NASA-CR-153,185

ICASE

NASA-CR-153185
19800015552

BOUNDARY CONDITIONS FOR THE NUMERICAL SOLUTION OF ELLIPTIC EQUATIONS IN EXTERIOR REGIONS

Alvin Bayliss

Max Gunzburger

and

Eli Turkel

Report No. 80-1

January 11, 1980

INSTITUTE FOR COMPUTER APPLICATIONS IN SCIENCE AND ENGINEERING
NASA Langley Research Center, Hampton, Virginia

Operated by the

UNIVERSITIES SPACE USRA RESEARCH ASSOCIATION

ENTER:
4B X ?+
.PRT - EM3287

DISPLAY 30/2/1
80N24044*# ISSUE 14 PAGE 1902 CATEGORY 64 RPT#: NASA-CR-153185
REPT-80-1 CNT#: NAS1-14101 DAAG29-78-C-0024 EY-76-C-02-3077 80/00/00
47 PAGES UNCLASSIFIED DOCUMENT

UTTL: Boundary conditions for the numerical solution of elliptic equations in exterior regions

AUTH: A/BAYLISS, A.; B/GUNZBURGER, M.; C/TURKEL, E. PAA: B/(Tennessee Univ.) ; C/(New York Univ.)

CORP: National Aeronautics and Space Administration. Langley Research Center, Hampton, VA. AVAIL.NTIS

SAP: HC A03/MF A01

CIO: UNITED STATES

MAJS: /*BOUNDARY CONDITIONS/*BOUNDARY VALUE PROBLEMS/*ELLIPTIC DIFFERENTIAL EQUATIONS/*NUMERICAL ANALYSIS/*PROBLEM SOLVING/*RADIATION DISTRIBUTION

MINS: / DIRICHLET PROBLEM/ HELMHOLTZ EQUATIONS/ LAPLACE EQUATION/ SOMMERFELD APPROXIMATION/ WAVE EQUATIONS

ABA: Author

ABS: Elliptic equations in exterior regions frequently require a boundary condition at infinity to ensure the well-posedness of the problem. Examples of practical applications include the Helmholtz equation and Laplace's equation. Computational procedures based on a direct discretization of the elliptic problem require the replacement of the condition on a finite artificial surface. Direct imposition of the

ENTER:
4B MORE
.PRT - EM3287

BOUNDARY CONDITIONS FOR THE NUMERICAL SOLUTION OF ELLIPTIC EQUATIONS IN EXTERIOR REGIONS

Alvin Bayliss
Institute for Computer Applications in Science and Engineering

Max Gunzburger*
University of Tennessee

Eli Turkel†
Courant Institute of Mathematical Sciences, New York University

ABSTRACT

Elliptic equations in exterior regions frequently require a boundary condition at infinity to ensure the well-posedness of the problem. Examples of practical applications include the Helmholtz equation and Laplace's equation. Computational procedures based on a direct discretization of the elliptic problem require the replacement of the condition at infinity by a boundary condition on a finite artificial surface. Direct imposition of the condition at infinity along the finite boundary results in large errors. A sequence of boundary conditions is developed which provides increasingly accurate approximations to the problem in the infinite domain. Estimates of the error due to the finite boundary are obtained for several cases. Computations are presented which demonstrate the increased accuracy that can be obtained by the use of the higher order boundary conditions. The examples are based on a finite element formulation but finite difference methods can also be used.

The authors' research was supported under NASA Contracts NAS1-14101 and NAS1-15810 while the first author was in residence at ICASE, NASA Langley Research Center, Hampton, VA 23665.

* Additional support for the second author was provided by the Army Research Office Contract No. DAAG 29-78-C-0024.

† The research for the third author was provided by the Department of Energy Grant No. DOE EY-76-C-02-3077.

I. Introduction

Elliptic problems in exterior regions arise in many branches of physics. For example, the flow of an incompressible irrotational fluid about a body is described by the Laplace equation (e.g. Lamb [19])

$$\Delta u = 0.$$

The same equation arises in the study of electrostatics exterior to given surfaces (e.g. Stratton [30]). A different example is the exterior scattering problem for either acoustics or electromagnetism. In this case one wishes to solve the Helmholtz equation

$$\Delta u + k^2 u = 0 \quad ,$$

with either Dirichlet or Neumann data specified on the bodies (Bowman, et al. [6], Muller [22]). For inhomogeneous media, k is a given function of the position. For some applications in plasma physics, k can be a nonlinear function.

In these cases, infinity can be regarded as a separate boundary. A condition at infinity is required to make the exterior problem well-posed. For the Laplace equation it is sufficient to impose a condition of regularity at infinity. In three dimensions this is

$$u = 0\left(\frac{1}{r}\right) \qquad r \to \infty \quad , \tag{1.1}$$

where r is the distance from a fixed (but arbitrary) origin (Kellogg [15]). For the Helmholtz equation one can impose the Sommerfeld radiation condition

(Sommerfeld [30])

$$\frac{\partial u}{\partial r} - i\,k\,u = o\left(\frac{1}{r}\right) \qquad r \to \infty \quad . \tag{1.2}$$

A more exact form of (1.2) is

$$\lim_{r \to \infty} \iint_{|y| = r} \left|\frac{\partial u}{\partial r} - i\,k\,u\right|^2 dS = 0 \quad , \tag{1.3}$$

where the integral is over spherical shells centered at $r = 0$ (Rellich [27], Hellwig [13]). The radiation condition ((1.2) - (1.3)) states that the solution corresponds to outgoing waves (see Wilcox [35], [36], for more details).

In many instances one is interested in problems with variable coefficients that approach a constant state at infinity. An extension of the theory of radiation conditions to problems with variable coefficients was developed by Vainberg [33]. The techniques to be described are valid for the variable coefficient case provided the coefficients approach constants at infinity at a sufficiently rapid rate.

A numerical solution of an elliptic problem in an exterior region must be able to incorporate the radiation condition at infinity within the computational procedure. Solution techniques based on eigenfunction expansions or asymptotic methods automatically accomplish this by the proper choice of expansion functions. When the free space Green's function which satisfies the radiation condition is known, (e.g. constant coefficients) the difficulty of imposing the radiation condition can be avoided by reformulating the problem as a Fredholm integral equation. Such formulations for the Helmholtz equation can be found in Chertock [9], Kleinman and Roach [16], and Burton and Miller [8]. Poggio and Miller [24] discuss a vector integral equation for the reduced Maxwell equations. Bayliss [4] shows that one can greatly increase the efficiency of the integral equation formulation by introducing an appropriate coordinate transform along the body. Schneck [28] has developed codes to solve the resultant integral equations for a range of applications.

The integral equation approach has several deficiencies. These methods are generally restricted to the constant coefficient case and require the inversion of a full matrix. This can result in storage difficulties, especially for three dimensional problems or problems with high frequencies. In addition, for many applications the matrix elements are expensive to compute [4]. Many mesh points are required to resolve the singularity in the kernel even for low frequencies.

For the Helmholtz equation, an additional difficulty with the integral equation formulation is the possibility of interior resonances. It is well known that for certain values of k the integral equation becomes singular ([9], [16]). These resonances are connected with eigenvalues of associated interior problems. Various attempts have been made to overcome this difficulty, but they generally increase the complexity of the integral equation approach (Ursell [32]). It will be shown that the proper formulation of radiation conditions can eliminate the possibility of eigenvalues.

An alternative to the integral equation method is to couple an interior solution with a global functional of the solution on an artificial boundary. The global functional can be obtained by integral formulas using the free space Green's function or by using an expansion, typically obtained from separation of variables, to represent the solution exterior to the artificial boundary. Marin [21], Zienkiewicz, et al. [37] and others have studied methods based on an integral relation over the artificial boundary, while Fix and Marin [10] have used a boundary condition based on separation of variables to solve problems in underwater acoustics.

These methods incorporate the exact radiation condition at the cost of a non-local boundary condition. A disadvantage of these methods is that the non-local coupling over the artificial boundary is equivalent to the full matrix that would be obtained from the integral equation. Furthermore, for the Helmholtz equation, spurious eigenvalues can also occur with this formulation. Goldstein [11] has suggested extending the boundary conditions of Engquist and Majda to the elliptic case. However, this method is restricted to only a range of frequencies depending on the expansion parameter. No calculations using this method have been carried out to date.

The method to be presented develops a sequence of local boundary conditions that are extensions of (1.1) and (1.2). These boundary conditions are then applied at a finite artificial boundary. As the order of accuracy of the boundary operator increases, the order of the highest derivative appearing in the boundary operator will also increase.

The artificial surface will generally be assumed, for the proofs, to be the sphere $r = r_1$. The resulting elliptic problem is then discretized and solved in the bounded region between the body and the artificial surface. The proposed boundary conditions are asymptotic in $1/r$. Hence, for a given accuracy one can bring the artificial boundary further in when using the higher order boundary conditions.

In many applications the solution is required only in the vicinity of the body. The far field solution can be calculated by a quadrature formula, such as Green's formula, once u and $\frac{\partial u}{\partial n}$ are known along the body. For problems in potential flow one frequently is only interested in the solution on the body. Because of this, we shall stress the accuracy of the boundary conditions as r_1 decreases. Furthermore, the error estimates will be for surface L^2 errors. These errors are due to the imposition of the generalized radiation conditions at a finite boundary.

These boundary conditions are related to a family of boundary conditions developed by Bayliss and Turkel [5] for time dependent problems. The boundary operators are differential relations which match the solution to an expansion in $1/r$ which is valid in a neighborhood of infinity. The boundary conditions generally involve derivatives of order greater than or equal to the order of the differential equation. Hence, these boundary conditions are different from the usual boundary conditions encountered in elliptic theory.

For the Laplace equation the resultant discretization can be solved by fast iterative methods leading to a substanial improvement over the integral equation methods. For Helmholtz type equations, the error will have a dependence on the number of wave lengths between the body and the artificial surface. In several test cases it has been possible to constrict the computational region as k increases. All numerical results in this study were obtained with a finite element program based on a band Gaussian solver. This has large storage requirements which limited the investigation of high frequencies. This storage can be reduced by the use of iterative methods. An iterative method for the Helmholtz equation based on a decay law for a corresponding hyperbolic problem was developed by Kriegsman and Morawetz [17]. Kriegsman and Morawetz have also implemented time dependent boundary conditions similar to those proposed here (private communication). Brandt [7] and Nicolaides [23] have developed iterative methods based on the multi-grid algorithm. These methods require Gaussian elimination on a coarse grid which provides some resolution of the solution. Hence, these methods have limited use for high frequencies. The scheme of Nicolaides can be combined with the finite element method described in the appendix. Extensions of the fast solvers based on capacitance methods are also feasible (Proskorowski and Widlund [25]).

In section 2 we develop the extension of the standard radiation conditions for both the Helmholtz and Laplace equations. Error estimates for Laplace's equation are given in section 3 and for the Helmholtz equation in section 4. These chapters can be skipped by those only interested in the computational procedure. In section 5 computational results are presented for both the Laplace equation and the Helmholtz equation. For the Helmholtz equation both constant and variable indices of refraction are considered. The details of the finite element procedure are given in the appendix.

II. Construction of Radiation Boundary Conditions

Let u be an outgoing solution to the three dimensional Helmholtz equation

$$\Delta u + k^2 u = 0 \quad , \tag{2.1}$$

exterior to a sphere $r = r_0$. It is known (Atkinson [2], Wilcox [34]) that u can be represented by a convergent expansion

$$u = \frac{e^{ikr}}{kr} \sum_{j=0}^{\infty} \frac{F_j(\theta,\phi)}{(kr)^j} \quad . \tag{2.2}$$

Here θ,ϕ denote the angular variables of an (r,θ,ϕ) spherical coordinate system. The series (2.2) is uniformly and absolutely convergent and can be differentiated term by term any number of times (Wilcox [34]). $F_j(\theta,\phi)$, $j \geq 1$ can be obtained from the radiation pattern, F_0, by the formula

$$F_j(\theta,\phi) = \frac{1}{(2i)^j j!} \prod_{\ell=0}^{j} [\ell(\ell-1) + Q]F_0(\theta,\phi) \qquad ,$$

where Q is the Beltrami operator in the angular coordinates θ and ϕ

$$Q = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \qquad .$$

The Sommerfeld radiation condition for any such solution is

$$-iku + u_r = o(\frac{1}{r}) \qquad (r \to \infty).$$

In fact it is clear from the expansion (2.2) that

$$-iku + u_r = O(\frac{1}{r^2}) \qquad (r \to \infty). \tag{2.3}$$

In numerical computations for which the exterior region is truncated at a finite value of r, say $r = r_1$, a possible boundary condition to impose is

$$-iku + u_r\Big|_{r=r_1} = 0 \qquad . \tag{2.4}$$

However, this condition is very inaccurate and in fact it can easily be seen that it is not exact even for the first term in the expansion (2.2).

We will develop here a sequence of linear differential operators B_m which provide more accurate extensions of the condition (2.4) by annihilating the first m terms in the expansion (2.2). Thus the condition that at $r = r_1$ the solution lies in the null space of the operator B_m can be considered as a procedure to match the solution to the first m terms in the expansion (2.2).

An example of such an operator is

$$B_1 u = (\frac{\partial}{\partial r} - i\,k + \frac{1}{r})u \quad .$$

It is easily verified that

$$B_1 \left[\frac{e^{ikr}}{kr} F(\theta,\phi)\right] = 0 \quad ,$$

for any function $F(\theta,\phi)$. Furthermore, it can be verified that for any function u having the expansion (2.2)

$$(2.5) \qquad B_1 u \Big|_{r=r_1} = 0(\frac{1}{r^3}) \quad .$$

To develop more accurate conditions we consider the sequence of operators

$$(2.6) \qquad B_m = \prod_{j=1}^{m} (\frac{\partial}{\partial r} - i\,k + \frac{2j-1}{r}) \equiv (\frac{\partial}{\partial r} - i\,k + \frac{2m-1}{r}) B_{m-1} \quad .$$

A straightforward calculation verifies that

$$B_m p = 0 \quad ,$$

for any function p of the form

$$p = \frac{e^{ikr}F(\theta,\phi)}{(kr)^{\ell}} \quad , \qquad \ell = 1,\ldots,m \quad .$$

Furthermore, if u is any function having an expansion of the form (2.2) then

$$B_m u \Big|_{r=r_1} \equiv h = 0\left(\frac{1}{r_1^{2m+1}}\right) \quad . \tag{2.7}$$

It is clear that the leading order term in h will involve only the term of order $m+1$ in the expansion (2.2) and thus the boundary condition $B_m u = 0$ will match the solution to the first m terms in the expansion (2.2). For any fixed k the errors in the boundary condition $B_m u$ will decrease at a faster rate (in $(r_1)^{-1}$) as $r_1 \to \infty$. This is thus analogous to the use of higher order difference approximations where the errors decrease at a faster rate in a mesh size h. Thus one can expect a significant increase in efficiency by applying the higher order boundary conditions. We point that the individual terms in (2.2) are not solutions to (2.1) (unless $k = 0$) however the series (2.2) provides a description of the behavior of the solution as $r \to \infty$ which is generally not the case for expansions based on complete sets of solutions to (2.1) (see Aziz and Kellogg [3]). We further point out that the operators B_m in (2.6) can be written as

$$(-i\,k + \frac{\partial}{\partial r})^m + \text{lower order terms} \quad , \tag{2.8}$$

and thus they can be considered as generalizations of the Sommerfeld radiation condition.

In the study of the Helmholtz equation we are interested in the behavior of the errors in different parameter ranges. Specifically,

1. The error for fixed k and m as the position of the artificial surface, i.e. r_1, varies.

2. The error for fixed k and r_1 as the order of the boundary operator m increases.

3. The error for fixed r_1 and m as the frequency k increases.

Case 2 is of greater importance than case 1 as it is generally more expensive to increase the size of the computational domain than to implement the higher order boundary conditions. Results to be established in sections 3 and 4 demonstrate that the higher order boundary condition can lead to significantly increased accuracy when applied at a fixed r_1.

The constants involved in the order relations (2.5) and (2.7) will, in general, depend on k. This is because for arbitrary problems the angular functions $F_j(\theta,\phi)$ can be expected to grow with k. Thus as k increases the errors in (2.5) and (2.7) will not, in general, be bounded uniformly in k. However, the quantity kr_1 is a natural non-dimensional quantity, which is in fact just the number of wave lengths to the artificial boundary $r = r_1$. The error obtained by taking only a fixed number of terms in the series (2.2) can be expected to depend significantly on this quantity. A consequence of this is that the radial resolution will not increase, or will increase slowly as k increases. Numerical results illustrating this will be presented in section 5.

We also consider the exterior Laplace equation. In this case it is well known that the analog of (2.2) holds, i.e., solutions have the multipole expansion

$$u = \frac{1}{r} \sum_{j=0}^{\infty} \frac{F_j(\theta,\phi)}{r^j} \quad . \tag{2.9}$$

It then follows that the differential operators obtained by setting $k = 0$ in (2.6)

$$B_m = \prod_{j=1}^{m} \left(\frac{\partial}{\partial r} + \frac{2j-1}{r}\right) \quad , \tag{2.10}$$

exactly annihilate the first m terms in (2.9). Similarly for any u with the expansion (2.9)

$$B_m u \Big|_{r = r_1} = O\left(\frac{1}{r^{2m+1}}\right) \quad . \tag{2.11}$$

Both (2.6) and (2.11) are valid for equations with variable coefficients provided the coefficients approach a constant state sufficiently rapidly at infinity. As indicated in the introduction we will be mainly interested in computing the solution on some surface. The solution at far fields points can then be obtained by a quadrature based on Green's formula. In the next two sections we prove theorems that demostrate that in some cases the expected surface L^2 errors are achieved.

For computational ease one can replace all radial derivatives beyond the first by tangential (angular) derivatives. This is done by using the differential equation and is especially important for finite element applications. The exact forms of B_1 and B_2 are given by (5.2).

The previous discussion has concentrated on the three dimensional Helmholtz and Laplace equations. For the two dimensional Helmholtz equation, the solution u has the convergent expansion (Karp [14])

$$u = H_0(kr) \sum_{j=0}^{\infty} \frac{F_j(\theta)}{r^j} + H_1(kr) \sum_{j=0}^{\infty} \frac{G_j(\theta)}{r^j} \quad , \tag{2.12}$$

where H_0 and H_1 are the Hankel functions of the first kind of order 0 and 1.

As this expansion is difficult to work with we use the asymptotic expansion [6]

$$(2.13) \qquad u \sim \sqrt{\frac{2}{\pi k r}}\; e^{i(kr - \frac{\pi}{2})} \sum_{j=0}^{\infty} \frac{f_j(\theta)}{r^j} \quad .$$

The boundary conditions based on (2.13) are

$$(2.14) \qquad B_m = \prod_{j=1}^{m} \left(\frac{\partial}{\partial r} + \frac{(2j - \frac{3}{2})}{r} - ik\right) \quad ,$$

which are analogous to (2.6).

We have concentrated on the homogenous Laplace and Helmholtz equations. The same boundary conditions can be used for the inhomogenous equation

$$(2.15) \qquad \Delta u + k^2 u = F \quad .$$

The estimates obtained in the next two sections apply to (2.15) provided that F decays sufficiently rapidly for large r.

Boundary conditions based on the operators B_m are nonstandard because of the high order of the derivatives involved. The regularity of the solutions up to the boundaries, using $B_m u = 0$ at the artificial surface, is guaranteed by the Agmon, Dougalis, Nirenberg theory [1]. Using the results of Lopatinskii [20] we need only consider the half plane problem without any lower order terms. Thus, we have reduced the problem to

$$(2.16) \qquad \begin{array}{lll} \Delta u = 0 & x \geq 0 & -\infty < y,\ z < \infty \ , \\ \dfrac{\partial^n u}{\partial x^n} = 0 & x = 0 & . \end{array}$$

The only solution to (2.16) that decays as $x \to \infty$ is $u = 0$. Hence, the complimentary condition of [1] is satisifed and regularity follows (see also [31]).

When estimates for the error are obtained it is important that the constants in the estimation do not grow too rapidly as the artificial boundary approaches infinity. It is also important, especially for the Helmholtz equation, to eliminate the possibility of spurious eigenvalues for the resulting interior problem. Indeed we wish to obtain estimates that are uniform in k and do not have poles at discrete values of k. Such estimates will be obtained in the next two sections.

III. Error Bounds for Laplace's Equation

We wish to obtain estimates for the L^2 surface error that occurs when the regularity condition at infinity is replaced by the condition $B_m u = 0$ at a finite boundary. In this section we concentrate on Laplace's equation. As discussed in the introduction the main interest is in the errors that occur in the solution and its derivative along the inner boundary.

For concreteness we shall consider the Neumann problem. All results are equally valid for the Dirichlet problem.

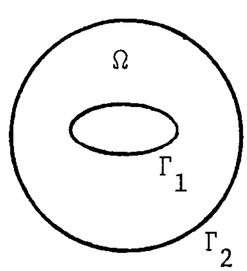

Figure 1.

The problem that we wish to solve is

$$(3.1)\qquad \begin{aligned} \Delta\, u &= 0 && \text{in } \Omega \;, \\ \frac{\partial u}{\partial n} &= g && \text{on } \Gamma_1 \;, \\ u &= 0(\tfrac{1}{r}) && r \to \infty \;. \end{aligned}$$

We replace this by the problem

$$(3.2)\qquad \begin{aligned} \Delta\, v &= 0 && \text{in } \Omega \;, \\ \frac{\partial v}{\partial n} &= g && \text{on } \Gamma_1 \;, \\ B_m v &= 0 && \text{on } \Gamma_2 \;, \end{aligned}$$

(see figure 1).

Let w be the error, $w = u - v$. Then w satisfies

$$(3.3)\qquad \begin{aligned} \Delta\, w &= 0 && \text{in } \Omega \;, \\ \frac{\partial w}{\partial n} &= 0 && \text{on } \Gamma_1 \;, \\ B_m w &= B_m u \equiv h && \text{on } \Gamma_2 \;. \end{aligned}$$

If Γ_2 is the sphere $r = r_1$ then by (2.6) $h = 0(\frac{1}{r_1^{2m+1}})$.

In this section we will only consider the case that the artificial surface Γ_2 is the sphere $r = r_1$. We will consider two cases. In theorem (3.1) we discuss the case that the body Γ_1 is also a sphere. In theorems (3.2) and (3.3) we consider general bodies, but only treat the boundary conditions B_1 and B_2. This is not a major restriction since B_1 and B_2 are the boundary conditions of the greatest practical importance.

Since we are interested in surface errors we introduce the notation

$$\|w\|^2_{(r)} = \iint\limits_{|y|=r} |w(y)|^2 dA_y \quad . \tag{3.4}$$

Introducing spherical coordinates (r,θ,ϕ) (3.4) becomes

$$\|w\|^2_{(r)} = \int_0^{2\pi}\int_0^{\pi} |w(r,\theta,\phi)|^2 r^2 \sin\theta \, d\theta d\phi \quad .$$

For simplicity we assume axial symmetry so that w is independent of ϕ. All the results are independent of this assumption.

For the first part we assume that the body is also a sphere. The coordinates are scaled so that the surface is the sphere $r = 1$. We then have

Theorem (3.1)

Let $g(\theta)$ be smooth and hence satisfy

$$\int_0^{\pi} g^2(\theta) \sin\theta \, d\theta < \infty. \tag{3.5}$$

Let w be the solution to (3.3). Then there exists a constant C, independent of m, such that

$$\|w\|_{(r)} \le \frac{Cr^{m+1}}{r_1^{2m+1} - 1} \quad , \tag{3.6a}$$

$$1 \le r \le r_1$$

$$\left\| \frac{\partial w}{\partial r} \right\|_{(r)} \le \frac{Cr^m}{r_1^{2m+1} - 1} \quad . \tag{3.6b}$$

Note:

(1) The bounds on the derivatives are necessary for the Dirichlet problem.

(2) It follows from (3.6a) that

$$\| w \|_{(r_1)} = O\left(\frac{1}{r_1^{m+1}}\right) \quad ,$$

$$\| w \|_{(1)} = O\left(\frac{1}{r_1^{2m+1}}\right) \quad .$$

Hence, the smallest errors occur along the inner surface. This is analogous to the Saint-Venant's principle. Lax [19] has considered decay laws for volume norms for positive elliptic operators.

(3) Since C is independent of m the estimate shows that we can improve the accuracy by fixing r_1 and increasing the order of the boundary operator.

Proof

We first consider the case that Dirichlet data is imposed, i.e., (3.1b) is replaced by $u = g$ on Γ_1. By assumption (3.5) and using axial symmetry we have that

(3.7) $$g(\theta) = \sum_{j=0}^{\infty} d_j P_j(\cos\theta) \quad ,$$

where P_j are the Legendre polynomials. It then follows that

$$\int_0^{\pi} |g^2(\theta)| \sin\theta \, d\theta = \sum_{j=0}^{\infty} d_j^2 \quad .$$

If $g(\theta)$ is sufficiently smooth it is also known that for any n (Gottlieb and Orszag [12])

$$|d_j| \leq \frac{C_n}{(j+1)^n} \qquad , \tag{3.8}$$

where C_n depends on n and g but not on j. Using separation of variables, the solution u to (3.1) is given by

$$u(r,\theta) = \sum_{j=0}^{\infty} \frac{d_j P_j(\cos\theta)}{r^{j+1}} \qquad , \tag{3.9a}$$

$$\frac{\partial u}{\partial r}(r,\theta) = -\sum_{j=0}^{\infty} \frac{(j+1)d_j P_j(\cos\theta)}{r^{j+2}} \qquad . \tag{3.9b}$$

It is easy to verify, by induction, that the boundary operators B_m given by (2.10) satisfy

$$B_m(r^k) = \prod_{\ell=1}^{m} (k+\ell)r^{k-m} \equiv A_{k,m} r^{k-m} \qquad . \tag{3.10}$$

Clearly $A_{k,m} = 0$ for $-m \leq k < 0$.

It follows from (3.2b), (3.9) and (3.10) that

$$B_m(w) = B_m(u) = \sum_{j=m}^{\infty} \frac{d_j P_j(\cos\theta) A_{-j,m}}{r^{j+m+1}} \qquad . \tag{3.11}$$

By separation of variables the error w has the form

$$w(r,\theta) = \sum_{j=0}^{\infty} q_j P_j(\cos\theta)[r^j - \frac{1}{r^{j+1}}] \qquad . \tag{3.12}$$

The operator B_m is applied to (3.10) and the result is evaluated at $r = r_1$. Using the completeness of the Legendre polynomials, this series can be equated term by term, with (3.11). We then have

$$(3.13) \qquad q_j = \begin{cases} 0 & j = 0,\ldots, m-1 \\ d_j\left(\dfrac{A_{-(j+1),m}}{A_{j,m}} r_1^{2j} - 1\right)^{-1} & j \geq m \end{cases} .$$

From the definition of $A_{-j,m}$ it is easily verified that

$$\left|\frac{A_{-(j+1),m}}{A_{j,m}}\right| > 1 ,$$

and so

$$(3.14) \qquad |q_j| \leq \frac{|d_j|}{r_1^{2j-1} - 1} \qquad j \geq m ,$$

and

$$|q_j(r^j - \frac{1}{r^{j+1}})| \leq \frac{|d_j| r^j}{r_1^{2j-1} - 1} \leq \frac{2|d_j| r^m}{r_1^{2m-1} - 1} \qquad \begin{array}{l} 1 \leq r \leq r_1 \\ j \geq m \end{array} ,$$

Since, $\| w \|^2_{(r)} = \sum_j |q_j(r^j - \frac{1}{r^{j+1}})|^2 r^2$, the result (3.6a) follows. By differentiating the series for w (3.12), and repeating the process, (3.6b) follows.

The proof for the case of Neumann data is similar. In this case (3.9) and (3.12) are replaced by

$$u(r,\theta) = - \sum_{j=0}^{\infty} \frac{d_j}{(j+1)} \frac{p_j(\cos \theta)}{r^{j+1}} ,$$

and

$$w(r,\theta) = \sum_{j=0}^{\infty} q_j P_j(\cos\theta)[r^j + \frac{j}{j+1} - \frac{1}{r^{j+1}}] \quad .$$

We next consider the case where (3.1) is to be solved exterior to an arbitrary domain Γ_1. We restrict the proofs by only considering $m = 1,2$. The proof relies on the generalized maximum principle discussed by Protter and Weinberger [26]. To apply these methods we assume that Γ_1 has the property that every $x \in \Gamma_1$ lies on the boundary of a ball contained in the exterior of Γ_1. We first need

Lemma 3.1

Let w satisfy

$$\begin{aligned} \Delta w &= 0 && \text{in } \Omega \quad , \\ \frac{\partial w}{\partial n} &= 0 && \text{on } \Gamma_1 \quad , \\ B_j w &= h && \text{on } \Gamma_2 \text{ for } j = 1,2 \quad . \end{aligned} \tag{3.15}$$

Suppose there exists functions z_1, z_2 such that

$$\begin{aligned} \Delta z_1 &\le 0 && \text{in } \Omega \quad , \\ \frac{\partial z_1}{\partial n} &\le 0 && \text{on } \Gamma_1 \quad , \\ B_j z_1 &\ge h && \text{on } \Gamma_2 \quad j = 1,2 \quad , \end{aligned} \tag{3.16}$$

and

$$\Delta z_2 \geq 0 \qquad \text{in } \Omega \quad ,$$

$$\frac{\partial z_2}{\partial n} \geq 0 \qquad \text{on } \Gamma_1 \quad ,$$

$$B_j z_2 \leq h \qquad \text{on } \Gamma_2 \qquad j = 1,2 \quad ,$$

then

$$z_2 \leq u \leq z_1 \qquad \text{in } \Omega \quad .$$

We make several observations

1. The normal derivative is taken in the direction away from the origin. Hence, for a sphere $\frac{\partial u}{\partial n} = \frac{\partial u}{\partial r}$.
2. Similar results hold when Dirichlet data is imposed on the inner body.
3. The results are valid for any uniformly elliptic equation in Ω.

Proof.

For $j = 1$ the lemma is a restatement of theorem 12 of [26]. When B_2 is used the result follows from the observation that the proof of Protter and Weinberger only requires that when w has a positive maximum on Γ_2 then $B_2 w$ is positive. This follows from the form of B_2.

Based on this lemma we have

Theorem 3.2

For an arbitrary body Γ_1 and using the boundary operator B_1 on Γ_2 the error satisfies

$$|w| \leq \frac{c}{r_1^2} \qquad \text{pointwise.} \tag{3.18}$$

Furthermore, using the operator B_2 on Γ_2 the error satisfies

$$(3.19)\qquad |w| \leq \frac{C}{r_1^3} \qquad \text{pointwise} \quad .$$

Proof.

The boundary condition $B_1 w$ can be expressed as

$$\left|\frac{\partial w}{\partial r} + \frac{w}{r}\right| = |h| \leq \frac{C}{2r_1^3} \quad .$$

We choose for the lemma $z_1 = \frac{C}{r_1^2}$ and $z_2 = -z_1$. Straightforward algebra shows that z_1 and z_2 satisfy (3.16) and (3.17) respectively. (3.18) then follows from the conlcusion of the lemma. For the boundary condition B_2 we choose $z_1 = \frac{C}{r_1^3}$ and $z_2 = -z_1$ and again (3.19) follows.

We note that the exact solution to the exterior problem decays at least as fast as $1/r$. Hence, the uniform error bounds given by (3.18) and (3.19) express a smaller relative error at the body Γ_1 then near the artificial surface $r = r_1$. For some applications one wishes error bounds for the normal derivative on Γ_1. The bounds can be obtained by deriving a Fredholm equation of the second kind for $\frac{\partial w}{\partial n}$ on Γ_1. A theorem valid for $k \geq 0$ will be given in the next section.

IV. Error Bounds for the Helmholtz Equation

The problem that we wish to solve is

(4.1a) $$\Delta u + k^2 u = 0 \qquad \text{exterior to } \Gamma_1 ,$$

(4.1b) $$\frac{\partial u}{\partial n} = g \qquad \text{on } \Gamma_1 ,$$

(4.1c) $$\frac{\partial u}{\partial r} - i k u = o(\frac{1}{r}) \qquad \text{as } r \to \infty .$$

As before we replace condition (4.1c) by

(4.1d) $$B_m v = 0 \qquad \text{on } \Gamma_2 ,$$

where v also satisfies (4.1a, 4.1b). Let w be the error, $w = u - v$. Then w satisfies

(4.2a) $$\Delta w + k^2 w = 0 \qquad \text{in } \Omega ,$$

(4.2b) $$\frac{\partial w}{\partial n} = 0 \qquad \text{on } \Gamma_1 ,$$

(4.2c) $$B_m w = B_m u \equiv h \qquad \text{on } \Gamma_2 ,$$

where B_m is given by (2.6) (see Figure 1). For simplicity we only consider the case of axial symmetry, however, all results hold for the general three dimensional problem as well as the for the Dirichlet problem. As in section 3 we restrict the proofs to the case that the artificial surface is the sphere $r = r_1$. We are interested in error estimates on surfaces and use the surface norm given by (3.4). We then have

Theorem 4.1.

Given equations (4.2) and $m = 1$ the error w has the bound

$$\|w\|_{(r_1)} \leq \frac{\|h\|_{(r_1)}}{k} \quad . \tag{4.3}$$

Proof.

Let $\overline{w}$ denote the complex conjugate of w. Then from Green's theorem and (4.2) we have

$$\int_{\Omega} |\operatorname{grad} w|^2 dV - k^2 \int_{\Omega} |w^2| dV = \int_{\Gamma_2} \overline{w} \frac{\partial w}{\partial r} dA \quad . \tag{4.4}$$

Using the definition of B_1 we also have

$$\int_{\Gamma_2} \overline{w} \frac{\partial w}{\partial r} dA = ik \int_{\Gamma_2} |w^2| dA + \int_{\Gamma_2} wh \, dA \quad . \tag{4.5}$$

We then substitute (4.5) into (4.4). Taking the imaginary part of the resulting equation yields

$$\|w\|^2_{(r_1)} = \int_{\Gamma_2} |w|^2 dA = \frac{1}{k} \int_{\Gamma_2} wh \, dA \leq \frac{\|w\|_{(r_1)} \|h\|_{(r_1)}}{k} \quad . \tag{4.6}$$

Dividing both sides by $\|w\|_{(r_1)}$ gives the estimate (4.3).

Since $h = B_1 u$ we know that $|h| \leq \frac{C}{r^3}$ where C depends only on g and k. Hence, (4.3) is equivalent to

$$\|w\|_{(r_1)} \leq \frac{C}{kr_1^2} \quad . \tag{4.7}$$

Using the definition of B_1 we also have

$$(4.8) \qquad \left\| \frac{\partial w}{\partial r} \right\|_{(r_1)} \le (k + \frac{1}{r}) \| w \|_{(r_1)} + \| h \|_{(r_1)}$$

$$\le (2 + \frac{1}{kr}) \| h \|_{(r_1)} \le \frac{C}{r^2}(2 + \frac{1}{kr}) \quad .$$

In theorem (4.1) we considered the boundary operator B_1. We now consider the operator B_2 but restrict the body Γ_1 to be a sphere. We then have

<u>Theorem 4.2</u>

Consider equation (4.2) with $m = 2$ and Γ_1 the sphere $r = 1$. Then the solution w satisfies the bound

$$(4.9) \qquad \| w \|_{(r_1)} \le (1 + \frac{kr_1}{4}) \frac{\| h \|_{(r_1)}}{k^2} \quad .$$

We note that by the construction of B_2 we have

$$|h| \le \frac{C}{r_1^5} \quad ,$$

where C depends only on g and k. It follows that

$$\| h \|_{(r_1)} \le \frac{C}{r_1^4} \quad ,$$

and (4.9) can be restated as

$$(4.10) \qquad \| w \|_{(r_1)} \le \frac{C}{r_1^3} \left(\frac{1}{r_1 k^2} + \frac{1}{4k} \right)$$

A similar result holds for the Dirichlet problem.

Proof

By separation of variables (assuming axial symmetry) the solution to (4.2) has the expansion

$$(4.11) \qquad w = \sum_{\ell=0}^{\infty} H_\ell(kr) P_\ell(\cos\theta) \quad ,$$

where H_ℓ are the spherical Bessel function and P_ℓ are the Legrendre polynomials. Hence H_ℓ satisfies the ordinary differential equation

$$(4.12) \qquad H_\ell'' + \frac{2}{r} H_\ell' + (k^2 - \frac{\lambda}{r^2}) H_\ell = 0 \quad ; \quad \lambda = \ell(\ell+1) \quad .$$

Similarly, by completeness, $B_m u \equiv h$ has an expansion

$$(4.13) \qquad h = \sum_{\ell=0}^{\infty} h_\ell P_\ell(\cos\theta) \quad .$$

By orthogonality it is sufficient to only consider one term in (4.11). We thus have reduced the problem to a one dimensional problem. Let $\phi = H_\ell(r)$, then

$$(4.14a) \qquad \phi'' + \frac{2}{r}\phi' + (k^2 - \frac{\lambda}{r^2})\phi = 0 \quad , \qquad 1 \le r \le r_1 \; ,$$

$$(4.14b) \qquad \phi'(1) = 0 \quad ,$$

$$(4.14c) \qquad B_2\phi = \phi'' + \frac{4}{r}\phi' + (\frac{2}{r} - k^2)\phi - 2ik(\phi' + \frac{2}{r}\phi) = h_\ell \qquad r = r_1 \quad .$$

We note that for the Dirichlet problem (4.14b) is replaced by $\phi(1) = 0$. For the Neumann problem we define q by $q = \phi(1)$. We then introduce a normalized variable

$$\psi = \phi/q \quad . \tag{4.15}$$

It follows form (4.14) that ψ is real. We then take the real and imaginary parts of (4.14c) and replace ϕ by ψ. Using (4.12) to eliminate the second derivatives, we obtain

$$\psi' + \frac{2}{r_1}\psi = -Im\left(\frac{h_\ell}{2qk}\right) \equiv \tilde{h}_1 \quad , \tag{4.16a}$$

and

$$\frac{2}{r}\psi' + \left(\frac{2}{r_1^2} + \frac{\lambda}{r_1^2} - 2k^2\right)\psi = Re\left(\frac{h_\ell}{q}\right) \equiv \tilde{h}_2 \quad , \tag{4.16b}$$

where both equations hold at $r = r_1$.

We need to consider two cases depending on which harmonic ℓ was chosen.

<u>Case I:</u> $\quad \dfrac{\lambda}{r_1^2} > k^2 \qquad\qquad \lambda = \ell(\ell+1)$.

In this case $\psi(1) = 1$, $\psi'(1) = 0$ together with (4.12) imply that ψ, ψ', ψ'' are all positive in a neighborhood of $r = 1$. This condition must persist at least until $r \geq r_*$ where $\psi''(r_*) < 0$, $\psi'(r_*) = 0$ and $\psi(r_*) > 0$. However, combining these conditions with (4.12) we see that $r_* > r_1$. Since we are only interested in $1 \leq r \leq r_1$ we conclude that ψ,ψ' are positive in the whole interval. In particular $\psi(r_1) > 0$, $\psi'(r_1) > 0$. Using (4.16) we have

$$\frac{2}{r}\,\psi(r_1) \le \psi' + \frac{2}{r_1}\psi \le |\tilde{h}_1| \le \frac{|h_\ell|}{2k|q|} \quad .$$

Since $\phi = q\psi$ we have

$$|\phi(r_1)| \le \frac{kr_1}{4}\left|\frac{h_\ell}{k^2}\right| \quad , \tag{4.17}$$

which is a stronger estimate than (4.9).

We now consider

<u>Case II:</u> $\qquad \dfrac{\lambda}{r_1^2} \le k^2 \quad .$

We now solve (4.16) for $\psi(r_1)$ and obtain

$$\psi(r_1)\left(\frac{\lambda}{r_1^2} - \frac{2}{r_1^2} - 2k^2\right) = \tilde{h}_2 - \frac{\tilde{h}_1}{r_1^k} \quad . \tag{4.18}$$

Since $\dfrac{\lambda}{r_1^2} \le k^2$ we have that

$$\left|\frac{\lambda}{r_1^2} - \frac{2}{r_1^2} - 2k^2\right| \ge k^2 + \frac{2}{r_1^2} \quad .$$

Hence, using (4.18) and $\phi = q\psi$ we have

$$k^2\left(1+ \frac{2}{r_1^2k^2}\right)\frac{|(r_1)|}{|q|} \le \frac{2|h_\ell|}{|q|}\left(1+\frac{1}{rk}\right) \quad ,$$

or

$$(4.19)\qquad |\phi(r_1)| \leq \frac{|h_\ell|}{k^2} \quad ,$$

which again is a stronger estimate than (4.9). We finally point out that (4.9) and (4.16a) imply

$$(4.20)\qquad \| \phi'(r_1) \| \leq \frac{\| h \|}{k}\left[\tfrac{1}{2} + \frac{2}{r_1 k}\left(1 + \frac{kr_1}{4}\right)\right] = 0\left(\frac{1}{r_1^3}\right),$$

since $h = 0\left(\frac{1}{r_1^5}\right)$.

The results of Theorems 4.1 and 4.2 can be stated as

$$(4.21)\qquad \| w \|_{(r_1)}, \ \| w_r \|_{(r_1)} = 0(1/r_1^{m+1}) \quad ,$$

for $m = 1$ and 2. We now extend these results from the outer surface $r = r_1$ to the body Γ_1. Introducing the notation

$$\| w \|_{(\Gamma_1)} = \sqrt{\int_{\Gamma_1} |w|^2 \, dA} \quad ,$$

for the surface L_2 norm; we then have

Theorem 4.2

For the problem (4.2) we have

$$(4.22)\qquad \| w \|_{(\Gamma_1)} \leq C\left[\| w \|_{(r_1)} + \| w_r \|_{(r_1)}\right] \quad ,$$

where C depends only on k and Γ_1.

Note: (1) An entirely analogous theorem holds for $\| w_n \|_{(r_1)}$ when the Dirichlet problem is considered.

(2) C is continuous in k and the result holds for $k = 0$.

(3) Since $u = O(\frac{1}{r})$ the relative error expressed in (4.22) is smaller than that expressed in (4.21).

Proof

Let $G(p,q)$ denote the free space Green's function

$$G(p,q) = \frac{e^{ik|p-q|}}{4\pi|p-q|} \quad . \tag{4.23}$$

Using Green's theorem applied to w in the region Ω (see figure 1) we have for $p \in \Omega$ (making use of (4.2b)

$$w(p) = \int_{|q|=r_1} G(p,q)w_n(q) - w(q)G_{n_q}(p,q)\, d\,A_q \tag{4.24}$$

$$+ \int_{q \in \Gamma_1} w(q)G_{n_q}(p,q)\, d\,A_q \quad ,$$

where the normal on Γ_1 points toward the exterior and the normal on $|q| = r_1$ is in the direction of increasing r. Upon letting p approach Γ_1 and using the standard jump relations of potential theory ([15]) we obtain

$$I(w) = \int_{|q|=r_1} (G(p,q)w_n(q) - w(q)G_{n_q}(p,q))\, d\,A_q \quad , \tag{4.25}$$

where I is the integral operator (see [9])

$$I(w) = \frac{w(p)}{2} - \int_{q \in \Gamma_1} G_{n_q}(p,q)w(q)\, d\,A_q \; .$$

It is clear that the right hand side of (4.25) satisfies (4.22). It is shown in [9] that $I(w)$ is invertible except for a discrete set of values of k and this establishes (4.22) except for these interior resonances. At the interior resonances we replace G by the modified Green's function of Ursell ([32]) and use the same proof.

V. Numerical Results

We consider the three dimensional Helmholtz equation in spherical coordinates with axial symmetry. Using r and θ as coordinates the equation becomes

$$\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2 \sin\theta}\ \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial u}{\partial\theta}\right) + k^2 u = 0 \quad . \tag{5.1}$$

The first two radiation boundary conditions are

$$B_1 u = \frac{\partial u}{\partial r} - i k u + \frac{u}{r} = 0 \quad , \tag{5.2a}$$

and

$$B_2 u = \frac{\partial^2 u}{\partial r^2} + \left(\frac{4}{r} - 2 i k\right) \frac{\partial u}{\partial r} + \left(\frac{2}{4} - 4 i k\right) \frac{u}{r} - k^2 u = 0 \quad . \tag{5.2b}$$

To eliminate $\frac{\partial^2 u}{\partial r^2}$, (5.2b) can be rewritten as

$$\frac{\partial u}{\partial r} = -\left(\frac{1}{r} - i k\right) u + \frac{\frac{\partial}{\partial\theta}\left(\frac{\partial u}{\partial\theta} \sin\theta\right)}{2r^2\left(\frac{1}{r} - i k\right)\sin\theta} \quad . \tag{5.2c}$$

We only consider the case that the body is a sphere, given by $r = r_0$. The radiation conditions are specified on the sphere $r = r_1$. On the body Neumann data

$$(5.3) \qquad \frac{\partial u}{\partial n} = h \qquad \text{on } \Gamma_1: \quad r = r_0$$

is given.

The Helmholtz equation is solved by a finite element code using linear elements. The radiation boundary condition is also written in weak form following an integration by parts. Details are given in the appendix. Richardson extrapolation in the theta direction is used for all results. This substantially increases the accuracy of the computed solutions, especially for the higher frequencies. The limiting factor in the method is the storage requirements of the banded Gauss solver. The use of higher order elements or iterative techniques would reduce the storage requirements.

We first consider acoustic scattering by a point source at a fixed axial point q. We then have

$$(5.4) \qquad \begin{array}{lll} \text{a)} & \Delta u + k^2 u = \delta(p-q) \quad , & r_0 < r < \infty \quad , \\ \text{b)} & \dfrac{\partial u}{\partial r} = 0 \quad , & r = r_0 \quad , \\ \text{c)} & \dfrac{\partial u}{\partial r} - iku = o(\frac{1}{r}) \quad , & r \to \infty \quad . \end{array}$$

Here, p denotes the dependent variable and q is the source point. (5.4) implies that the scatterer is hard, i.e., the normal acoustic velocity is zero on the body.

The singularity in (5.4) is eliminated by introducing v given by

$$v = u - \frac{e^{ik|p-q|}}{4\pi|p-q|} \quad .$$

The equations for v are then

$$
(5.5) \qquad
\begin{aligned}
&a) \quad \Delta v + k^2 v = 0, \\
&b) \quad \frac{\partial v}{\partial r} = - \frac{\partial}{\partial r} \left(\frac{e^{ik|p-q|}}{4\pi|p-q|} \right) \Bigg|_{r = r_0}, \\
&c) \quad \frac{\partial v}{\partial r} - i k v = o(\frac{1}{r}), \qquad r \to \infty.
\end{aligned}
$$

To solve this system according to the previously described procedure, we replace (5.5c) by

$$
(5.5d) \qquad B_1 v = 0, \qquad r = r_1,
$$

or

$$
(5.5e) \qquad B_2 v = 0, \qquad r = r_1.
$$

The "exact" solution was generated by using an integral equation code with a fine grid. This code had been previously checked by comparisons with analytic solutions presented in [6] to verify its accuracy.

In Table I we present the relative surface L^2 errors for various k. The data in this table was obtained with a fixed number of points $(N = 5)$ in the radial direction. For these computations the body has radius $r_0 = \frac{1}{2}$. The source is located on the axis at $r = .6$. Similar results have been obtained for a wide range of source positions.

The results given in Table I indicate that for the problem considered the error due to the artificial boundary decreases as k increases. Specifically the grid in the normal direction can be chosen independent of k.

One can also bring in the artificial surface so that it coincides with the inner boundary. In this case only an ordinary differential equation needs to be solved. However, this resulted in substantial errors and accurate solutions could not be obtained.

The results of Table I show that the first order boundary condition (5.2a) is not good enough for many computations. Except for the lowest of frequencies 10 percent accurate solutions could not be obtained using (5.2a) because of storage difficulties that arise from using a large r_1.

We next consider the Helmholtz equation with a variable k. We choose k in (5.4a) as

$$k = \begin{cases} 4\left(1 - \dfrac{r - r_0}{.15}\right) & r_0 \leq r \leq r_0 + .15 \\ 3 & r_0 + .15 \leq r. \end{cases}$$

We choose $r_0 = \frac{1}{2}$ and consider a sequence of outer boundary positions r_1. The "exact" solution is generated by choosing the outer boundary sufficiently far away so that the solutions obtained by using the first or second order boundary conditions differed by less than 3 percent. The solution obtained by using B_2 at this r_1 was taken as the "exact" solution.

Since k is variable inside the region the Green's function is not known. Hence, one can not use Green's formula to calculate the far field solution given u and $\frac{\partial u}{\partial n}$ at $r = r_0$. Instead u and $\frac{\partial u}{\partial n}$ on the outer boundary can be used to find the far field solution, since k is constant beyond the outer boundary. The value of $\frac{\partial u}{\partial n}$ on the outer boundary can be calculated from u and its tangential derivatives by using the boundary conditions (5.2a or 5.2c). The tangential derivatives can be eliminated by integration by parts in the Green's formula.

In figure 2 we plot the relative surface errors over the outer surface for different values of r_1. The improvement achieved by using B_2 (5.2c) rather than B_1 (5.2a) is evident.

As the final example we consider Laplace's equation. The exact solutions are generated by imposing Neumann data corresponding to a monopole or dipole centered at an axial point p_s inside r_1 and displaced from the origin of coordinates. The solution is

$$u = \frac{1}{4\pi|p-p_s|}, \tag{5.7a}$$

and

$$u = \frac{\cos\theta'}{|p-p_s|^2}, \tag{5.7b}$$

for the monopole and dipole respectively. Here θ' denotes the polar angle in a polar coordinate system centered at p_s.

It is well known that general solutions to Laplace's equation in exterior domains can be expressed as a superposition of surface monopoles or surface dipoles ([15]). Hence, the model problems (5.7) are relevant to realistic problems especially when p_s is chosen near the body surface.

In table 2 we present the surface errors, over the inner surface ($r = \frac{1}{2}$), for several different cases. The solution types M and D denote the monopole (5.7a) or dipole (5.7b) solution respectively.

The first order condition is exact for a monopole centered at the origin while the second order boundary condition is exact for both monopoles and dipoles centered at the origin. When the second order condition is used for the displaced dipole (5.7b) it is more accurate than the first order condition is for a displaced monopole (5.7a). For small p_s the dipole has no $1/r$ contribution and the first order condition is expected to be inaccurate. These results again confirm the substantial improvements that can be obtained by the use of (5.2c). The decay rate of the error as a function of r_1, as predicted in Theorem (3.1) has also been computationally verified.

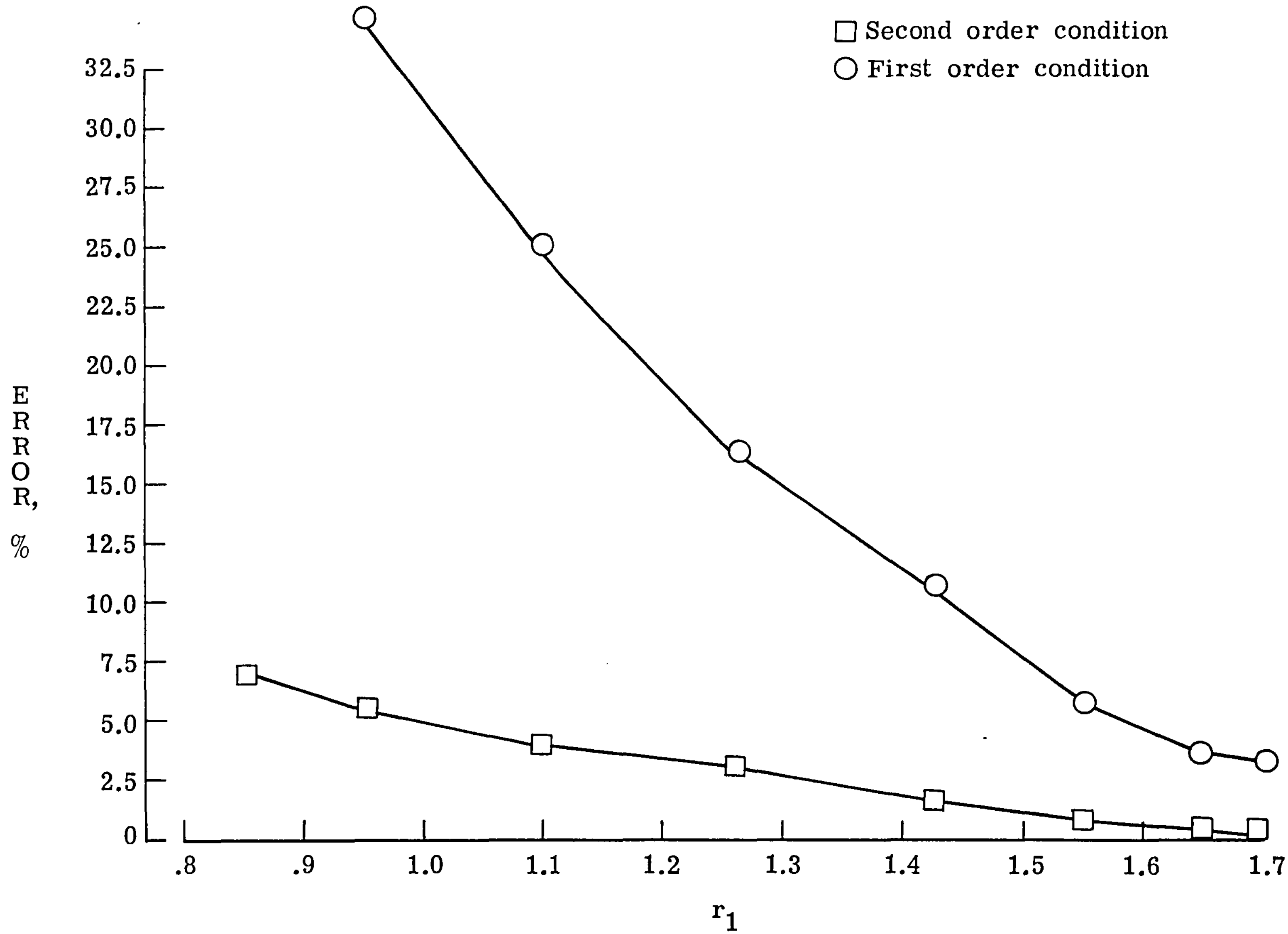

Figure 2.- Errors for variable coefficient problem.

TABLE 1

Relative surface L^2 errors for the Helmholtz equation

kr_0	r_1	m	error
11	.645	1	18.6
11	.645	2	5.4
23.6	.575	1	31.5
23.6	.575	2	6.5

TABLE 2

Relative surface L^2 errors for the Laplace equation

Solution type	p_s	r_1	m	error
M	.2	.57	1	14.7
M	.2	.57	2	1.1
M	.2	.64	1	9.4
M	.2	.64	2	0.6
D	.2	.57	1	65.0
D	.2	.57	2	8.9
D	.2	.64	1	38.3
D	.2	.64	2	4.9
M	.4	.60	1	25.4
M	.4	.60	2	4.1
M	.4	.65	1	17.7
M	.4	.65	2	2.7
D	.4	.60	1	35.4
D	.4	.60	2	10.5
D	.4	.65	1	21.6
D	.4	.65	2	7.2

APPENDIX

In this section we consider the problem of implementing the boundary conditions corresponding to B_1 and B_2. From (2.6) we see that these conditions have the general form

$$B_1 u = \frac{\partial u}{\partial r} + \gamma_1 u = 0, \tag{A.1}$$

and

$$B_2 u = \frac{\partial^2 u}{\partial r^2} + \beta_1 \frac{\partial u}{\partial r} + \gamma_1 u = 0. \tag{A.2}$$

Here α_1, β_1, and γ_1 are complex functions depending only on k and r and not on the angular variables which are given explicitly in (5.2a) and (5.2b).

For simplicity we will consider only axially symmetric problems, so that the Helmholtz equation

$$\Delta u + k^2 u = 0, \tag{A.3}$$

may be written as

$$\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}(\sin\theta \frac{\partial u}{\partial \theta}) + k^2 u = 0. \tag{A.4}$$

The presence of the $\frac{\partial^2 u}{\partial r^2}$ term in (A.2) is nonstandard and difficult to implement directly. Since the boundary will be the sphere $r = r_1$ it is convenient to eliminate the $\frac{\partial^2 u}{\partial r^2}$ term in (A.2) by using (A.4) so that only tangential second derivatives appear in the boundary condition.

This can also be done for arbitrary shapes of the artificial boundary. The result can be express in the form

(A.5) $$B_2 u = \gamma_2 \frac{\partial u}{\partial r} + \frac{\beta_2}{\sin\theta} \frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta}) + \alpha_2 u = 0,$$

where α_2, β_2, γ_2 depend only on k and r and not on θ and are given explicitly in (5.2c). The functional form of (A.5) also includes the boundary operator B_1 (with $\beta_2 = 0$).

The computational problem is to solve (A.3) in a region Ω exterior to an inner boundary Γ_1 and interior to the sphere $r = r_1$. On $r = r_1$ we impose (A.5) while on Γ_1 we may impose either Dirichlet or Neumann data. For concreteness we assume that Neumann data is specified, i.e.

(A.6) $$\frac{\partial u}{\partial n} = g(r,\theta) \qquad \text{on } \Gamma_1.$$

The numerical method employed is a Galerkin finite element technique which we now describe.

Consider the following weak formulation of the problem (A.3), (A.5), (A.6). We seek a function u in a Hilbert space H_m such that

(A.7) $$B(u,v) = F(v),$$

for all v in H_m where

(A.8) $$B(u,v) = \iint_\Omega [\nabla u \cdot \nabla v - k^2 uv] r^2 \sin\theta \, d\theta \, dr + \int_{r=r_1} [\frac{\beta_2}{\gamma_2} \frac{\partial u}{\partial\theta} \frac{\partial v}{\partial\theta} - \frac{\alpha_2}{\gamma_2} uv] r_1^2 \sin\theta \, d\theta,$$

and

$$F(v) = -\int_{\Gamma_1} g(r,\theta) v \, d\, s.$$

The boundary integral terms in (A.8) come from using (A.5) and integrating by parts in θ. We note that $r^2 \sin\theta$ comes from the three dimensional volume element. Our approximation problem is to choose a finite dimensional subspace S^h of H_m and then seek a $u^h \in S^h$ such that

$$B(u^h, v^h) = F(v^h), \tag{A.9}$$

for all $v^h \in S^h$.

It is easy to see that if u is a sufficiently smooth solution to (A.7) then u will be a solution to (A.3), (A.5) and (A.6). For $m = 1$ the above weak formulation almost leads to a standard finite element problem, once S^h is chosen to be some finite element space. Indeed, for $m = 1$, $\beta_2 = 0$ and we may choose $H_1 = H^1(r)$, i.e., the Sobolev space of functions with one distributional derivative. The only complication is the appearance of the term $(r^2 \sin\theta)$ in the integrals. For $m = 2$, we need more smoothness on the boundary $r = r_1$ due to the first term in the boundary integral in (A.8). The choice $H_2 = H^1(\Omega) \times H^1(r{=}r_1)$ suffices. For either $m = 1$ or $m = 2$ we may choose S^h to be the finite element space defined by subdividing Ω into triangular elements and then restricting the function in S^h to be continuous in Ω and linear in each triangle, i.e. a piecewise linear finite element space. Then we compute u^h in the standard manner, i.e. we choose a (local) basis for S^h, expand u^h in terms of this basis, and let v^h in (A.9) range over the basis to obtain a system of algebraic equations for the nodal values of u^h.

Numerical experiments confirm that when both the θ and r grids are refined that h^2 convergence rates are obtained. These convergence rates were verified for both the first order $B_1 u = 0$ and second order $B_2 u = 0$ boundary conditions. Hence, the second order derivatives that appear in B_2 did not cause any deterioration in the rate of convergence. When only the θ mesh was refined and the errors were measured on the inner boundary a convergence rate of order h was observed.

The computations presented in this paper were intended to exhibit the improvements due to increasing the order of the boundary operators. For this reason, it was desired to minimize discretization errors due to the finite element approximation. It has been verified that the higher order conditions did not affect the rate of convergence of the discretization scheme.

REFERENCES

[1] S. AGMON, A. DOUGALIS, and L. NIRENBERG, *Estimates near the boundary for solutions of elliptic partial differential equations satisfying general boundary conditions, I.*, Comm. Pure Appl. Math., 12 (1959, pp. 623-727.

[2] F. V. ATKINSON, *On Sommerfeld's "Radiation Condition"*, The Philosophical Magazine, 40 (1949), pp. 645-651.

[3] A. K. AZIZ and B. KELLOGG, *A scattering problem in the Helmholtz equation*, Advances in Computer Methods for Partial Differential Equations III, IMACS, 1979.

[4] A. BAYLISS, *On the use of coordinate stretching in the numerical computation of high frequency scattering*, J. Sound Vibration, 60 (1978), pp. 543-553.

[5] A. BAYLISS and E. TURKEL, *Radiation boundary conditions for wave-like equations*, ICASE Report No. 79-26, to appear.

[6] J. J. BOWMAN, T. B. A. SENIOR, and L. E. USLENGHI, editors, *Electromagnetic and Acoustic Scattering by Simple Shapes*, North-Holland Publishing Company, Amsterdam, 1969.

[7] A. BRANDT, *Multi-level adaptive solutions to boundary-value problems*, Math. of Comput., 31 (1977), pp. 333-390.

[8] A. J. BURTON and G. F. MILLER, *The application of integral equation methods to the numerical solution of some exterior boundary-value problems*, Proc. Royal Society London A323 (1971), pp. 201-210.

[9] G. CHERTOCK, *Integral equation methods on sound radiation and scattering from arbitrary surface*, Report 3938, David W. Taylor Naval Ship Research and Development Center, June 1971.

[10] G. J. FIX and S. P. MARIN, *Variational methods for underwater acoustic problems*, J. Comput. Phys., 28 (1978), pp. 253-270.

[11] C. I. GOLDSTEIN, *Numerical methods for Helmholtz type equations in unbounded regions*, Brookhaven report, BNL-26543, May 1979.

[12] D. GOTTLIEB and S. ORSZAG, *Numerical Analysis of Spectral Methods: Theory and Applications*, SIAM Regional Conference Series in Appl. Math., 1977.

[13] G. HELLWIG, *Partial Differential Equations*, Blaisdell Publishing Company, New York, 1964.

[14] S. N. KARP, *A convergent "far-field" expansion for two dimensional radiation functions*, Comm. Pure Appl. Math. 14 (1961), pp. 427-434.

[15] O. B. KELLOGG, *Foundations of Potential Theory*, Dovan Publications, New York, 1953.

[16] R. E. KLEINMAN and G. F. ROACH, *Boundary integral equations for the three dimensional Helmholtz equation*, SIAM Review, 16 (1974), pp. 214-236.

[17] G. KRIEGSMANN and C. S. MORAWETZ, *Numerical solutions of exterior problems with the reduced wave equation*, J. Comput. Phys., 28 (1978), pp. 181-197.

[18] H. LAMB, *Hydrodynamics*, Dover Publications, New York, 1945.

[19] P. D. LAX, *A Phragmén-Lindelöf theorem in harmonic analysis and its application to some questions in the theory of elliptic equations*, Comm. Pure Appl. Math., 10 (1957), pp. 123-151.

[20] Ya. B. LOPATINSKII, *On a method of reducing boundary problems for a system of differential equations of elliptic type to regular equations*, Ukrain. Mat. Z., 5 (1953), pp. 123-151.

[21] S. P. MARIN, *A finite element method for problems involving the Helmholtz equation in two dimensional exterior regions*, Ph.D. Thesis, Carnegie-Mellon University, March 1978.

[22] C. MÜLLER, *Foundations of the Mathematical Theory of Electromagnetic Waves*, Springer-Verlag, New York, 1969.

[23] R. A. NICOLAIDES, *On some theoretical and practical asnects of multi-grid methods*, Math. Comput., 33 (1979), pp. 933-952.

[24] A. J. POGGIO and E. K. MILLER, *Integral equation solutions of three dimensional scattering problems*, Computer Techniques for Electromagnetics, R. Mittra, ed., Pergamon Press, Oxford, 1973, pp. 159-265.

[25] W. PROSKOROWSKI and O. WIDLUND, *On the numerical solution of Helmholtz's equation by the capacitance matrix method*, Math. Comput., 30, (1976), pp. 433-468.

[26] M. H. PROTTER and F. WEINBERGER, *Maximum Principles in Differential Equations*, Prentice Hall, Englewood Cliffs, NJ, 1967.

[27] F. RELLICH, *Uber das asymptotishce verhatlen der Rosungen von $\Delta u + \lambda u = 0$ in unendlichen gebieten*, Jahresber Deutsch. Math. Verein, 53 (1943), pp. 57-65.

[28] H. SCHNECK, *Improved integral formulation for acoustic radiation problems*, J. Acoustical Society of America, 44 (1968), pp. 41-58.

[29] A. SOMMERFELD, *Partial Differential Equations in Physics*, Academic Press, New York, 1964.

[30] J. A. STRATTON, *Electromagnetic Theory*, McGraw-Hill, New York, 1941.

[31] M. TAYLOR, *Pseudo-Differential Operators*, Springer-Verlag Lecture in Math., 416, 1974.

[32] F. URSELL, *On the exterior problems in acoustics*, Proc. Cambridge Philos. Soc., 74 (1973), pp. 117-125.

[33] B. VAINBERG, *Principles of radiation, limit absorption and limit amplitude in the general theory of partial differential equations*, Russian Mathematical Surveys, 21 (1966), pp. 115-193.

[34] C. H. WILCOX, *A generalization of theorems of Rellich and Atkinson,* Proc. Amer. Math. Soc., (1955), pp. 271-276.

[35] C. H. WILCOX, *Spherical means and radiation conditions*, Arch. Rat. Mech., 3 (1959(, pp. 133-148.

[36] C. H. WILCOX, *Scattering Theory for the D Alembert Equation in Exterior Domains*, Springer-Verlag Lecture Notes in Math., 442, 1975.

[37] O. C. ZIENKIEWICZ, D. W. KELLY, and P. BETTESS, *Marriage a la mode - the best of both worlds finite elements and boundary integrals,* Energy Methods in Finite Element Analysis, R. Glowinski, E. Y. Rodin, O. C. Zienkiewicz, ed., John Wiley and Sons, New York, 1978, pp. 81-108.

INSTITUTE FOR COMPUTER APPLICATIONS
IN SCIENCE AND ENGINEERING
Mail Stop 132 C
NASA Langley Research Center
Hampton, Virginia 23665