

A COLLOCATION METHOD FOR SOLVING THE EXTERIOR NEUMANN PROBLEM

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Dedicated to Professor Gheorghe Micula at his 60th anniversary

Abstract. In this paper we study the numerical solution of a boundary integral equation reformulation of the exterior Neumann problem. We give a brief outline of the problem and its solvability. Then, we propose a collocation method based on interpolation and give an error analysis. Numerical examples for the piecewise constant collocation method (centroid rule) conclude the paper.

1. The Exterior Neumann Problem

Let D denote a bounded open simply-connected region in \mathbb{R}^3 , and let S denote its boundary. Let $\bar{D} = D \cup S$ and denote by $D_e = \mathbb{R}^3 - \bar{D}$ the region complementary to D . Let $\bar{D}_e = D_e \cup S$. At a point $P \in S$, let \mathbf{n}_P denote the unit normal directed into D , provided that such a normal exists. Also assume that S is a piecewise smooth surface that can be decomposed into a finite union of smooth surfaces intersecting each other along common edges at most. In addition, assume that S has a triangulation $\mathcal{T}_n = \{\Delta_{n,k} \mid 1 \leq k \leq n\}$ with mesh size h (such a triangulation can be obtained as the image of a composition of bijections m_k from the unit simplex σ onto a planar triangle Δ_k and bijections F_j from a right triangle onto each smooth piece S_j of S ; for details, see Micula [7, Chapter 3]).

The Exterior Neumann Problem

Find $u \in C^1(\bar{D}_e) \cap C^2(D_e)$ that satisfies

$$\begin{aligned} \Delta u(P) &= 0, P \in D_e \\ \frac{\partial u(P)}{\partial \mathbf{n}_P} &= f(P), P \in S \end{aligned} \tag{1}$$

$$u(P) = O(P^{-1}), \frac{\partial u(P)}{\partial r} = O(|P|^{-2}), \text{ as } r = |P| \rightarrow \infty \text{ uniformly in } \frac{P}{|P|}$$

with $f \in C(S)$ a given boundary function.

Received by the editors: 29.09.2003.

2000 *Mathematics Subject Classification.* 65N35, 65N30, 65P05, 35Q60.

The boundary value problem (1) has been studied extensively (see Mikhlin [8, Ch. 18], G nter [5, Ch. 3], Colton [4, Section 5.3]). Here we only give a very brief outlook at results on the solvability of the problem (1).

The Divergence Theorem (see Atkinson [2, Theorem 7.1.2]) can be used to obtain a representation formula for functions that are harmonic inside the region D_e . Let $u \in C^1(\overline{D_e}) \cap C^2(D_e)$ and assume that $\Delta u(P) = 0$ at all $P \in D_e$. Then

$$\begin{aligned} \int_S \frac{\partial u(Q)}{\partial n_Q} \frac{dS(Q)}{|P-Q|} - \int_S u(Q) \cdot \frac{\partial}{\partial n_Q} \left[\frac{1}{|P-Q|} \right] dS_Q \\ = \begin{cases} [4\pi - \Omega(P)]u(P) & , P \in S \\ 4\pi u(P) & , P \in D_e \end{cases} \end{aligned} \quad (2)$$

(see Atkinson [1].) In formula (2), $\Omega(P)$ denotes the *interior solid angle* at $P \in S$, defined in Atkinson [2, p. 430]. If S is smooth, then $\Omega(P) = 2\pi$. For a cube, the corners have interior solid angle of $\frac{1}{2}\pi$, and the edges have interior solid angles of π .

To study the solvability of (1), consider representing its solution as a *single layer potential*

$$u(A) = \int_S \frac{\rho(Q)}{|A-Q|} dS_Q, \quad A \in D_e \quad (3)$$

The function ρ in (3) is called a *single layer density* function. The function $u(A)$ in (3) is harmonic for all $A \notin S$. For well-behaved density functions and for $A \notin S$, the integrand in (3) is nonsingular. Even though for the case $A = P \in S$, the integrand in (3) becomes singular, it is relatively straightforward to show that the integral exists and moreover, if ρ is bounded on S , then

$$\sup_{A \in \mathbb{R}^3} |u(A)| \leq c \|\rho\|_\infty \quad (4)$$

For a complete description of the properties of the single layer potential, see G nter [5, Chapter 2].

Now for the function u of (3), impose the boundary condition from (1) to get

$$\lim_{\substack{A \rightarrow P \\ A \in D_e}} \mathbf{n}_P \cdot \nabla \left[\int_S \frac{\rho(Q)}{|A-Q|} dS_Q \right] = f(P), \quad P \in S \quad (5)$$

for all $P \in S$ at which the normal \mathbf{n}_P exists (which implies $\Omega(P) = 2\pi$). Using a limiting argument, we obtain the second kind integral equation

$$2\pi\rho(P) + \int_S \rho(Q) \cdot \frac{\partial}{\partial \mathbf{n}_P} \left[\frac{1}{|P-Q|} \right] dS_Q = f(P), \quad P \in S^* \quad (6)$$

The set S^* is to contain all points $P \in S$ at which a normal is defined. If S is a smooth surface, then $S^* = S$; otherwise, $S - S^*$ is a set of measure 0. The kernel

function in (6) is given by

$$\frac{\partial}{\partial \mathbf{n}_P} \left[\frac{1}{|P-Q|} \right] = \frac{\mathbf{n}_P \cdot (P-Q)}{|P-Q|^3} = \frac{\cos \theta_P}{|P-Q|^2} \quad (7)$$

where θ_P denotes the angle between \mathbf{n}_P and $(P-Q)$. Equation (6) can now be written as

$$\rho(P) + \frac{1}{2\pi} \int_S \rho(Q) \cdot \frac{\cos \theta_P}{|P-Q|^2} dS_Q = \hat{f}(P), \quad P \in S \quad (8)$$

where $\hat{f}(P) = \frac{1}{2\pi} f(P)$. For simplicity, we will write $f(P)$ instead of $\hat{f}(P)$.

Write the equation (8) in operator form:

$$(\mathcal{I} - K)\rho = f \quad (9)$$

The properties of the integral operator \mathcal{K} and, implicitly, the solvability of equation (1) have been studied intensively in the literature, especially for the case that S is a smooth surface. For S sufficiently smooth, \mathcal{K} is a compact operator from $C(S)$ to $C(S)$ and from $L^2(S)$ to $L^2(S)$. These results are contained in many textbooks, for example see Kress [6, Chapter 6], or Mikhlin [8, Chapters 12 and 16]. We will just state the following solvability result.

Theorem 1.1. *Let S be a C^2 surface. Then the equation (9) has a unique solution $\rho \in X$ for each given function $f \in X$, with $X = C(S)$ or $X = L^2(S)$.*

This theorem then leads to a solvability result for the Exterior Neumann Problem (1)

Theorem 1.2. *Let S be a smooth surface with $\overline{D_e}$ a region to which the Divergence Theorem can be applied. Assume the function $f \in C(S)$. Then, the Neumann problem (1) has a unique solution $u \in C^\infty(D_e)$.*

For the case when S is only piecewise smooth, the properties of \mathcal{K} and the solvability of (8) are not yet fully understood. We will assume that Theorem 1.1 is true for the piecewise smooth surfaces that we will consider in our work.

2. A Collocation Method

We want to study the numerical solution of (8) using an integral equation reformulation of (1) have been used before (see Atkinson and Chien [3] or Atkinson [2, Section 9.2]), but with the collocation nodes on the boundary of each triangular element. There are problems with defining the normal at the collocation points which are common to more than one triangular face, especially if the surface itself is approximated. This in turn means it is difficult to evaluate the kernel function in equation (8). For these reasons it makes sense to try collocation methods that use only interior collocation node points. We will use interpolation of order r (the collocation nodes will be the same as the interpolation nodes), of the form

$$q_{i,j} = \left(\frac{i + (r-3i)\alpha}{r}, \frac{j + (r-3j)\alpha}{r} \right), \quad i, j \geq 0, \quad i + j \leq r \quad (10)$$

for some $0 < \alpha < 1/3$ (these are points interior to the unit simplex, but they get mapped into points interior to each triangle in \mathcal{T}_n). For corresponding *Lagrange* functions (see Micula [7, pg. 7-11]), for $g \in C(S)$ define an operator \mathcal{P}_n by

$$\mathcal{P}_n g(P) = \sum_{j=1}^{f_r} g(m_k(q_j)) l_j(s, t), \quad (s, t) \in \sigma, \quad P = m_k(s, t) \in \Delta_k \quad (11)$$

This interpolates $g(P)$ over each triangular element $\Delta_k \in S$, with the interpolating function polynomial in the parameterization variables s and t . Since $\mathcal{P}_n g$ is not continuous in general, we need to enlarge $C(S)$ to include the piecewise polynomial approximations $\mathcal{P}_n g$. To do this, we consider the equation (9) within the framework of the function space $L^\infty(S)$ with the uniform norm $\|\cdot\|_\infty$. Then, $\mathcal{P}_n : L^\infty(S) \rightarrow L^\infty(S)$ is a bounded projection operator.

Define a collocation method with (10). Denote $v_{k,j} = m_k(q_j)$. Substitute

$$\begin{aligned} \rho_n(P) &= \sum_{j=1}^{f_r} \rho_n(v_{k,j}) l_j(s, t) \\ P &= m_k(s, t) \in \Delta_k, \quad k = 1, \dots, n \end{aligned} \quad (12)$$

into (8). To determine the values $\{\rho_n(v_{k,j})\}$, force the equation resulting from the substitution to be true at the collocation nodes $\{v_1, \dots, v_{nf_r}\}$. This leads to the linear system

$$\begin{aligned} \rho_n(v_i) &- \frac{1}{2\pi} \sum_{k=1}^n \sum_{j=1}^{f_r} \rho_n(v_{k,j}) \int_{\sigma} \frac{\cos \theta_{v_i}}{|v_i - m_k(s, t)|^2} \\ &\cdot |(D_s m_k \times D_t m_k)(s, t)| d\sigma = f(v_i), \quad i = 1, \dots, nf_r \end{aligned} \quad (13)$$

which we write abstractly as

$$(\mathcal{I} - P_n \mathcal{K}) \rho_n = P_n f \quad (14)$$

which will be compared to (9). We have the following result.

Theorem 2.1. *Let S be a C^2 surface as described earlier, with $F_j \in C^{r+2}$. Then for all sufficiently large n , say $n \geq n_0$, the operators $\mathcal{I} - P_n \mathcal{K}$ are invertible on $L^\infty(S)$ and have uniformly bounded inverses. For the solution ρ of (9) and the solution ρ_n of (13)*

$$\|\rho - \rho_n\|_\infty \leq \|(\mathcal{I} - P_n \mathcal{K})^{-1}\| \cdot \|\rho - P_n \rho\|_\infty, \quad n \geq n_0 \quad (15)$$

Furthermore, if $f \in C^{r+1}(S)$, then

$$\|\rho - \rho_n\|_\infty = O(h^{r+1}), \quad n \geq n_0 \quad (16)$$

For the proof, see, for example, Atkinson [1]).

So interpolation of order r , leads to an error of order $O(h^{r+1})$. But superconvergent methods can be developed. Next, we want to explore in more detail the collocation method based on piecewise constant interpolation (the centroid method)

and show that it is superconvergent at the collocation points. Define the operator \mathcal{P}_n by

$$\mathcal{P}_n g(P) = g(P_k), P \in \Delta_k, k = 1, \dots, n \quad (17)$$

for $g \in C(S)$. Then, \mathcal{P}_n is a bounded operator on $C(S)$ with $\|\mathcal{P}_n\| = 1$. Define a collocation method with (17). Substitute

$$\rho_n(P) = \rho_n(P_k), P = m_k(s, t) \in \Delta_k, k = 1, \dots, n \quad (18)$$

into (8). To determine the values $\{\rho_n(P_k)\}$, force the equation resulting from the substitution to be true at the collocation nodes $\{P_k \mid k = 1, \dots, n\}$. This leads to the linear system

$$\begin{aligned} \rho_n(P_i) + \frac{1}{2\pi} \sum_{k=1}^n \rho_n(P_k) \cdot \int_{\sigma} \frac{\cos \theta_{P_k}}{|P_k - m_k(s, t)|^2} \\ \cdot |(D_s m_k \times D_t m_k)(s, t)| d\sigma = f(P_k), i = 1, \dots, n \end{aligned} \quad (19)$$

which can be rewritten abstractly as

$$(\mathcal{I} + P_n \mathcal{K}) \rho_n = P_n f \quad (20)$$

which will be compared to (9).

By Theorem 2.1., for the true solution ρ of (9) and the solution ρ_n of the collocation equation (20), we have

$$\|\rho - \rho_n\|_{\infty} = O(h), \quad n \geq n_0 \quad (21)$$

For $g \in C(\sigma)$, consider the interpolation formula (17), which has degree of precision 0. Integrating it over σ , we obtain

$$\int_{\sigma} g(s, t) d\sigma \approx \int_{\sigma} \mathcal{L}_{\tau} g(s, t) d\sigma = \frac{1}{2} g\left(\frac{1}{3}, \frac{1}{3}\right) \quad (22)$$

which has degree of precision 1.

For $\tau \subset \mathbb{R}^2$, a planar triangle and for a function $g \in C(\tau)$, the function

$$\mathcal{L}_{\tau} g(x, y) = g\left(m_{\tau}\left(\frac{1}{3}, \frac{1}{3}\right)\right) = g(P_{\tau}) \quad (23)$$

the constant polynomial interpolating g at the node $m_{\tau}\left(\frac{1}{3}, \frac{1}{3}\right) = P_{\tau}$ (the centroid of τ). We have the following.

Lemma 2.2. *Let τ be a planar right triangle and assume the two sides which form the right angle have length h . Let $g \in C^2(\tau)$. Let $\Phi \in L^1(\tau)$ be differentiable with the first derivatives $D_x \Phi, D_y \Phi \in L^1(\tau)$. Then*

$$\left| \int_{\tau} \Phi(x, y) (\mathcal{I} - \mathcal{L}_{\tau}) g(x, y) d\tau \right| \leq ch^2 \left[\int_{\tau} (|\Phi| + |D\Phi|) d\tau \right] \cdot \max_{\tau} \{|Dg|, |D^2g|\} \quad (24)$$

For the proof, see Micula [7, pg 74-75].

This result can be extended to general triangles, provided

$$\sup_n \left[\max_{\Delta_{n,k} \in \mathcal{T}_n} r(\Delta_{n,k}) \right] < \infty \quad (25)$$

where

$$r(\tau) = \frac{h(\tau)}{h^*(\tau)} \quad (26)$$

with $h(\tau)$ and $h^*(\tau)$ denoting the diameter of τ and the radius of the circle inscribed in τ , respectively.

Corollary 2.3. *Let τ be a planar triangle of diameter h , let $g \in C^2(\tau)$, and let $\Phi \in L^1(\tau)$ with both first derivatives in $L^1(\tau)$. Then*

$$\left| \int_{\tau} \Phi(x, y) (\mathcal{I} - L_{\tau}) g(x, y) \right| \leq c(r(\tau)) h^2 \left[\int_{\tau} (|\Phi| + |D\Phi|) d\tau \right] \cdot \max_{\tau} \{ \|Dg\|_{\infty}, \|D^2g\|_{\infty} \} \quad (27)$$

where $c(r(\tau))$ is some multiple of $r(\tau)$ of (26).

Since formula (22) has degree of precision 1 (odd) over σ , extending it to a square would not improve the degree of precision, which means the same error bound as in Lemma 2.2 is true for a parallelogram formed by two symmetric triangles.

We want to apply the above results to the individual subintegrals in

$$\mathcal{K}g(P_i) = \frac{1}{2\pi} \sum_{k=1}^n \int_{\sigma} \frac{\cos \theta_{P_k}}{|P_k - m_k(s, t)|^2} \rho(m_k(s, t)) \cdot |(D_s m_k \times D_t m_k)(s, t)| d\sigma \quad (28)$$

with the role of g played by $\rho(m_k(s, t)) |(D_s m_k \times D_t m_k)(s, t)|$, and the role of Φ played by $\frac{\cos \theta_{P_k}}{|P_k - m_k(s, t)|^2}$. For the derivatives of this last function, we have

Theorem 2.4. *Let i be an integer and S be a smooth C^{i+1} surface. Then*

$$\left| D_Q^i \left(\frac{\cos \theta_P}{|P - Q|^2} \right) \right| \leq \frac{c}{|P - Q|^{i+1}}, \quad P \neq Q \quad (29)$$

with c a generic constant independent of P and Q .

For details of the proof, see Micula [7, pg.76].

For the error at the collocation node points, we have the following.

Theorem 2.5. *Assume the hypotheses of Theorem 2.1, with each $F_j \in C^2$. Assume $\rho \in C^2$. Assume the triangulation \mathcal{T}_n of S satisfies (25) and is symmetric. For those integrals in (28) for which $P_i \in \Delta_k$, assume that all such integrals are evaluated with an error of $O(h^2)$. Then*

$$\max_{1 \leq i \leq n} |\rho(P_i) - \hat{\rho}_n(P_i)| \leq ch^2 \log h \quad (30)$$

Proof. We will bound

$$\max_{1 \leq i \leq n} |\mathcal{K}(I - P_n)u(v_i)|$$

For a given node point v_i , denote Δ^* the triangle containing it and denote:

$$\mathcal{T}_n^* = \mathcal{T}_n - \{\Delta^*\}$$

By our assumption, the error in evaluating the integral of (28) over Δ^* will be $O(h^2)$.

Partition \mathcal{T}_n^* into parallelograms to the maximum extent possible. Denote by $\mathcal{T}_n^{(1)}$ the set of all triangles making up such parallelograms and let $\mathcal{T}_n^{(2)}$ contain the remaining triangles. Then

$$\mathcal{T}_n^* = \mathcal{T}_n^{(1)} \cup \mathcal{T}_n^{(2)}.$$

It is easy to show that the number of triangles in $\mathcal{T}_n^{(1)}$ is $O(n) = O(h^{-2})$, and the number of triangles in $\mathcal{T}_n^{(2)}$ is $O(\sqrt{n}) = O(h^{-1})$.

It can be shown that all but a finite number of the triangles in $\mathcal{T}_n^{(2)}$, bounded independent of n , will be at a minimum distance from v_i . That means that the triangles in $\mathcal{T}_n^{(2)}$ are “far enough” from v_i , so that the function $G(v_i, Q)$ is uniformly bounded for Q being in a triangle in $\mathcal{T}_n^{(2)}$ (where we denote by $G(P, Q) = \frac{\cos \theta_P}{|P - Q|^2}$).

First, consider the contribution to the error coming from the triangles in $\mathcal{T}_n^{(2)}$. By Lemma 2.2. the error over each such triangle is $O(h^2 \|D^2 g\|_\infty)$, since the area of each triangle is $O(h^2)$ and using our earlier observation. Having $O(h^{-1})$ such triangles in $\mathcal{T}_n^{(2)}$, the total error coming from triangles in $\mathcal{T}_n^{(2)}$ is $O(h^3 \|D^2 g\|_\infty)$.

Next, consider the contribution to the error coming from triangles in $\mathcal{T}_n^{(1)}$. By Lemma 2.2., the error will be of size $O(h^2)$ multiplied times the integral over each such parallelogram of the maximum of the first derivatives of $G(v_i, Q)$ with respect to Q . Combining these we will have a bound

$$ch^2 \int_{S-\Delta^*} (|G| + |DG|) dS_Q \quad (31)$$

By Theorem 2.4., the quantity in (31) is bounded by

$$ch^2 \int_{S-\Delta^*} \left(\frac{1}{|P - Q|} + \frac{1}{|P - Q|^2} \right) dS_Q \quad (32)$$

Using a local representation of the surface and then using polar coordinates, the expression in (32) is of order

$$ch^2 (h + \log h)$$

Thus, the error arising from the triangles in $\mathcal{T}_n^{(1)}$ is $O(h^2 \log h)$. Combining the error arising from the integrals over Δ^* , $\mathcal{T}_n^{(1)}$, and $\mathcal{T}_n^{(2)}$, we have (30). \square

3. Numerical Examples

As a smooth surface consider the ellipsoid

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 + \left(\frac{z}{c}\right)^2 = 1 \quad (33)$$

with $(a, b, c) = (1, 1, 1)$ (the surface $E1$), and $(a, b, c) = (2, 3, 5)$ (the surface $E2$).

We solve the equation (1) with the function $f(P)$ so chosen that the true solution is

$$u = \frac{1}{\sqrt{x^2 + y^2 + z^2}} \quad (34)$$

In Tables 1 and 2 we give

$$|u(P) - u_n(P)| \quad (35)$$

where $P = P_{ij} = \tau_i \left(\frac{a}{\sqrt{3}}, \frac{b}{\sqrt{3}}, \frac{c}{\sqrt{3}} \right) \in D_e(E_j)$ (the exterior of E_j), where $\tau_1 = 1.1$, $\tau_2 = 2$, and $\tau_3 = 10$ (points situated further and further away from the boundary of the ellipsoid). The results are consistent with a convergence rate of $O(h^2 \log h)$ predicted by Theorem 2.5. which illustrates the superconvergence.

As a simple piecewise smooth surface, we use again the unit cube

$$S = [0, 1] \times [0, 1] \times [0, 1] \quad (36)$$

$P = P_{11}$			$P = P_{21}$		$P = P_{31}$	
n	$ u(P) - u_n(P) $	Ratio	$ u(P) - u_n(P) $	Ratio	$ u(P) - u_n(P) $	Ratio
4	8.52 E-1		5.05 E-1		1.02 E-1	
16	9.29 E-2	9.16	6.05 E-2	8.35	1.20 E-2	8.53
64	1.10 E-2	8.44	8.32 E-3	7.27	1.63 E-3	7.36
256	2.67 E-3	4.12	1.88 E-3	4.40	3.71 E-4	4.39

TABLE 1. Errors in solving the Neumann Problem on $E1$

$P = P_{12}$			$P = P_{22}$		$P = P_{32}$	
n	$ u(P) - u_n(P) $	Ratio	$ u(P) - u_n(P) $	Ratio	$ u(P) - u_n(P) $	Ratio
4	2.87 E-1		1.56 E-1		2.70 E-2	
16	5.94 E-2	4.84	2.91 E-2	5.36	5.09 E-3	5.30
64	1.24 E-2	4.77	5.85 E-3	4.98	9.99 E-4	5.10
256	3.02 E-3	4.12	1.29 E-3	4.53	2.07 E-4	4.82

TABLE 2. Errors in solving the Neumann Problem on $E2$

The function f is chosen so that the true solution is

$$u = \frac{1}{\sqrt{(x-0.5)^2 + (y-0.5)^2 + (z-0.5)^2}} \quad (37)$$

n	$P = P_1$		$P = P_2$		$P = P_3$	
	$ u(P) - u_n(P) $	Ratio	$ u(P) - u_n(P) $	Ratio	$ u(P) - u_n(P) $	Ratio
12	8.98 E-1		2.92 E-1		3.62 E-2	
48	4.11 E-1	2.17	9.18 E-2	3.18	3.01 E-3	12.01
192	1.96 E-1	2.02	3.61 E-2	2.54	3.61 E-4	8.33
768	9.89 E-2	1.98	1.68 E-2	2.14	1.18 E-4	3.05

TABLE 3. Errors in solving the Neumann Problem on the unit cube

In Table 3 we give the results for $|u(P) - u_n(P)|$ for $P = P_i = (\tau_i, \tau_i, \tau_i) \in D_e(S)$, $i = 1, 2, 3$. The ratios approach 2 as n increases, which is consistent with a rate of convergence of $O(h)$ as predicted by Theorem 2.1. (with $r = 0$). As shown in the table, the further away from the boundary of S the point P is, the better the approximation.

We conclude by noting that the ideas used in this paper to study the numerical solution of the exterior Neumann problem (1) apply very well to studying the numerical solutions of the interior Neumann problem and the (interior or exterior) Dirichlet problem as well. For the interior Neumann problem (analogous to (1), only with D instead of D_e), an auxiliary condition on $f(P)$ is needed for solvability (namely, $\int_S f(Q) dS = 0$). Also, this problem does not have a unique solution in the sense that two solutions differ by a constant, and the integral equation corresponding to (8) is no longer uniquely solvable.

The equation coming from the Dirichlet problem is similar, but the interest in solving it using collocation methods with only interior collocation points is not so great in this case, since the kernel does not involve the normal \mathbf{n}_P , but the normal \mathbf{n}_Q .

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