34	28	−2.03E−1	0.53	52	−6.36E−2	0.85
64	−2.04E−1	0.39	124	−6.49E−2	0.77	244	−5.61E−3	1.57
256	−1.16E−1	0.41	508	−1.97E−2	0.85	1012	−4.51E−4	1.77
1024	−6.51E−2	0.42	2044	−5.81E−3	0.88	4084	−3.41E−5	1.85
4096	−3.61E−2	0.43	8188	−1.67E−3	0.90			

Table 6: Evaluation of f_3 with $\alpha = -1$

3.5 Generalizations

We have presented results for only the planar wedge, while using polynomial interpolation of degree two to approximate the integrand and the integration region. Any other degree of interpolation could also have been used. In such cases, the definition of the nodes will change appropriately. But the definition of the triangulation will remain the same, and we will use the '$La+u$' refinement.

In addition to using quadratic interpolation, we have also examined the use of linear, cubic and quartic interpolation. For linear and cubic interpolation, the function value at the origin is needed in the numerical integration. We simply let $f(0,0)=0$. The results are consistent with the kind of results we have obtained for the quadratic case, and they are as follows.

Suppose that we use interpolation of degree d to approximate both the integrand and the wedge S. Let $\{q_1,\ldots,q_v\}$ be the node points in the unit simplex and let $\{l_1,\ldots,l_v\}$ be the basis functions in the Lagrange form, where $v=\frac{(d+1)(d+2)}{2}$. The points $\{q_1,\ldots,q_v\}$ will be equally spaced over σ and of the form $(\frac{i}{d},\frac{j}{d})$, $0\le i+j\le d$. Define the interpolating operation

$$\mathcal{P}_N h(s,t)=\sum_{j=1}^{v} h(q_j)l_j(s,t)$$

The numerical integration we use is based on integrating this interpolation polynomial, i.e.

$$\begin{aligned}\int_\sigma h(s,t)ds\,dt &\approx \int_\sigma \mathcal{P}_N h(s,t)ds\,dt\\ &= \sum_{j=1}^{v}\tilde{\omega}_j^{(d)}h(q_j)\end{aligned}$$

Assume that the integrand is of the form (3.1). Then with the '$La+u$' refinement, we have

$$\left| \int_S f(q)\, dS - \sum_{K=1}^{N_n} \sum_{j=1}^{v} \tilde{\omega}_{j,K}^{(d)} f(v_{j,K}) \right| \le \begin{cases} O(\frac{\ln N_n}{N_n^{d^*}}) & \text{if } p_1 = d^* \\ O(\frac{1}{N_n^p}) & \text{otherwise} \end{cases}$$

where N_n is the number of triangular elements in the triangulation. The order $p = \min\{p_1, d^*\}$, $p_1 = \frac{(\alpha+2)(L+1)}{2}$, $d^* = \frac{d+2}{2}$ when d is an even number, and $d^* = \frac{d+1}{2}$ when d is an odd number. The proof is completely analogous to that given earlier for the quadratic case. In addition, we need the results for smooth integrands as stated in [16] and [18].

The results can be generalized to other integration regions S, for example, a wedge with the central angle larger than π, triangles, squares, regions containing the origin as an interior point, etc. We also can generalize this to curved surfaces in $\mathbf{R}^3$, with the integrand having a point singularity of the type given in (3.1). We omit statements of these results, as they are straightforward. We note however that for curved surfaces, we include the interpolatory approximation of it as discussed earlier in (3.6).

CHAPTER IV

A NUMERICAL INTEGRATION METHOD FOR POTENTIAL INTEGRALS

4.1 Introduction

In practice, we have to evaluate many integrals when we solve integral equations with the collocation method, and usually these integrals must be done by time-consuming numerical integrations. Integrals involved in the integral equations are either the single layer integral

$$\int_S \frac{f(Q)}{\mid P - Q \mid} dS_Q$$

or the double layer integral

$$\int_S f(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q .$$

Both are singular at $Q = P$. The use of a standard quadrature method may be very inefficient. The method we use to compensate for the bad behaviour of such integrands is to place more node points near the singular point in order to improve the performance of a standard quadrature methods. In Chapter 3, the interpolation-based numerical integration associated with an '$La + u$' refinement for functions of the form

$$f(x, y) = r^{\alpha} \varphi(\theta) h(r) g(x, y), \quad \alpha > -2$$

has been studied. In this formula, (r, θ) are the polar coordinates corresponding to the Cartesian coordinates (x, y). It was shown that if L is a positive integer greater than $\frac{4}{\alpha+2}-1$, then the order of convergence is $O(\frac{1}{N^2})$ with N the total number of triangles at level n. In the present chapter, we extend this result to the single layer and double layer integrals over a surface in $\mathbf{R}^3$.

4.2 Error analysis for single layer integrals

We consider first the error in evaluating a single layer integral

$$\int_S \frac{f(Q)}{\mid P-Q \mid} dS_Q$$

The kernel of the single layer integral has degree of singularity -1, and the corresponding value of L is 4. Our analysis begins with the integration region S a smooth triangular element in $\mathbf{R}^3$, i.e. there is a mapping $m : \sigma \xrightarrow[\text{onto}]{1-1} S$, $m \in C^6(\sigma)$. Assume $m(0,0)=P$, as most often, we will be interested only in the case that P is a node point of a given triangulation of S. Let $\{\triangle_K \mid 1 \le K \le N_n\}$ be the irregular triangulation of S obtained by performing n loops of the '$4a+u$' refinement about the point P. Write

$$\begin{aligned}
&\int_S f(Q)\frac{1}{\mid P-Q \mid} dS_Q \\
=\ &\sum_{K=1}^{N_n} \int_{\triangle_K} f(Q)\frac{1}{\mid P-Q \mid} dS_Q \\
=\ &\sum_{K=1}^{N_n} \int_{\sigma} f(m_K(s,t))\frac{1}{\mid P-m_K(s,t) \mid} \mid D_s m_K \times D_t m_K \mid d\sigma \qquad (4.1) \\
\approx\ &\sum_{K=1}^{N_n} \sum_{j=4}^{6} \frac{1}{6} f(m_K(\rho_j))\frac{1}{\mid P-m_K(\rho_j) \mid} \mid D_s \widetilde{m}_K \times D_t \widetilde{m}_K \mid_{\rho_j}
\end{aligned}$$

where $m_K : \sigma \to \triangle_K$ is defined by the composition of m with an affine map from σ to $\widehat{\triangle}_K$. $\widetilde{m}_K$ is the quadratic interpolation of m_K. The element $\widehat{\triangle}_K$ is the pre-image under the map m_K. Note we are including the use of the approximating surface.

Lemma 4.1 Assume that $f \in C^4(S)$. Then

$$\left| \int_S f(Q) \frac{1}{\mid P - Q \mid} dS_Q \; - \sum_{K=1}^{N_n} \sum_{j=4}^{6} \widetilde{\omega}_{j,K} f(v_{j,K}) \frac{1}{\mid P - v_{j,K} \mid} \right| \leq O(\frac{1}{N_n^2}) \qquad (4.2)$$

where

$$\widetilde{\omega}_{j,K} = \frac{1}{6} \mid D_s \widetilde{m}_K \times D_t \widetilde{m}_K \mid_{\rho_j} .$$

and N_n is the total number of triangles at level n.

Proof. From Section 2.4, we know the structure of the '$4a+u$' refinement. At level $n > 1$, it divides the unit simplex into $4n-4$ regions $\widehat{B}_0, \widehat{B}_1, \ldots, \widehat{B}_{4n-5}$. The regions $\widehat{B}_l$ are as before. Each $\widehat{B}_l$ is uniformly divided, and additional facts on the '$4a+u$' refinement are also given in Section 2.4.

The analysis of the error is given in two steps. First, estimate the integration error in (4.2) contributed by B_{4n-5}, and second give the error analysis over the union of $B_0, B_1, \ldots, B_{4n-6}$. When examining the error, we need the following estimates: for $(s,t) \in \sigma$,

$$\begin{aligned} \mid D_s m_K(s,t) \times D_t m_K(s,t) \mid &= O(\widehat{\delta}_K^2) & (4.3) \\ \mid D_s \widetilde{m}_K(s,t) \times D_t \widetilde{m}_K(s,t) \mid &= O(\widehat{\delta}_K^2) & (4.4) \\ \mid D_s m_K(s,t) \times D_t m_K(s,t) \mid - \mid D_s \widetilde{m}_K(s,t) \times D_t \widetilde{m}_K(s,t) \mid &= O(\widehat{\delta}_K^4) & (4.5) \end{aligned}$$

where $\widehat{\delta}_K = diam(\widehat{\triangle}_K)$. See Chien [16].

Case 1. $\triangle_K \subset B_{4n-5}$:

The partition of $\widehat{B}_{4n-5}$ is exactly shown in Figure 6. Let $\{\widehat{\triangle}_K \mid K = 1, \ldots, 16\}$ denote the sixteen triangles in $\widehat{B}_{4n-5}$, and let $\widehat{\triangle}_1$ contain the point corresponding to P. By $\widehat{\delta}_{4n-5}$, denote the diameter of $\widehat{\triangle}_K$, $\widehat{\delta}_{4n-5} = \frac{1}{2^{n+(4n-5)}}$.

(a) We first estimate the error of

$$\left| \int_{\triangle_1} f(Q) \frac{1}{\mid P - Q \mid} dS_Q - \sum_{j=4}^{6} \widetilde{\omega}_{j,1} f(v_{j,1}) \frac{1}{\mid P - v_{j,1} \mid} \right|.$$

$$\begin{aligned}
\left| \int_{\triangle_1} f(Q) \frac{1}{\mid P - Q \mid} dS_Q \right| &\leq \int_{\sigma} \frac{\mid f(m_1(s,t)) \mid}{\mid P - m_1(s,t) \mid} \mid D_s m_1 \times D_t m_1 \mid ds\, dt \\
&\leq O(\widehat{\delta}^2_{4n-5}) \int_{\sigma} \frac{1}{\mid P - m_1(s,t) \mid} ds\, dt \\
&\leq O(\widehat{\delta}^2_{4n-5}) O(\widehat{\delta}^{-1}_{4n-5}) \\
&= O(\frac{1}{2^{5n}})
\end{aligned}$$

The third inequality is obtained in the thesis of Chien [16, p. 44]. In addition,

$$\begin{aligned}
\left| \sum_{j=4}^{6} \widetilde{\omega}_{j,1} \frac{f(v_{j,1})}{\mid P - v_{j,1} \mid} \right| &\leq O(\widehat{\delta}^2_{4n-5}) O(\widehat{\delta}^{-1}_{4n-5}) \\
&\leq O(\widehat{\delta}_{4n-5}) = O(\frac{1}{2^{5n}})
\end{aligned}$$

Therefore,

$$\left| \int_{\triangle_1} f(Q) \frac{1}{\mid P - Q \mid} dS_Q - \sum_{j=4}^{6} \widetilde{\omega}_{j,1} f(v_{j,1}) \frac{1}{\mid P - v_{j,1} \mid} \right| \leq O(\frac{1}{2^{5n}}).$$

(b) The error over $\triangle_K$ $(K = 2, \ldots, 16)$ can be obtained by using Taylor's error formula. Let

$$m_K(s,t) = m(u\widehat{v}_1 + t\widehat{v}_2 + s\widehat{v}_3) = \begin{bmatrix} x^1(u\widehat{v}_1 + t\widehat{v}_2 + s\widehat{v}_3) \\ x^2(u\widehat{v}_1 + t\widehat{v}_2 + s\widehat{v}_3) \\ x^3(u\widehat{v}_1 + t\widehat{v}_2 + s\widehat{v}_3) \end{bmatrix}$$

where $\widehat{v}_1$, $\widehat{v}_2$ and $\widehat{v}_3$ are three vertices of $\widehat{\triangle}_K$ in $\mathbf{R}^2$, and $u = 1 - s - t$, $(s,t) \in \sigma$, $x^i \in C^6(R_j)$, $i = 1,2,3$. We can write $\widehat{v}_i = (v_{i,x},\ v_{i,y})$. Hence,

$$x_s^i = \frac{\partial x^i}{\partial s} = \frac{\partial x^i}{\partial x}(v_{3,x} - v_{1,x}) + \frac{\partial x^i}{\partial y}(v_{3,y} - v_{1,y})$$

and

$$x_t^i = \frac{\partial x^i}{\partial t} = \frac{\partial x^i}{\partial x}(v_{2,x} - v_{1,x}) + \frac{\partial x^i}{\partial y}(v_{2,y} - v_{1,y}) \ .$$

Write

$$D_s m_K \times D_t m_K = \begin{bmatrix} x_s^1(s,t) \\ x_s^2(s,t) \\ x_s^3(s,t) \end{bmatrix} \times \begin{bmatrix} x_t^1(s,t) \\ x_t^2(s,t) \\ x_t^3(s,t) \end{bmatrix} = \begin{bmatrix} x_s^2(s,t)x_t^3(s,t) - x_s^3(s,t)x_t^2(s,t) \\ x_s^3(s,t)x_t^1(s,t) - x_s^1(s,t)x_t^3(s,t) \\ x_s^1(s,t)x_t^2(s,t) - x_s^2(s,t)x_t^1(s,t) \end{bmatrix}$$

$$= \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \begin{bmatrix} x_x^2 x_y^3 - x_x^3 x_y^2 \\ x_x^3 x_y^1 - x_x^1 x_y^3 \\ x_x^1 x_y^2 - x_x^2 x_y^1 \end{bmatrix}$$

where $\|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\|$ is two times the area of $\widehat{\triangle}_K$. Define

$$J(m_K(s,t)) = \begin{bmatrix} x_x^2 x_y^3 - x_x^3 x_y^2 \\ x_x^3 x_y^1 - x_x^1 x_y^3 \\ x_x^1 x_y^2 - x_x^2 x_y^1 \end{bmatrix}$$

After the above computation, we have that

$$D_s m_K \times D_t m_K = \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \cdot J(m_K(s,t))$$

and the integral in (4.1) can be expressed as

$$\int_\sigma f(m_K(s,t)) \frac{1}{\mid P - m_K(s,t) \mid} \mid D_s m_K \times D_t m_K \mid d\sigma$$

$$= \ \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \cdot \int_\sigma f(m_K(s,t)) \frac{1}{\mid P - m_K(s,t) \mid} \mid J(m_K(s,t)) \mid d\sigma$$

Let

$$h(m_K(s,t)) \ = \ f(m_K(s,t)) \frac{1}{\mid P - m_K(s,t) \mid} \mid J(m_K(s,t)) \mid \ . \tag{4.6}$$

Then h is smooth on $\triangle_K$ and $m_K : \sigma \xrightarrow[\text{onto}]{1-1} \triangle_K$ is also smooth, and we have

$$\int_\sigma f(m_K(s,t)) \frac{1}{\mid P - m_K(s,t) \mid} \mid D_s m_K \times D_t m_K \mid d\sigma$$

$$- \ \frac{1}{6} \sum_{j=4}^{6} f(m_K(\rho_j)) \frac{1}{\mid P - m_K(\rho_j) \mid} \mid D_s m_K \times D_t m_K \mid_{\rho_j}$$

$$= \ \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \cdot \int_\sigma f(m_K(s,t)) \frac{1}{\mid P - m_K(s,t) \mid} \mid J(m_K(s,t)) \mid d\sigma$$

$$- \ \frac{1}{6} \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \sum_{j=4}^{6} f(v_{j,K}) \frac{1}{\mid P - v_{j,K} \mid} \mid J(v_{j,K}) \mid$$

$$= \ \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \left[\int_\sigma h(m_K(s,t)) \, d\sigma - \frac{1}{6} \sum_{j=4}^{6} h(m_K(\rho_j)) \right]$$

$$= \ \|(\widehat{v}_3 - \widehat{v}_1) \times (\widehat{v}_2 - \widehat{v}_1)\| \int_\sigma \left[h(m_K(s,t)) - \sum_{j=1}^{6} h(m_K(\rho_j)) l_j(s,t) \right] d\sigma \tag{4.7}$$

Moreover,

$$h(m_K(s,t)) - \sum_{j=1}^{6} h(m_K(\rho_j)) l_j(s,t) = H_{h,K}(s,t;\zeta,\eta) \tag{4.8}$$

where

$$H_{h,K}(s,t;\zeta,\eta)$$

$$= \frac{1}{3!}\left[(s\frac{\partial}{\partial s}+t\frac{\partial}{\partial t})^3 h(m_K(\zeta,\eta)) - \sum_{j=1}^{6}(s_j\frac{\partial}{\partial s}+t_j\frac{\partial}{\partial t})^3 h(m_K(\zeta_j,\eta_j))l_j(s,t)\right]$$

In this, $\rho_j = (s_j,t_j)$, (ζ,η) is on the line segment from (0,0) to (s,t), and (ζ_j,η_j) is on the line segment from (0,0) to (s_j,t_j). Notice that (ζ,η) and (ζ_j,η_j) belong to σ.

We would like to examine one term in $H_{h,K}$, that associated with s^3, and it will show the general behavior of $H_{h,K}$.

$$\frac{\partial^3}{\partial s^3}h(m_K(\zeta,\eta)) = \frac{\partial^3}{\partial s^3}\left(\frac{f(m_K(s,t))}{\mid P-m_K(s,t)\mid}\mid J(m_K(s,t))\mid\right)\Bigg|_{\substack{s=\zeta\\ t=\eta}}$$

$$= f(m_K(\zeta,\eta))\mid J(m_K(\zeta,\eta))\mid \frac{\partial^3}{\partial s^3}\left(\frac{1}{\mid P-m_K(s,t)\mid}\right)\Bigg|_{\substack{s=\zeta\\ t=\eta}} \tag{4.9}$$

$$+3\left\{\frac{\partial}{\partial s}\left(f(m_K(s,t))\mid J(m_K(s,t))\mid\right)\frac{\partial^2}{\partial s^2}\left(\frac{1}{\mid P-m_K(s,t)\mid}\right)\right\}\Bigg|_{\substack{s=\zeta\\ t=\eta}} \tag{4.10}$$

$$+3\left\{\frac{\partial^2}{\partial s^2}\left(f(m_K(s,t))\mid J(m_K(s,t))\mid\right)\frac{\partial}{\partial s}\left(\frac{1}{\mid P-m_K(s,t)\mid}\right)\right\}\Bigg|_{\substack{s=\zeta\\ t=\eta}} \tag{4.11}$$

$$+\frac{1}{\mid P-m_K(s,t)\mid}\frac{\partial^3}{\partial s^3}\left(f(m_K(s,t))\mid J(m_K(s,t))\mid\right)\Bigg|_{\substack{s=\zeta\\ t=\eta}} \tag{4.12}$$

The magnitudes of (4.9), ..., (4.12) vary from $O(\frac{\widehat{\delta}^3_{4n-5}}{d_K^4})$ to $O(\frac{\widehat{\delta}^3_{4n-5}}{d_K})$, and $O(\frac{\widehat{\delta}^3_{4n-5}}{d_K^4})$ is the dominant term in (4.9), ..., (4.12), with $d_K \equiv dist(P,\triangle_K)$. It follows that the coefficient of s^3 in $H_{h,K}$ is of size $O(\frac{\widehat{\delta}^3_{4n-5}}{d_K^4})$. Consequently,

$$| H_{h,K}(s,t;\zeta,\eta) | \leq \ O(\frac{\widehat{\delta}^3_{4n-5}}{d_K^4}) \tag{4.13}$$

for any $(s,t) \in \sigma$.

Let $d_{4n-5} = \min\{d_K \mid K = 2,\ldots,16\}$. By a straightforward argument, $d_{4n-5} = O(\widehat{\delta}_{4n-5})$. Therefore,

$$\left| \int_{\triangle_K} f(Q)\frac{1}{| P - Q |}\, dS_Q - \sum_{j=4}^{6} \omega_{j,K} f(v_{j,K})\frac{1}{| P - v_{j,K} |} \right|$$

$$\begin{aligned}
&\leq \ O(\widehat{\delta}^2_{4n-5}) \int_\sigma | h(m_K(s,t)) - \sum_{j=1}^{6} h(v_{j,K}) l_j(s,t) | \, d\sigma \\
&= \ O(\widehat{\delta}^2_{4n-5}) \int_\sigma | H_{f,K}(s,t;\zeta,\eta) | \, d\sigma \\
&\leq \ O(\widehat{\delta}^2_{4n-5}) O(\frac{\widehat{\delta}^3_{4n-5}}{d^4_{4n-5}}) \\
&\leq \ O(\widehat{\delta}_{4n-5}) = O(\frac{1}{2^{5n}})
\end{aligned}$$

where

$$\omega_{j,K} = \frac{1}{6} \mid D_s m_K(s,t) \times D_t m_K(s,t) \mid_{\rho_j} .$$

This is the error from the numerical integration. The error from the approximate surface $\widetilde{m}_K$ is

$$| \sum_{j=4}^{6} \ \omega_{j,K} f(v_{j,K})\frac{1}{| P - v_{j,K} |} - \sum_{j=4}^{6} \ \widetilde{\omega}_{j,K} f(v_{j,K})\frac{1}{| P - v_{j,K} |} \ |$$

$$\begin{aligned}
&\leq \ \sum_{j=4}^{6} | \ \omega_{j,K} - \widetilde{\omega}_{j,K} \ | \ \frac{| \ f(v_{j,K}) \ |}{| \ P - v_{j,K} \ |} \\
&\leq \ O(\widehat{\delta}^4_{4n-5}) O(\frac{1}{d_K}) \\
&= \ O(\widehat{\delta}^3_{4n-5}) \ \leq \ O(\frac{1}{2^{5n}})
\end{aligned}$$

The second inequality is from (4.5). Thus the error contributed by B_{4n-5} is $O(\frac{1}{2^{5n}})$.

Case 2. $\triangle_K \subset B_l$, $l = 0, 1, \ldots, 4n-6$:

There are two types of triangles in B_l. Those triangles that are part of symmetric pairs of triangles (cf. Figure 2) are of the first type and remaining triangles are of the second type. By analysis of the '$4a+u$' refinement in Section 2.4, the number of triangles of the first type is $O(N_l)$, where N_l is the number of triangles in B_l. Then N_l is proportional to 4^{n-i}, where l is decomposed as $l = 4i + i_1$ for $0 \le i_1 < 4$.

Since h is smooth on B_l, then by Taylor's error formula we have

$$h(m_K(s,t)) - \sum_{j=1}^{6} h(m_K(\rho_j)) l_j(s,t) = H_{h,K}(s,t) + G_{h,K}(s,t;\zeta,\eta) \tag{4.14}$$

where

$$\begin{aligned} &H_{h,K}(s,t) \\ &= \frac{1}{3!}\left[(s\frac{\partial}{\partial s} + t\frac{\partial}{\partial t})^3 h(m_K(0,0)) - \sum_{j=1}^{6}(s_j\frac{\partial}{\partial s} + t_j\frac{\partial}{\partial t})^3 h(m_K(0,0)) l_j(s,t)\right] \\ &G_{h,K}(s,t;\zeta,\eta) \\ &= \frac{1}{4!}\left[(s\frac{\partial}{\partial s} + t\frac{\partial}{\partial t})^4 h(m_K(\zeta,\eta)) - \sum_{j=1}^{6}(s_j\frac{\partial}{\partial s} + t_j\frac{\partial}{\partial t})^4 h(m_K(\zeta_j,\eta_j)) l_j(s,t)\right] \end{aligned}$$

We examine (4.14) and we can find the following.

First, $H_{h,K}(s,t)$ is a polynomial of degree three. Second, the coefficients of $H_{h,K}(s,t)$ are combinations of $(\widehat{v}_{2,K} - \widehat{v}_{1,K})$ and $(\widehat{v}_{3,K} - \widehat{v}_{1,K})$. $\widehat{v}_{j,K}$'s are vertices of $\widehat{\triangle}_K$. For instance, the coefficient of s^3 is

$$\frac{1}{3!}\frac{\partial^3}{\partial s^3} h(m_K(0,0))$$

$$= \frac{1}{3!}\left[\frac{\partial^3}{\partial x^3}h(m_K(\rho_1))(v_{3K,x}-v_{1K,x})^3 + \frac{\partial^3}{\partial y^3}h(m_K(\rho_1))(v_{3K,y}-v_{1K,y})^3\right)$$

$$+ 3\,\frac{\partial^3}{\partial x^2 \partial y}h(m_K(\rho_1))(v_{3K,x}-v_{1K,x})^2(v_{3K,y}-v_{1K,y})$$

$$+ 3\,\frac{\partial^3}{\partial x \partial^2 y}h(m_K(\rho_1))(v_{3K,x}-v_{1K,x})(v_{3K,y}-v_{1K,y})^2\Bigg] \tag{4.15}$$

where $\hat{v}_{j,K} = (v_{jK,x}, v_{jK,y})$ for $j = 1,2,3$. For every symmetric pair of triangles, say $\widehat{\triangle}_1$ and $\widehat{\triangle}_2$, in $\hat{B}_l$ (see Figure 2, with $k = 1$ and $l = 2$), let

$$\begin{aligned} m_1(s,t) &= (\hat{v}_{3,1}-\hat{v}_{1,1})s + (\hat{v}_{2,1}-\hat{v}_{1,1})t + \hat{v}_{1,1} \\ m_2(s,t) &= (\hat{v}_{3,2}-\hat{v}_{1,2})s + (\hat{v}_{2,2}-\hat{v}_{1,2})t + \hat{v}_{1,2} \end{aligned}$$

Then

$$\begin{aligned} \hat{v}_{1,1}-\hat{v}_{2,1} &= -(\hat{v}_{1,2}-\hat{v}_{2,2}) \\ \hat{v}_{1,1}-\hat{v}_{3,1} &= -(\hat{v}_{1,2}-\hat{v}_{3,2})\,. \end{aligned}$$

We now have for $H_{h,1}$ and $H_{h,2}$, that the coefficient of s^3 in $H_{h,1}$ is

$$\frac{1}{3!}\left[\frac{\partial^3}{\partial x^3}h(m_1(\rho_1))(v_{31,x}-v_{11,x})^3 + \frac{\partial^3}{\partial y^3}h(m_1(\rho_1))(v_{31,y}-v_{11,y})^3\right.$$

$$+ 3\,\frac{\partial^3}{\partial x^2 \partial y}h(m_1(\rho_1))(v_{31,x}-v_{11,x})^2(v_{31,y}-v_{11,y})$$

$$\left.+ 3\,\frac{\partial^3}{\partial x \partial^2 y}h(m_1(\rho_1))(v_{31,x}-v_{11,x})(v_{31,y}-v_{11,y})^2\right] \tag{4.16}$$

and the coefficient of s^3 in $H_{h,2}$ is

$$\frac{1}{3!}\left[\frac{\partial^3}{\partial x^3}h(m_2(\rho_1))(v_{32,x}-v_{12,x})^3+\frac{\partial^3}{\partial y^3}h(m_2(\rho_1))(v_{32,y}-v_{12,y})^3\right.$$

$$+3\,\frac{\partial^3}{\partial x^2\partial y}h(m_2(\rho_1))(v_{32,x}-v_{12,x})^2(v_{32,y}-v_{12,y})$$

$$\left.+3\,\frac{\partial^3}{\partial x\partial^2 y}h(m_2(\rho_1))(v_{32,x}-v_{12,x})(v_{32,y}-v_{12,y})^2\right] \tag{4.17}$$

Adding (4.16) and (4.17) gives us zero, and an analogous argument holds for the remaining coefficients. This means that cancellation happens on any symmetric pair of triangles. It follows that

$$\left|\int_{\widehat{\triangle}_1\cup\widehat{\triangle}_2} f(Q)\frac{1}{\mid P-Q\mid}\,dS_Q-\sum_{K=1}^{2}\sum_{j=4}^{6}\omega_{j,K}f(v_{j,K})\frac{1}{\mid P-v_{j,K}\mid}\right|$$

$$\leq\;O(\widehat{\delta}_l^2)\sum_{K=1}^{2}\int_\sigma\mid G_{h,K}(s,t;\zeta,\eta)\mid ds\,dt$$

where $\widehat{\delta}_l$ is the diameter of $\widehat{\triangle}_1$ and $\widehat{\triangle}_2$. This argument is based on Chien [16].

Using a similar calculation,

$$\mid G_{h,K}(s,t;\zeta,\eta)\mid\leq O(\frac{\widehat{\delta}_l^4}{d_K^5})$$

For $\triangle_K\subset B_l$,

$$\widehat{\delta}_l=\frac{1}{2^{n+l}}$$

$$\mathrm{dist}(\rho_1,\widehat{B}_l)=O(\frac{1}{2^{5i}})$$

where ρ_1 is the origin of the unit simplex and $\widehat{B}_l$ is pre-image of B_l under the map m. Decompose l as $l=4i+i_1$ for $0\leq i_1<4$. Let

$$d_l=\min\{d_K\mid\triangle_K\subset B_l\}$$

Then $d_l=O(\frac{1}{2^{5i}})$. And the number of triangles of the first type in B_l is $O(2^{2n-2i})$.

Adding the error contributed by triangles of the first type, we have

$$\begin{aligned}
&\left| \sum_{\triangle_K\ of first\ type} \left(\int_{\triangle_K} f(Q)\frac{1}{\mid P-Q\mid} dS_Q - \sum_{j=4}^{6} \omega_{j,K} f(v_{j,K}) \frac{1}{\mid P - v_{j,K}\mid} \right) \right| \\
\leq\ & O(N_l) O(\frac{\widehat{\delta}_K^6}{d_K^5}) \leq O(2^{2n-2i}\frac{1}{2^{6n+6l}}2^{25i}) \\
\leq\ & O(2^{-4n-\frac{l}{4}}) \qquad (4.18)
\end{aligned}$$

For the remaining triangles in B_l, those of the second type, the error contributed by each of them is $O(\frac{\widehat{\delta}_K^5}{d_K^4})$. The number of triangles of the second is proportional to 2^{n-i}. Therefore,

$$\begin{aligned}
&\left| \sum_{\triangle_K\ of second\ type} \left(\int_{\triangle_K} f(Q)\frac{1}{\mid P-Q\mid}\ dS_Q - \sum_{j=4}^{6} \omega_{j,K} f(v_{j,K}) \frac{1}{\mid P - v_{j,K}\mid} \right) \right| \\
\leq\ & O(2^{n-i}\frac{1}{2^{5n+5l}}2^{20i})\ \leq O(2^{-4n-\frac{l}{4}}) \qquad (4.19)
\end{aligned}$$

Combine (4.18) and (4.19),

$$\left| \int_{B_l} f(Q)\frac{1}{\mid P-Q\mid}\ dS_Q\ - \sum_K \sum_{j=4}^{6}\ \omega_{j,K} f(v_{j,K}) \frac{1}{\mid P - v_{j,K}\mid} \right| \leq O(2^{-4n-\frac{l}{4}}) \qquad (4.20)$$

Consequently,

$$\begin{aligned}
E_1\ =\ & \sum_{l=0}^{4n-5} \left| \int_{B_l} f(Q)\frac{1}{\mid P-Q\mid} dS_Q\ - \sum_K \sum_{j=4}^{6}\ \omega_{j,K} f(v_{j,K}) \frac{1}{\mid P - v_{j,K}\mid} \right| \\
\leq\ & O(2^{-4n})
\end{aligned}$$

Next, let us consider

$$E_2 = \sum_{l=0}^{4n-5} \sum_{\substack{K \\ \triangle_K \subset B_l}} \sum_{j=4}^{6} \left(\omega_{j,K} \frac{f(m_K(\rho_j))}{\mid P - m_K(\rho_j)\mid} - \widetilde{\omega}_{j,K} \frac{f(m_K(\rho_j))}{\mid P - m_K(\rho_j)\mid} \right)$$

Define

$$e_{2,K}(s,t) = \frac{f(m_K(s,t))}{\mid P - m_K(s,t) \mid}(\mid D_s m_K(s,t) \times D_t m_K(s,t) \mid$$

$$- \quad \mid D_s \widetilde{m}_K(s,t) \times D_t \widetilde{m}_K(s,t) \mid)$$

From the argument given in [16, p. 89],

$$\sum_{j=4}^{6} e_{2,K}(\rho_j) = O(\frac{\widehat{\delta}_K^5}{d_K^2}) + O(\frac{\widehat{\delta}_K^6}{d_K^3})$$

With the usual cancellation over symmetric pairs and the discussion of the first part of this case,

$$\sum_{\substack{K \\ \triangle_K \subset B_l}} \sum_{j=4}^{6} \left(\omega_{j,K} \frac{f(m_K(\rho_j))}{\mid P - m_K(\rho_j) \mid} - \widetilde{\omega}_{j,K} \frac{f(m_K(\rho_j))}{\mid P - m_K(\rho_j) \mid} \right)$$

$$\leq \quad O(2^{2n-2i}) O(\frac{\widehat{\delta}_l^6}{d_K^3}) + O(2^{n-i}) O(\frac{\widehat{\delta}_l^5}{d_K^2})$$

$$\leq \quad O(2^{-4n-11i})$$

$$E_2 = O(\frac{1}{2^{4n}}).$$

Thus, (4.2) follows because $N_n = O(2^{2n})$. ■

The formula (4.2) implies a bound $\frac{c}{N_n^2}$ for the integration error. The constant c depends on the surface S and the integrand function f. More precisely, it depends on the maximum value of f, the maximum values of the k-th derivatives of f for $k = 1, 2, 3$ and 4, and the maximum values of m_K which are parametrizations of the surface and its k-th derivatives for $k = 1, \ldots, 5$.

We now consider the numerical evaluation of single layer integrals at the node points of a given triangulation of the surface S.

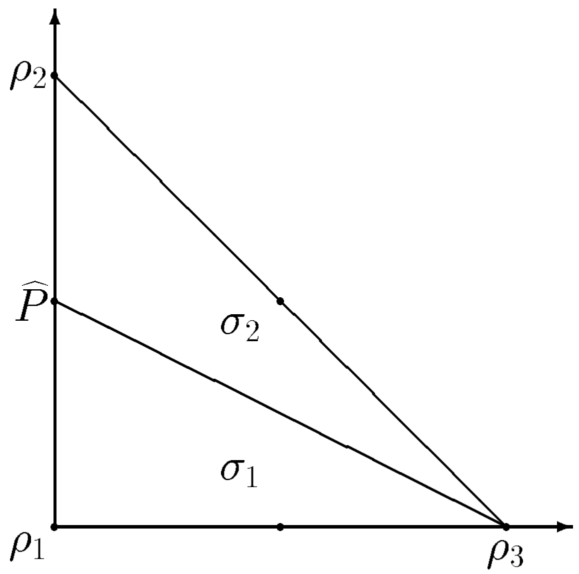


Figure 7: Splitting triangles

Theorem 4.2 Let S be a piecewise smooth surface in $\mathbf{R}^3$. Let $\{\triangle_K \mid 1 \le K \le N_0\}$ be a triangulation obtained by a uniform refinement of S. Let P be a node point on S associated with $\{\triangle_K\}$. If P is a vertex, let $\{\triangle_K\}$ be our initial triangulation of S. If P is a midpoint of a side of $\triangle_K$, split each of the triangles containing P into two triangles (see Figure 7), and let the new triangulation still be denoted by $\{\triangle_K\}$. Let $\{\triangle_{K,n} \mid 1 \le K \le N_n\}$ be the triangulation obtained by performing n loops of '$4a+u$' refinement about P on the initial given triangulation $\{\triangle_K\}$, with N_n the number of elements in $\{\triangle_{K,n}\}$. Assume that $f \in C^4(S)$. Then

$$\left| \int_S f(Q) \frac{1}{\mid P - Q \mid} dS_Q \ - \sum_{K=1}^{N_n} \sum_{j=4}^{6} \tilde{\omega}_{j,K} f(v_{j,K}) \frac{1}{\mid P - v_{j,K} \mid} \right| \le O(\frac{1}{N_n^2}) \tag{4.21}$$

Proof. The integrand in (4.21) varies from singular to quite smooth. To handle this varied behavior, we classify triangles in the initial triangulation $\{\triangle_K\}$ into two groups. Let T_1 be the collection of triangles $\triangle_K$ containing P, let T_2 be the collection of triangles $\triangle_K$ with $P \notin \triangle_K$. Let E_i denote the error contributed by T_i for $i = 1, 2$.

1) Since the number of triangles $\triangle_K$ in T_1 is finite, in fact, at most 6, and the error contributed by each triangle $\triangle_K$ is $O(\frac{1}{N_n^2})$ by 4.1. Then $E_1 = O(\frac{1}{N_n^2})$.

2) Triangles in T_2 form a quasi-uniform refinement and are away from the point P with a fixed distance or greater. By Corollary 4.5 in Chien's thesis [16], we have $E_2 = O(\widehat{\delta}_n^4)$ where $\widehat{\delta}_n$ is the mesh size of $\{\widehat{\triangle}_{K,n}\}$ corresponding to T_2. Since $\widehat{\delta}_n = O(\frac{1}{2^n})$, $N_n = O(2^{2n})$. Therefore, $E_2 = O(\frac{1}{N_n^2})$. ∎

4.3 Error analysis for double layer integrals

An analogous result holds for the double layer integrals over smooth surfaces. Using the triangulation scheme in Section 4.2, the double layer integral can be written as

$$\begin{aligned}
&\int_S f(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q \\
= \; & \sum_{K=1}^{N_n} \int_{\triangle_{K,n}} f(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q \\
= \; & \sum_{K=1}^{N_n} \int_{\sigma} f(m_K(s,t)) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - m_K(s,t) \mid} \right] \mid D_s m_K \times D_t m_K \mid \, d\sigma \quad (4.22)
\end{aligned}$$

For $Q = m_K(s,t)$,

$$\nu(s,t) = \nu_Q = \pm \frac{D_s m_K \times D_t m_K}{\mid D_s m_K \times D_t m_K \mid}$$

with the sign chosen so that ν_Q points into the bounded domain D.

Without loss of generality, we assume the sign of ν_Q is always positive, and (4.22) then becomes

$$
\begin{aligned}
&\int_S f(Q) \frac{\partial}{\partial \nu_Q} \left[\frac{1}{\mid P - Q \mid} \right] dS_Q \\
= \quad & \sum_{K=1}^{N_n} \int_\sigma f(m_K(s,\,t)) \frac{(P - m_K(s,\,t)) \cdot (D_s m_K \times D_t m_K)}{\mid P - m_K(s,\,t) \mid^3}\, d\sigma \\
\approx \quad & \sum_{K=1}^{N_n} \sum_{j=4}^{6} \frac{1}{6} f(m_K(\rho_j)) \frac{(P - m_K(\rho_j)) \cdot (D_s m_K \times D_t m_K) \mid_{\rho_j}}{\mid P - m_K(\rho_j) \mid^3}
\end{aligned}
\tag{4.23}
$$

Using the fact that if P and $m_K(s,t)$ are close enough, then

$$
\mid \cos\theta \mid \leq \text{constant} \cdot \mid P - m_K(s,t) \mid \tag{4.24}
$$

where θ is the angle between the vectors $(D_s m_K(s,t) \times D_t m_K(s,t))$ and $(P - m_K(s,t))$. See Mikhlin [37, p. 349]. The singularity of the integrand in (4.22) is $O(\mid P - Q \mid^{-1})$ as $Q \to P$. We can follow the same form of the proof as in Theorem 4.2, with Corollary 4.7 from [16] used to bound E_2, to show the error for evaluating the double layer integral at any node point is $O(\frac{1}{N_n^2})$.

Theorem 4.3 Let S be a smooth surface in $\mathbf{R}^3$. Assume that $\{\triangle_K\}$, P, $\{\triangle_{K,n}\}$, f, N_n are as in Theorem 4.2. Then

$$
\begin{aligned}
&\Bigg| \int_S f(Q) \frac{\partial}{\partial \nu_Q} \left(\frac{1}{\mid P - Q \mid} \right) dS_Q \\
&\quad - \sum_{K=1}^{N_n} \sum_{j=4}^{6} \frac{1}{6} f(v_{j,K}) \frac{(P - v_{j,K}) \cdot (D_s \widetilde{m}_K \times D_t \widetilde{m}_K) \mid_{\rho_j}}{\mid P - v_{j,K} \mid^3} \Bigg| = O(\frac{1}{N_n^2})
\end{aligned}
\tag{4.25}
$$

For piecewise smooth surfaces with a given triangulation $\{\triangle_K\}$, a triangle $\triangle_K$ in the triangulation either contains the node point P, or its distance from P is greater than some positive number. Therefore, the integration error E_2 contributed by those triangles in T_2, as defined before, is $O(\frac{1}{N_n^2})$. To estimate the error E_1, it is suffice to consider the error contributed by one triangle containing P. No matter where the node point P is, such a triangle, say $\triangle_K$, is always a smooth portion of the surface. Locally we can apply (4.24) to the integrand and reduce the degree of singularity to -1. Then using the analysis given in Theorem 4.2, we have

Theorem 4.4 Assume that S is a piecewise smooth surface in $\mathbf{R}^3$. Then the error formula (4.25) holds.

4.4 Numerical examples

Two smooth surfaces were used in our experiments. Surface #1 (denoted by $S\#1$) was the ellipsoid

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

with $a, b, c > 0$.

The ellipsoid is convex and symmetric. For that reason, we also devised and used a surface which is not symmetric and which is slightly non-convex. Surface #2 ($S\#2$) is defined by

$$(x, y, z) = \rho(\xi, \eta, \zeta)(A\xi, B\eta, C\zeta), \qquad \xi^2 + \eta^2 + \zeta^2 = 1$$

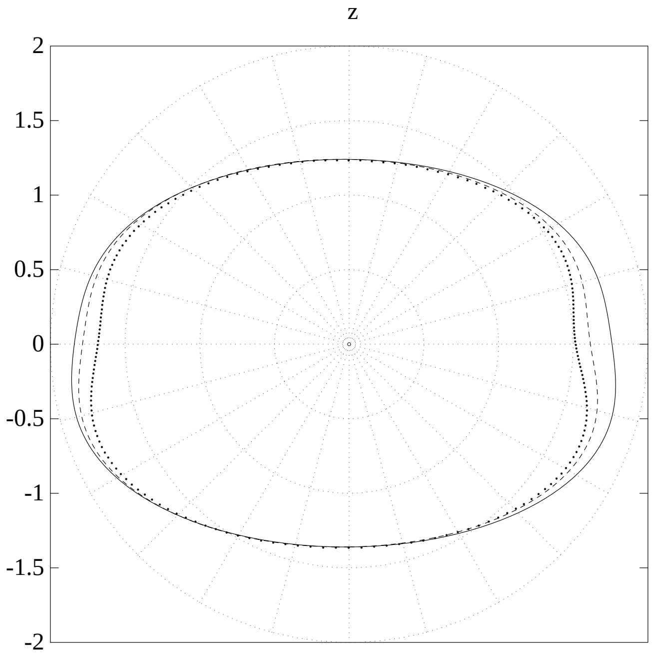
with

$$\rho(\xi, \eta, \zeta) = 1 - [(\xi - .1)^2 + 2(\eta - .1)^2 - 3(\zeta - .1)^2]/\alpha$$

and $A,\ B,\ C > 0$, $\alpha \geq 5$. The case we use here is $\alpha = 10$ and $(A, B, C) = (2, 2, 1)$. Figure 8 gives the cross-sections of $S\#2$ when intersecting S with vertical planes containing the z-axis, intersecting at angles of $\phi = 0,\ \pi/4,\ \pi/2$ with respect to the positive x-axis.

We approximate the solid angle

$$\Omega(P) \;=\; \int_S \frac{\partial}{\partial \nu_Q}\left[\frac{1}{\mid P - Q \mid}\right] dS_Q\,, \qquad P \in S \tag{4.26}$$



solid curve: $\phi = 0$, dash curve: $\phi = \pi/4$, dot curve: $\phi = \pi/2$

Figure 8: Cross sections of "squash" surface

using the method analyzed in Section 4.3. The expression on the right hand side of (4.26) is the double layer integral with $f(P) \equiv 1$. For a smooth surface S, the solid angle $\Omega(P) = 2\pi$ at all points $P \in S$.

The parameters for the surface $S\#1$ are $(a, b, c) = (2, 2.5, 3)$. We initially divide the surface into eight triangular elements. Each of these elements is a portion of the surface within one octant. The approximate values of the solid angle for $S\#1$ are given in Table 7 at the following representative nodes.

$$v_1 = (0, 0, 3), \quad v_2 = (2, 0, 0), \quad v_3 = (0, 2.5, 0)$$
$$v_7 = (\sqrt{2}, 0, \sqrt{4.5}), \quad v_8 = (\sqrt{2}, \sqrt{3.125}, 0), \quad v_9 = (0, \sqrt{3.125}, \sqrt{4.5})$$

The subscripts refer to the indexing of node points used in our triangulation package.

The first three nodes are vertices and last three points are midpoints corresponding to the initial triangulation. The column labeled *Order* again gives the value

$$p_n = \frac{\ln |E_n/E_{n+1}|}{\ln(N_{n+1}/N_n)}$$

where E_n is the error at level n of '$4a+u$' refinement. The empirical rate of convergence is approximately $O(\frac{1}{N_n^2})$, equivalently, $p_n \to 2$.

i	E_1	E_2	E_3	E_4	E_5
1	2.11	2.97E−2	3.61E−4	−2.03E−5	−2.59E−6
2	1.64	3.99E−2	1.94E−3	1.01E−4	5.63E−6
3	1.71	2.27E−2	3.25E−4	−2.54E−6	−9.10E−7
7	2.64	6.43E−1	1.60E−2	4.35E−4	9.53E−6
8	2.65	4.97E−1	1.29E−2	3.69E−4	5.57E−6
9	2.96	9.68E−1	2.41E−2	6.72E−4	1.35E−5
i	p_1	p_2	p_3	p_4	
1	1.28	2.79	2.02	1.48	
2	1.12	1.92	2.07	2.07	
3	1.30	2.69	3.40	0.74	
7	1.02	1.44	2.33	2.69	
8	1.21	1.43	2.30	2.57	
9	0.81	1.44	2.32	2.75	

Table 7: Solid angle approximation on an ellipsoid at selected v_i

Similar results for the approximate solid angle are true for $S\#2$. See Table 8. The approximate values of the solid angle are given at the following representative nodes.

$v_1 = (0, 0, 1.24)$, $v_2 = (1.84, 0, 0)$, $v_3 = (0, 1.68, 0)$

$v_7 = (1.5156, 0, 0.7578)$, $v_8 = (1.2621, 1.2621, 0)$, $v_9 = (0, 1.4649, 0.7325)$

i	E_1	E_2	E_3	E_4	E_5
1	2.41	6.32E−2	3.65E−3	2.17E−4	1.29E−5
2	−7.63E−1	2.72E−2	−1.04E−4	−2.06E−5	−2.00E−6
3	−2.02	1.80E−2	8.95E−5	2.98E−6	−2.17E−7
7	2.95	9.02E−1	1.76E−2	4.86E−4	1.14E−5
8	2.43	1.76E−1	1.03E−2	3.40E−5	−3.62E−6
9	2.84	8.93E−1	1.68E−2	4.65E−4	1.04E−5
i	p_1	p_2	p_3	p_4	
1	1.10	1.81	1.98	2.02	
2	1.06	3.41	1.14	1.67	
3	1.42	3.36	2.38	1.88	
7	0.86	1.54	2.32	2.64	
8	1.90	1.11	3.70	1.58	
9	0.84	1.55	2.32	2.67	

Table 8: Solid angle approximation on a “squash” surface at selected v_i

Below we give examples for piecewise smooth surfaces. We again use the numerical integration method (4.25) to approximate the interior angle $\Omega(v)$ at points $v \in S$. We describe two piecewise smooth surfaces. Surface #3 (S#3) is an elliptical paraboloid with a cap

$$\begin{aligned} \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 &= z, \qquad 0 \le z \le c \\ \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 &\le c, \qquad z = c \end{aligned}$$

where $a, b, c > 0$. Surface #4 (S#4) is an "L-block", described as follows. Define

$$L_0 = [0,1] \times [0,2] \cup [0,2] \times [0,1] \subset \mathbf{R}^2$$

$$D_0 = [0,1] \times L_0 \subset \mathbf{R}^3$$

$$D = \{(ax, by, cz) \mid (x,y,z) \in D_0\}$$

where $a, b, c > 0$. Let S be the boundary of D.

Results for the elliptical paraboloid are given in Table 9 at the following representative nodes.

$$\begin{array}{lll} v_1 = (0,0,0), & v_2 = (2,0,1), & v_6 = (0,0,1) \\ v_7 = (1,0,.25), & v_8 = (\sqrt{2},\sqrt{2},1), & v_{15} = (1,0,1) \end{array}$$

The parameters for the surface are $(a,b,c) = (2,2,1)$. In this case the number of triangles in the initial triangulation is 32. In Table 9, *Order* and E_n are as before. The empirical rate of convergence is approximately $O(\frac{1}{N_n^2})$. Since the representative nodes are from the coarsest triangulation of S, they are either on the edge or away from the edge. The pattern to the rate at which the error decreases agrees with the theoretical result.

The results for a polyhedral surface were much better. Table 10 contains results for the L-block at the following representative nodes.

$$\begin{aligned} &v_1 = (0,0,0), && v_7 = (0,0,1), && v_9 = (0,1,1) \\ &v_{17} = (.5,0,1.5), && v_{20} = (.5,0,1), && v_{33} = (.5,1,1) \end{aligned} \tag{4.27}$$

The parameters for the surface are $(a,b,c) = (1,1,1)$. Initially we divide the surface into 112 triangles. There is no approximation of the surface in this case, and thus all error are due to the numerical integration being used. In addition, there are no singular integrals, as the double layer kernel function $\kappa(P,Q)$ is identically zero when P and Q belong to the same planar surface. The resulting errors are very small.

When compared with the numerical results given in [12], our method for evaluating the solid angles of the piecewise smooth surfaces shows a regular pattern to the rate at which the error decreases. For smooth surfaces, this numerical integration scheme also gives the better approximation in the sense that the errors decrease faster than those produced by the similar method in [12].

i	$\Omega(v_i)$	E_1	E_2	E_3	E_4	E_5
1	2π	4.52E−1	1.75E−2	7.38E−4	3.50E−5	1.84E−6
2	$\pi/2$	3.09E−2	−8.54E−4	−2.75E−4	−2.46E−5	−1.83E−6
6	2π	2.19E−1	3.46E−2	3.76E−3	3.48E−4	2.92E−5
7	2π	6.07E−1	1.07E−2	−7.94E−5	−2.56E−5	−2.75E−6
8	$\pi/2$	1.88E−1	3.36E−3	3.35E−5	−4.26E−6	−5.32E−7
15	2π	−2.37E−1	−1.32E−2	−6.33E−4	−4.78E−5	−3.50E−6
i		p_1	p_2	p_3	p_4	
1		1.41	2.08	2.15	2.12	
2		1.56	0.75	1.71	1.87	
6		0.80	1.46	1.68	1.78	
7		1.58	3.17	0.80	1.60	
8		1.57	2.98	1.45	1.49	
15		1.13	1.97	1.82	1.88	

Table 9: Solid angle approximation on an elliptical paraboloid at selected v_i

i	$\Omega(v_i)$	E_1	E_2	E_3	E_4	E_5
1	$\pi/2$	$-7.79\text{E}{-5}$	$-5.14\text{E}{-6}$	$-3.18\text{E}{-7}$	$-1.98\text{E}{-8}$	$-1.24\text{E}{-9}$
7	π	$2.02\text{E}{-4}$	$9.51\text{E}{-6}$	$5.81\text{E}{-7}$	$3.61\text{E}{-8}$	$2.25\text{E}{-9}$
9	$3\pi/2$	$4.82\text{E}{-4}$	$2.42\text{E}{-5}$	$1.48\text{E}{-6}$	$9.19\text{E}{-8}$	$5.74\text{E}{-9}$
17	2π	$2.26\text{E}{-2}$	$1.41\text{E}{-4}$	$5.66\text{E}{-6}$	$3.47\text{E}{-7}$	$2.16\text{E}{-8}$
20	2π	$1.71\text{E}{-2}$	$5.25\text{E}{-5}$	$1.47\text{E}{-6}$	$9.22\text{E}{-8}$	$5.77\text{E}{-9}$
33	3π	$2.62\text{E}{-2}$	$1.07\text{E}{-4}$	$4.00\text{E}{-6}$	$2.51\text{E}{-7}$	$1.57\text{E}{-8}$
i		p_1	p_2	p_3	p_4	
1		1.56	1.91	1.98	2.00	
7		1.63	1.89	1.98	2.00	
9		1.50	1.87	1.97	2.00	
17		2.79	2.18	1.98	2.00	
20		3.08	2.42	1.97	1.99	
33		2.92	2.23	1.97	1.99	

Table 10: Solid angle approximation on an L-block at selected v_i

CHAPTER V

THE COLLOCATION METHOD

5.1 Introduction

This chapter is devoted to numerical methods for boundary integral equations. We consider the numerical solution of boundary integral equations of the second kind for solving Laplace's equation $\Delta u = 0$ on connected regions D in $\mathbf{R}^3$. The collocation method with piecewise quadratic approximations is the numerical method being used. Atkinson and Chien [12] have analyzed the collocation method with piecewise quadratic interpolation for both the surface S and unknown solution ρ. Superconvergence results for the approximate solutions were shown for the smooth surface case.

The aim of this chapter is to analyze a corresponding discrete collocation method based on the numerical scheme introduced in Chapter 4. The main result is that the superconvergence result of [12] is still valid for the discrete collocation method when a proper integration scheme is chosen. It is given for the boundary integral equations associated with the interior Dirichlet problem and the exterior Neumann problem.

Following the discussion in Section 2.3, the integral equations (2.2) and (2.5) are different only in their right hand inhomogeneous term. With (2.5), we can study the error in the numerical solution of the integral equation by using problems for which we know the true solution of (2.4). With equation (2.2), we do not know the true solution in general (except when $f \equiv 1$); and thus the numerical solution must be checked indirectly by evaluating (2.1) numerically and comparing it to a known solution u. Our numerical examples are given for the exterior Neumann problem.

5.2 The collocation method

Any collocation method for solving an integral equation $(\lambda + \mathcal{K})\rho = g$ can be written as

$$(\lambda + \mathcal{P}_N\mathcal{K})\rho_n = \mathcal{P}_N g\,, \qquad \lambda = 2\pi \tag{5.1}$$

The function g can be the function f of (2.2) or $\mathcal{S}f$ of (2.5). For our work, the operator $\mathcal{P}_N$ is the projection operator defined by (2.15). We discuss results for this approximation; and then in the next section, we give error results for the discrete collocation method which is based on the numerical integration scheme given in Chapter 4.

For S smooth, the solvability of (5.1) is determined from the standard theory for projection methods given in Section 2.3. With (a) compactness for $\mathcal{K} : C(S) \to C(S)$, and (b) pointwise convergence on $C(S)$ of the projections $\mathcal{P}_N$ to I (by Theorem 2.6), we have that

$$\|(I - \mathcal{P}_N)\mathcal{K}\| \to 0 \quad \text{as} \quad n \to \infty$$

Together with Theorem 2.4, we have that if $(\lambda + \mathcal{K})^{-1}$ exists on $C(S)$, then $(\lambda + \mathcal{P}_N\mathcal{K})^{-1}$ exists and is uniformly bounded for all sufficiently large N, say $N \geq N_0$.

In [12], Atkinson and Chien considered the iterated collocation solution

$$\hat{\rho}_n = \frac{1}{\lambda}(g - \mathcal{K}\rho_n)$$

It satisfies the equations

$$(\lambda + \mathcal{K}\mathcal{P}_N)\hat{\rho}_n \;=\; g \tag{5.2}$$

$$\mathcal{P}_N\hat{\rho}_n \;=\; \rho_n \tag{5.3}$$

The questions of stability for (5.1) and (5.2) are linked by the identities

$$(\lambda + \mathcal{K}\mathcal{P}_N)^{-1} = \frac{1}{\lambda}[I - \mathcal{K}(\lambda + \mathcal{P}_N\mathcal{K})^{-1}\mathcal{P}_N] \tag{5.4}$$

$$(\lambda + \mathcal{P}_N\mathcal{K})^{-1} = \frac{1}{\lambda}[I - \mathcal{P}_N(\lambda + \mathcal{K}\mathcal{P}_N)^{-1}\mathcal{K}] \tag{5.5}$$

The existence of uniform boundedness of $(\lambda + \mathcal{K}\mathcal{P}_N)^{-1}$ then follows from (5.4).

For the errors in ρ_n and $\hat{\rho}_n$, use

$$\rho - \rho_n = \lambda(\lambda + \mathcal{P}_N\mathcal{K})^{-1}(\rho - \mathcal{P}_N\rho)$$

$$\rho - \hat{\rho}_n = -(\lambda + \mathcal{K}\mathcal{P}_N)^{-1}\mathcal{K}(\rho - \mathcal{P}_N\rho)$$

The quantity $\mathcal{K}(\rho - \mathcal{P}_N\rho)$ sometimes converges to zero more rapidly than does $\rho - \mathcal{P}_N\rho$. Using (5.3), this will show that ρ_n is superconvergent to ρ at the collocation node points, and we will make use of this in the following sections.

Theorem 5.1 Consider the integral equation (2.2) and (2.5) with solution ρ. Let S be a smooth surface in $\mathbf{R}^3$, and assume the unknown function $\rho \in C^4(S)$. Then

$$\max_{1 \le i \le N_v} \mid \rho(v_i) - \rho_n(v_i) \mid = O\left(\widehat{\delta}_n^4 \ln \widehat{\delta}_n\right) \tag{5.6}$$

where $\widehat{\delta}_n$ is the mesh size of the triangulation $\{\widehat{\triangle}_{K,n} \mid 1 \le K \le N_n\}$ of the R_j's obtained by the quasi-uniform refinement. The set $\{v_i \mid 1 \le i \le N_v\}$ is the collection of the node points of the triangulation $\{\triangle_{K,n}\}$ with N_v the number of distinct node points.

Proof. See [12]. ∎

5.3 A discrete collocation method

The linear system for (5.2) becomes

$$2\pi\hat{\rho}_n(v_i) + \sum_{K=1}^{N_n}\sum_{j=1}^{6}\hat{\rho}_n(v_{j,K})\int_\sigma \kappa(v_i, m_K(s,t))l_j(s,t) \mid D_s m_K \times D_t m_K \mid d\sigma$$

$$= \quad g(v_i)\,, \qquad i = 1, \ldots . N_v\,. \tag{5.7}$$

where $\kappa(P,Q)$ denotes the kernel function for the double layer integral operator. The collocation integrals in the matrix of coefficients of (5.7) are given by

$$\int_\sigma \kappa(v_i, m_K(s,t))l_j(s,t) \mid D_s m_K \times D_t m_K \mid d\sigma \tag{5.8}$$

and these must be evaluated numerically for $i = 1, \ldots, N_v$, $j = 1, \ldots, 6$, and $K = 1, \ldots, N_n$. For the exterior Neumann problem, we also need to evaluate the corresponding single layer integrals

$$\int_\sigma \frac{f(m_K(s,t))}{\mid v_i - m_K(s,t) \mid} \mid D_s m_K \times D_t m_K \mid d\sigma \tag{5.9}$$

We consider two cases in evaluating (5.8), depending on whether v_i is inside or outside of $\triangle_{K,n}$. The numerical integration method being used is (3.4). We also use the approximate surface $\widetilde{m}_K$. The following scheme is based on the error analyses in Chapter 4.

If $v_i \in \triangle_{K,n}$, then $\kappa(v_i, Q)$ is singular. We use the '$4a+u$' refinement to further divide the element $\triangle_{K,n}$. Assuming the collocation node v_i is a vertex, say $v_i = m_K(0,0)$. We perform n loops of '$4a+u$' refinement about $(0,0)$ on σ, then integrate (5.8) with (3.6) applied to the integral over each of the corresponding subintegrals. If the collocation node v_i is a midpoint of a side, then we divide $\triangle_{K,n}$ into two parts as in Theorem 4.2 and treat the integral over each part as described above.

For $v_i \notin \triangle_{K,n}$, the integrand in (5.8) is analytic; but it is increasingly peaked as the distance between v_i and $\triangle_{K,n}$ decreases. The analysis in Chapter 4 suggested using (3.6) with n levels of quasi-uniform refinement. In fact, it is sufficient to integrate (5.8) using lower levels of quasi-uniform refinement with the needed accuracy when $\triangle_{K,n}$ is far away from the point v_i. Since the triangulation for the collocation method becomes finer as n increases. We do it in the following way.

If

$$0 < dist(v_i, \triangle_{K,n}) \leq (2-1)\delta_n\,,$$

where δ_n is the mesh size of $\{\triangle_{K,n}\}$ as defined in (2.12), then integrate (5.8) using (3.6) with n levels of uniform subdivision of $\triangle_{K,n}$ [thus dividing $\triangle_{K,n}$ into 4^n congruent subtriangles, with (3.6) applied to the integral over each of the corresponding subintegrals]. If $v_i \notin \triangle_{K,n}$ and

$$(2-1)\delta_n < dist(v_i, \triangle_{K,n}) \leq (2^2-1)\delta_n\,,$$

then integrate (5.8) using (3.6) with $\max\{n-1, 1\}$ levels of uniform subdivision of $\triangle_{K,n}$. If $v_i \notin \triangle_{K,n}$ and

$$(2^2-1)\delta_n < dist(v_i, \triangle_{K,n}) \leq (2^3-1)\delta_n\,,$$

then integrate (5.8) using (3.6) with $\max\{n-2, 1\}$ levels of uniform subdivision of $\triangle_{K,n}$. Continue with this in the obvious way. This method of numerical integration for $v_i \notin \triangle_{K,n}$ was suggested in [12], without analysis.

Consider the error from evaluating (5.8) and (5.9) over S associated with the resulting triangulation. We have found that it is $O(\widehat{\delta}_n^4)$. The argument is more complicated than the one used in Theorem 4.2, because many more triangles are within a small distance of the point v_i. Let T_i, E_i $(i = 1, 2)$ be as defined before. Then the error bounds for E_1 can be obtained in the same way as for Theorem 4.2

because each triangle in T_1 is divided by n loops of '$4a+u$' refinement about v_i.

For the error from T_2, the collection of triangles not containing v_i, we note that the size of triangles in T_2 varies. The triangle becomes larger as the distance from v_i increases. We examine the structure of T_2 based on the triangulation $\triangle_{K,n}$. Define

$$\begin{aligned} d_n &= \min_K \{d_{K,n} \mid d_{K,n} > 0\} \\ d_{K,n} &= dist(v_i, \triangle_{K,n}) \\ \widehat{\delta}_n &= \text{the mesh size of } \{\widehat{\triangle}_{K,n}\} \end{aligned} \tag{5.10}$$

Then $d_n = O(\widehat{\delta}_n)$ and $\widehat{\delta}_n = O(\frac{\widehat{\delta}}{2^n})$, with $\widehat{\delta}$ the mesh size of the original parametrization domains $\{R_j\text{'s}\}$. For simplicity, we take $d_{K,n} \doteq d_n, 2d_n, \ldots$, depending on how far the $\triangle_{K,n}$ is from the point v_i. And the number of $\triangle_{K,n}$ at distance $i \cdot d_n$ is proportional to i. Define

$$A_m^{(n)} = \{\triangle_{K,n} \mid (2^m - 1) \cdot d_n \le d_{K,n} < (2^{m+1} - 1) \cdot d_n\}$$

for $m = 1, 2, \ldots, m(n)$. The value of $m(n)$ is at most n because we only consider triangles near the node point v_i. With the refinement we used, we know that each triangle in $A_m^{(n)}$ is divided into 4^{n-m} subtriangles uniformly. Denote triangles in $A_m^{(n)}$ by $\triangle^*_{K,n}$.

Define

$$A_{mj}^{(n)} = \{\triangle^*_{K,n} \subset A_m^{(n)} \mid$$
$$(2^m - 1) \cdot d_n + j \frac{\widehat{\delta}_n}{2^{n-m}} \le dist(v_i, \triangle^*_{K,n}) < (2^m - 1) \cdot d_n + (j+1) \frac{\widehat{\delta}_n}{2^{n-m}}\}$$
$$j = 0, 1, \ldots, t_m - 1.$$

where $t_m \leq O(2^n)$ because $d_n = O(\widehat{\delta}_n)$. Let c_{mj}, c'_{mj} be the numbers of triangles of the first type and the second type at distance $(2^m - 1)\cdot d_n + j\frac{\widehat{\delta}_n}{2^{n-m}}$, respectively. Then $c_{mj} = O(2^m 2^{n-m}) = O(2^n)$, $c'_{mj} = O(1)$. In addition, $\widehat{\delta}^*_{K,n}$, the mesh size of $A^{(n)}_{mj}$, is $\frac{\widehat{\delta}_n}{2^{n-m}}$. Let $d^*_{K,n} \equiv dist(v_i, \triangle^*_{K,n})$, $d^*_{K,n} \geq (2^m - 1)\cdot d_n + j\frac{\widehat{\delta}_n}{2^{n-m}}$ for triangles $\triangle^*_{K,n} \subset A^{(n)}_{mj}$.

The error from the numerical integration over triangles of the first type in $A^{(n)}_m$ is bounded by

$$\begin{aligned}
\sum_{j=0}^{t_m-1} O(2^n) O\left(\frac{\widehat{\delta}^{*\,6}_{K,n}}{d^{*\,5}_{K,n}}\right) &\leq \sum_{j=0}^{t_m-1} O(2^n) O\left(\left[\frac{\widehat{\delta}_n}{2^{n-m}}\right]^6 \frac{1}{\left[(2^m-1)\cdot d_n + j\frac{\widehat{\delta}_n}{2^{n-m}}\right]^5}\right) \\
&\leq \sum_{j=0}^{t_m-1} O\left(\frac{\widehat{\delta}^6_n}{2^{6n-6m}} \frac{1}{(2^m-1)^5 \cdot d_n^5}\right) \\
&\leq \sum_{j=0}^{t_m-1} O\left(\widehat{\delta}_n \frac{1}{2^{6n-6m}} \frac{1}{2^{5m}}\right) \\
&\leq O(2^n) O(2^n) O\left(\frac{1}{2^n} \frac{1}{2^{6n-6m}} \frac{1}{2^{5m}}\right) \\
&= O\left(\frac{1}{2^{4n}} \frac{1}{2^{n-m}}\right)
\end{aligned}$$

The error from the numerical integration over triangles of the second type in $A^{(n)}_m$ is bounded by

$$\begin{aligned}
\sum_{j=0}^{t_m-1} O(1) O\left(\frac{\widehat{\delta}^{*\,5}_{K,n}}{d^{*\,4}_{K,n}}\right) &\leq \sum_{j=0}^{t_m-1} O(2^n) O\left(\left[\frac{\widehat{\delta}_n}{2^{n-m}}\right]^5 \frac{1}{\left[(2^m-1)\cdot d_n + j\frac{\widehat{\delta}_n}{2^{n-m}}\right]^4}\right) \\
&\leq \sum_{j=0}^{t_m-1} O\left(\widehat{\delta}_n \frac{1}{2^{5n-5m}} \frac{1}{2^{4m}}\right)
\end{aligned}$$

$$\leq \quad O(2^n)O(\frac{1}{2^n}\frac{1}{2^{5n-m}}) \;=\; O(\frac{1}{2^{4n}}\frac{1}{2^{n-m}})$$

Consequently, the error from $A_m^{(n)}$ is $O(\frac{1}{2^{4n}}\frac{1}{2^{n-m}})$.

The error from the numerical integration over T_2 is bounded by

$$\sum_{m=1}^{n} O(\frac{1}{2^{4n}}\frac{1}{2^{n-m}}) = O(\frac{1}{2^{4n}}) = O(\widehat{\delta}_n^4)$$

By a similar calculation, we can show that the error from the approximate surface $\widetilde{m}$ over T_2 is also $O(\frac{1}{2^{4n}}) = O(\widehat{\delta}_n^4)$.

Combining the above error analysis, we give the global error for the single layer and double layer integrals in the following theorem.

Theorem 5.2 Let S, $\{\triangle_{K,n}\}$, $\{v_i\}$, $\widehat{\delta}_n$ be as in Theorem 5.1. Assume $f \in C^4(S)$. Let $\widetilde{\mathcal{S}}_n(f)$, $\widetilde{\mathcal{D}}_n(f)$ be the numerical integration associated with the scheme given in this section for the single layer integral and double layer integral, respectively. Then

$$\max_{1\leq i\leq N_v}\left|\int_S \frac{f(Q)}{\mid v_i - Q\mid} dS_Q - \widetilde{\mathcal{S}}_n(f)\right| \;=\; O(\widehat{\delta}_n^4) \tag{5.11}$$

$$\max_{1\leq i\leq N_v}\left|\int_S f(Q)\frac{\partial}{\partial \nu_Q}\left[\frac{1}{\mid v_i - Q\mid}\right] dS_Q - \widetilde{\mathcal{D}}_n(f)\right| \;=\; O(\widehat{\delta}_n^4) \tag{5.12}$$

The method being used has retained the rate of convergence that is true with uniform meshes for smooth integrands. Nonetheless, the integration of (5.8) and (5.9) are still the most expensive parts of our computation. Several methods have been tried for evaluating (5.8) and (5.9). Besides the method suggested in Atkinson and Chien [12], a method with automatic error control could be based on what was described in Atkinson [7] and [10]. Numerical quadratures with no approximation of the surface was presented in Guermond and Fontaine [30] and Guermond [31]. But we believe our method is easier to implement and gives a better approximation.

With the preceding numerical integration scheme, we have obtained a discrete collocation method corresponding to (5.7). The resulting linear system is denoted by

$$(2\pi I + \widetilde{K}_N)\widetilde{\rho}_n \;=\; \widetilde{g}_n \tag{5.13}$$

with

$$\begin{aligned} \widetilde{\rho}_{n,i} \;&\equiv\; \widetilde{\rho}_n(v_i)\,, \qquad\qquad i = 1,\ldots,N_v\,, \\ \widetilde{g}_{n,i} \;&\equiv\; \begin{cases} f_n(v_i) & \text{if } \; g = f \\ \widetilde{\mathcal{S}}_n(f)(v_i) & \text{if } \; g = \mathcal{S}f \end{cases} \end{aligned}$$

where $\widetilde{\mathcal{S}}_n(f)(v_i)$ is the preceding numerical integration for the single layer integral at $P = v_i$. We call $\widetilde{\rho}_n$ the discrete collocation solution, and it is more explicitly computable than ρ_n or $\hat{\rho}_n$.

The error analyses of layer potentials help us establish the rate of convergence of the discrete collocation method.

Theorem 5.3 Consider the integral equations (2.2) and (2.5) with solution ρ. Let S be a smooth surface in $\mathbf{R}^3$, and assume the unknown function $\rho \in C^4(S)$. Then

$$\max_{1\leq i\leq N_v} \mid \rho(v_i) - \widetilde{\rho}_n(v_i) \mid = \; O(\widehat{\delta}_n^4 \ln \widehat{\delta}_n) \tag{5.14}$$

Proof. We use a perturbation analysis, based on regarding the system (5.13) as a perturbation of the corresponding linear system

$$(2\pi I + K_N)\rho_n \;=\; g_n \tag{5.15}$$

where $g_n = (g(v_i))$, for the projection method analyzed in Theorem 5.1 which used the exact surface S. As noted earlier following (5.4), $(2\pi + \mathcal{K}\mathcal{P}_N)^{-1}$ is uniformly bounded for all sufficiently large N. Also, since the iterated collocation equation can be considered as being a Nyström method, we have that $(2\pi I + K_N)^{-1}$ exists by Theorem 2.8. Moreover, we can bound $\|(2\pi I + K_N)^{-1}\|$ in terms of c by following a standard derivation.

For any $G \in \mathbf{R}^{N_v}$ with N_v the number of node points, we choose a function $g \in C(S)$ with

$$g(v_j) \;=\; G_j, \qquad\qquad j = 1, \ldots, N_v$$

and

$$\|g\|_\infty \;=\; \|G\|_\infty$$

By Theorem 2.8, the solution of the approximating equation

$$(2\pi + \mathcal{K}\mathcal{P}_N)\rho_n \;=\; g_n$$

in $C(S)$, and the solution of the linear system

$$(2\pi I + K_N)Z \;=\; G$$

in $\mathbf{R}^{N_v}$ are related by $\rho_n(P_j) = Z_j$, $j = 1, \ldots, N_v$. Therefore,

$$\begin{aligned} \|(2\pi I + K_N)^{-1}G\|_\infty &= \|Z\|_\infty \;\le\; \|\rho_n\|_\infty \\ &= \|(2\pi + \mathcal{K}\mathcal{P}_N)^{-1}g\|_\infty \;\le\; \|(2\pi + \mathcal{K}\mathcal{P}_N)^{-1}\|_\infty \, \|g\|_\infty \\ &= \|(2\pi + \mathcal{K}\mathcal{P}_N)^{-1}\|_\infty \, \|G\|_\infty \end{aligned}$$

This implies that

$$\|(2\pi I + K_N)^{-1}\| \;\le\; \|(2\pi + \mathcal{K}\mathcal{P}_N)^{-1}\| \;\le\; c \;<\; \infty\,, \qquad N \ge N_0 \tag{5.16}$$

where the matrix norm is the standard row norm.

The present analysis uses the result

$$\|K_N - \widetilde{K}_N\| \;=\; O(\frac{1}{2^{4n}}) = O(\widehat{\delta}_n^4) \tag{5.17}$$

with the matrix row norm. The proof of this is essentially the same as that for (5.12). Using (5.17) and the invertibility of $2\pi I + K_N$ with the uniform boundedness of

$(2\pi I+K_N)^{-1}$, for all sufficiently large N, the geometric series theorem implies that

$$\left[I-(2\pi I+K_N)^{-1}(K_N-\widetilde{K}_N)\right]^{-1}$$

exists and is bounded by

$$\frac{1}{1-\|(2\pi I+K_N)^{-1}(K_N-\widetilde{K}_N)\|}. \tag{5.18}$$

Therefore,

$$2\pi I+\widetilde{K}_N=(2\pi I+K_N)\left[I-(2\pi I+K_N)^{-1}(K_N-\widetilde{K}_N)\right]$$

is invertible and the inverse of $2\pi I+\widetilde{K}_N$ is uniformly bounded for some sufficiently large N_0.

By straightforward manipulation of (5.13) and (5.15), we have

$$\rho_n-\widetilde{\rho}_n \;=\; (2\pi I+\widetilde{K}_N)^{-1}\left[\widetilde{K}_N-K_N\right]g_n+(2\pi I+\widetilde{K}_N)^{-1}\left[g_n-\widetilde{g}_n\right] \tag{5.19}$$

The first term on the right side is $O(\widehat{\delta}_n^4)$, from (5.17). The second term is either zero or $O(\widehat{\delta}_n^4)$, from (5.11). When considered with Theorem 5.1, this shows the result (5.14). ■

Note that this result was proven in Atkinson and Chien [12] for only the case with exact integration over the true surface.

5.4 Numerical examples

We begin with the solution of (2.4) for the ellipsoid ($S\#1$)

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

with $(a,b,c)=(2,2.5,3)$. The exterior Neumann problem (2.4) was solved with the function f so chosen that the true solution is known. The two cases used here are

$$u_1(P)=\frac{1}{r},\quad u_2(P)=\frac{1}{r}e^{x/r^2}\cos(z/r^2) \tag{5.20}$$

with $P = (x, y, z)$ and $r = \mid P \mid$. In this case, $\rho = u$; and we use u and u_N in our discussion. Table 11 contains the maximum error at the node points for solving boundary integral equation (2.5). The results are consistent with an asymptotic rate for the error of $O(\widehat{\delta}_n^4)$ or $O(\widehat{\delta}_n^4 \ln \widehat{\delta}_n)$, in agreement with the theoretical result in Theorem 5.3.

N	$\|u_1 - u_{1N}\|_\infty$	Ratio	$\|u_2 - u_{2N}\|_\infty$	Ratio
8	1.53E−2		1.12E−2	
32	1.43E−3	10.7	2.72E−3	4.1
128	9.50E−5	15.1	2.51E−4	10.8
512	6.02E−6	15.7	1.62E−5	15.5

Table 11: Maximum errors on ellipsoid $S\#1$

We give results for the surface $S\#2$.

$$(x, y, z) = \rho(\xi, \eta, \zeta)(A\xi, B\eta, C\zeta), \qquad \xi^2 + \eta^2 + \zeta^2 = 1$$

with

$$\rho(\xi, \eta, \zeta) = 1 - [(\xi - .1)^2 + 2(\eta - .1)^2 - 3(\zeta - .1)^2]/\alpha$$

and A, B, $C > 0$, $\alpha \geq 5$. The case we use here is $\alpha = 10$ and $(A, B, C) = (2, 2, 1)$. The Neumann data f was chosen from (5.20). In Table 12, the asymptotic pattern for the maximum error at the node points appears to be $O(\widehat{\delta}_n^3)$; and to check in more detail whether the error is truly $O(\widehat{\delta}_n^3)$ or $O(\widehat{\delta}_n^4)$, Tables 13 and 14 give the errors for u_{1N} and u_{2N} at a representative sampling of the 18 nodes used in the coarsest triangulation of S (for $N = 8$),

$v_1 = (0, 0, 1.24)$, $v_2 = (1.84, 0, 0)$, $v_5 = (0, -1.52, 0)$

$v_7 = (1.5156, 0, 0.7578)$, $v_8 = (1.2621, 1.2621, 0)$, $v_{12} = (-1.1421, -1.1421, 0)$

$v_{13} = (0, -1.3849, 0.6925)$, $v_{15} = (1.6356, 0, -0.8178)$, $v_{18} = (0, -1.5049, -0.7525)$

along with the ratios by which these errors decrease, respectively. The columns E_1, E_2, E_3, and E_4 denote the errors for the parameter $N = 8$, 32, 128, and 512, respectively. When looking at the individual errors, there is a pattern of an $O(\widehat{\delta}_n^4)$ rate of convergence at a large number of the points.

N	$\|u_1 - u_{1N}\|_\infty$	Ratio	$\|u_2 - u_{2N}\|_\infty$	Ratio
8	6.56E−2		6.64E−2	
32	5.33E−3	12.3	4.75E−3	14.0
128	8.66E−4	6.2	1.35E−3	3.5
512	1.10E−4	7.9	1.98E−4	6.8

Table 12: Maximum errors on surface $S\#2$

i	E_1	E_2	E_3	E_4
1	−2.51E−2	−5.02E−3	−4.73E−4	−3.14E−5
2	−4.09E−2	−4.18E−3	−2.79E−4	−1.78E−5
5	−6.56E−2	−5.33E−3	−3.27E−4	−2.24E−5
7	−3.11E−2	−2.96E−3	−7.80E−5	1.31E−5
8	−3.20E−2	−4.44E−3	−3.77E−4	−2.62E−5
12	−3.27E−2	−5.23E−3	−4.59E−4	−3.35E−5
13	−2.91E−2	−3.01E−3	−1.48E−4	2.91E−6
15	−2.65E−2	−2.39E−3	−7.59E−5	9.22E−6
18	−2.21E−2	−2.38E−3	−1.49E−4	−2.97E−6
i	$\|E_1/E_2\|$	$\|E_2/E_3\|$	$\|E_3/E_4\|$	
1	5.0	10.6	15.1	
2	9.8	15.0	15.7	
5	12.3	16.3	14.6	
7	10.5	37.9	6.0	
8	7.2	11.8	14.3	
12	6.3	11.3	13.7	
13	9.7	20.3	50.9	
15	11.1	31.5	8.2	
18	9.3	16.0	50.1	

Table 13: Errors at representative v_i on $S\#2$, for $u = u_1$

i	E_1	E_2	E_3	E_4
1	−4.28E−2	−8.06E−4	1.77E−4	1.42E−5
2	−4.75E−2	−4.62E−3	−4.63E−4	−3.24E−5
5	−4.45E−2	−2.10E−4	−1.30E−4	−1.40E−5
7	−5.75E−2	−3.17E−3	−3.53E−4	−1.79E−5
8	−6.61E−2	−3.96E−3	−4.67E−4	−2.86E−5
12	−2.73E−2	−3.84E−4	−1.87E−4	−2.09E−5
13	−4.53E−2	1.03E−4	−1.27E−4	−1.97E−5
15	−5.08E−2	−2.31E−3	−3.24E−4	−2.04E−5
18	−3.98E−2	2.81E−4	−1.11E−4	−1.90E−5
i	$\|E_1/E_2\|$	$\|E_2/E_3\|$	$\|E_3/E_4\|$	
1	53.1	4.6	12.5	
2	10.3	10.0	14.3	
5	211.9	1.6	9.3	
7	18.1	9.0	19.7	
8	16.7	8.5	16.3	
12	71.1	2.1	8.9	
13	439.8	0.8	6.4	
15	22.0	7.1	15.9	
18	141.6	2.5	5.8	

Table 14: Errors at representative v_i on $S\#2$, for $u = u_2$

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