THE BELL SYSTEM TECHNICAL JOURNAL
Vol. 57, No. 8, October 1978
Printed in U.S.A.

Boundary Integral Solutions of Laplace's Equation

By J. L. BLUE

(Manuscript received January 26, 1978)

Although Laplace's equation is simple, the region over which it is to be solved is often complicated. Both the shape of the region and the boundary conditions can induce solutions Φ which are singular at isolated points on the boundary of the region.

Boundary integral equation methods are well-suited to the problem, reducing a two-dimensional partial differential equation to a one-dimensional integral equation. Unfortunately, the standard boundary integral equation methods lead to an ill-conditioned set of linear equations, restricting the achievable accuracy in the approximate solution.

This paper describes an improved boundary integral method. A new integral equation is derived. Laplace's equation is reduced to solving two coupled, one-dimensional integral equations. The resulting linear equations are well-conditioned.

A program package for solving Laplace's equation has been developed. The package solves Laplace's equation in two dimensions or in three dimensions with axial symmetry. The region may extend to infinity, and may be multiply-connected. In addition to smooth basis functions, the program automatically includes appropriate singular basis functions, greatly improving the achievable accuracy for regions with corners.

I. INTRODUCTION

Laplace's equation frequently arises in modeling physical problems, especially in electromagnetism, in thermal flow, and in fluid flow. In two dimensions, Laplace's equation is

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = 0,$$

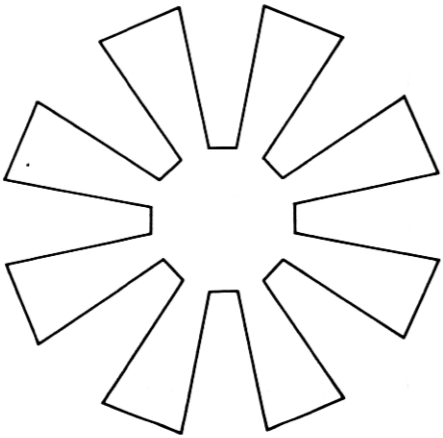

Fig. 1—Region used in an analysis of an electrostatic lens.

and in three dimensions,

$$\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}+\frac{\partial^2\Phi}{\partial z^2}=0.$$

To complete the specification of a particular problem, a region on which to solve Laplace's equation must be specified, plus boundary conditions on the boundary of the region.

As compensation for the simplicity of the partial differential equation, the region over which Laplace's equation is to be solved is often complicated. Figure 1 shows the region used by the author in an unpublished analysis of an electrostatic lens. The solution is singular at the re-entrant corners. (By singular, we mean that Φ has a finite limit as the corner is approached, but that some derivatives of Φ do not have a finite limit.) The singularity is a consequence of the region itself, not of any particular boundary conditions. In fact, the solution is singular unless very special boundary conditions are prescribed.

Even with a rectangular region, the solution can be singular at isolated points. Figure 2 is an example, a thin-film capacitor with metal top and bottom contacts. To obtain its capacitance, Laplace's equation must be solved inside the rectangle. The boundary conditions are $\Phi = 1$ on the top contact, $\Phi = 0$ on the bottom contact, and zero normal derivative, $\partial\Phi/\partial n = 0$, on the remainder of the boundary. (The definition of the normal derivative is given in the next section.) At the center edge of the top contact, the solution is singular.

Standard methods for elliptic partial differential equations include finite difference and finite element methods. Both methods require a grid, usually rectangular or triangular, everywhere inside the region. Thus the region must be bounded. Both methods are difficult to apply

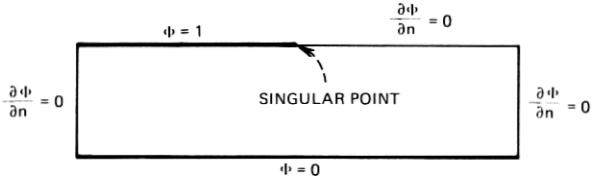

Fig. 2—Region used in an analysis of a thin-film capacitor. The potential is singular at the center of the top side.

to complicated regions; if the true solution has singularities, accuracy is usually poor unless heroic measures are taken. Neither method is suitable for a package for general regions and boundary conditions.

Laplace's equation is the simplest elliptic partial differential equation, and has been the subject of a great deal of analysis. Special methods for Laplace's equation are available, methods that do not work for general elliptic partial differential equations.

Special methods for Laplace's equation include the so-called "fast Poisson solvers."[1] They can quickly solve $\nabla^2\Phi(x,y) = f(x,y)$ if the region and boundary conditions are sufficiently simple. However, even Fig. 2 is not simple enough because of the mixed boundary conditions on the top boundary. The fast Poisson solvers have great utility for special problems, but are not appropriate for a general Laplace package. Recent research (Ref. 2, for example) indicates how these methods may be extended in the future.

1.1 The boundary integral equation method

The most useful special method for Laplace's equation is the boundary integral equation method. The basic method has been known for many years,[3,4] but has enjoyed a renewed popularity since the advent of large digital computers. A few representative references are Refs. 5 to 9. A two-dimensional partial differential equation is reduced to a one-dimensional integral equation. Similarly, a three-dimensional partial differential equation can be reduced to a two-dimensional integral equation. The integral equation involves only the geometry and the values of Φ and $\partial\Phi/\partial n$ on the boundary. Multiply-connected regions pose no added difficulty. After the integral equation has been solved approximately, another integral can be done to evaluate $\nabla\Phi$ and Φ at any point inside the region.

The boundary integral equation method has been quite successful, providing fast and inexpensive solutions for Laplace's equation in two dimensions. The usual implementation does have several difficulties. First, the integral equation is a Fredholm integral equation of the first kind for $\partial\Phi/\partial n$, and consequently is ill-conditioned. (For either a Dirichlet or a Neumann problem, a well-conditioned integral equation is

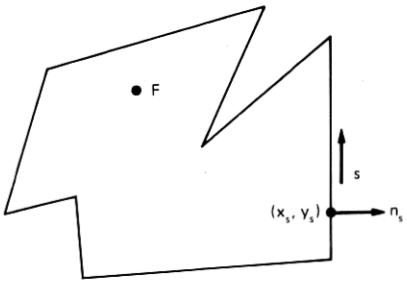

Fig. 3—Illustration of the definitions of s, x_s, y_s, $\mathbf{n}_s$, and F.

available, but not for mixed boundary conditions.) Matrices generated for approximate solutions to the integral equation are ill-conditioned, and $\partial\Phi/\partial n$ cannot be found accurately. Second, three-dimensional problems with axial symmetry are essentially two-dimensional problems, but no provision is made for their solution. (The next two objections do not apply to Ref. 9.) Third, the unknown Φ and $\partial\Phi/\partial n$ are approximated by low-order polynomials on sections of the boundary. Convergence requires many coefficients if accuracy of more than a few percent is required. Finally, no provision is provided for dealing with singularities.

The present paper describes an improved boundary integral method which counters all the above difficulties. Two coupled integral equations are used; the combination leads to a well-conditioned matrix. Both Φ and $\partial\Phi/\partial n$ can be obtained accurately. Higher-order approximations for the unknown Φ and $\partial\Phi/\partial n$ are used. Corner singularities are recognized automatically, and special approximating functions are used. Axisymmetric problems are solved by the same program. Typical problems cost only a few dollars to run. A reliable estimate of the accuracy of the approximate Φ is available.

1.2 The Laplace package

The method described in this paper has been implemented in the Laplace program package. A user's guide for the Laplace package, with several examples, is available separately.[10] The program package is written in EFL,[11] an extended Fortran language. The output of the EFL compiler is portable Fortran.

The package solves Laplace's equation in two dimensions or in three dimensions with axial symmetry. Two-dimensional regions must be bounded by straight-line segments. Three-dimensional regions must be figures of revolution whose cross section in the (r,z) plane is bounded by straight-line segments. The region may extend to infinity, but the boundary must not extend to infinity. The region may be multiply-

connected. On each line segment, either Φ or $\partial\Phi/\partial n$ may be specified as a boundary condition. In addition to smooth basis functions, the program automatically includes the appropriate singular basis functions greatly improving the achievable accuracy for regions with corners.

Section II discusses the mathematical basis for the boundary integral equation method. Section III describes the implementation of the method. Possible extensions to the program package are discussed in Section IV. Section V has results for a sample problem. The appendix derives the new integral equation used.

II. INTEGRAL EQUATION FORMULATION

In this section, Laplace's equation is formulated as a pair of coupled integral equations. The two-dimensional partial differential equation is reduced to a pair of one-dimensional integral equations.

We wish to solve

$$\nabla^2\Phi(x,y) = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = 0 \tag{P1a}$$

for (x,y) in a region D with boundary Γ. D may be multiply-connected, in which case Γ has several distinct parts. For now, we discuss only the two-dimensional "interior" problem, with D a finite region. At the conclusion of this section, we discuss the two-dimensional "exterior" problem, with D an infinite region, and the three-dimensional axisymmetric problem, both interior and exterior.

As in Fig. 3, let (x_s,y_s) be the coordinates of the point at arc length s, and denote $\phi(s) = \Phi(x_s,y_s)$. We will use Φ for the potential of a general point, and ϕ for a point on Γ. Let $\mathbf{n}_s$ be the outward-pointing unit normal vector at s. For a point s not at a vertex of Γ, define

$$\psi(s) \equiv \lim_{(x,y)\to(x_s,y_s)} \mathbf{n}_s \cdot \nabla\Phi(x,y).$$

The notation $\partial\phi/\partial n_s$ is also used for the right side of the above definition.

For the problem to be well-posed, a boundary condition must be given at each point of Γ.[12] The Laplace package allows the specification

$$\phi(s) = b_1(s) \text{ on part of } \Gamma, \text{ say } \Gamma_1 \tag{P1b}$$

$$\psi(s) = b_2(s) \text{ on the remainder of } \Gamma, \text{ say } \Gamma_2. \tag{P1c}$$

For any fixed point $F = (x_F,y_F)$, the Green's function, or fundamental solution to Laplace's equation, is

$$G(x,y;x_F,y_F) = -\tfrac{1}{2}\ln\left[(x - x_F)^2 + (y - y_F)^2\right].$$

Except at point F, $\nabla^2 G(x,y;x_F,y_F) = 0$.

Now let (x,y) be any point strictly inside D. Green's boundary identity is[3]

$$2\pi\Phi(x,y) = \int_\Gamma [\psi(s)G(x_s,y_s;x,y) - \phi(s)\mathbf{n}_s \cdot \nabla_s G(x_s,y_s;x,y)]ds.$$

The gradient operator, ∇_s, operates on the x_s and y_s. The above equation is usually abbreviated as

$$2\pi\Phi(x,y) = \int_\Gamma \left[\psi(s)G - \phi(s)\frac{\partial G}{\partial n_s}\right] ds, \tag{1}$$

with the arguments of G left implicit.

If (x,y) is a point at arc length t on a smooth part of Γ, it may be shown[3,13] that

$$\pi\phi(t) = \fint_\Gamma \left[\psi(s)G - \phi(s)\frac{\partial G}{\partial n_s}\right] ds. \tag{2}$$

The integral is now a Cauchy principal-value integral at $s = t$.

Suppose that the correct $\phi(s)$ and $\psi(s)$ are not known, but only approximate values $\phi^*(s)$ and $\psi^*(s)$ are known. Then the function $\Phi^*(x,y)$ defined by

$$2\pi\Phi^*(x,y) = \int_\Gamma \left[\psi^*(s)G - \phi^*(s)\frac{\partial G}{\partial n_s}\right] ds$$

exactly obeys Laplace's equation for (x,y) strictly inside D. Φ^* will not obey the correct boundary conditions as (x,y) approaches the boundary unless $\phi^*(s)$ and $\psi^*(s)$ are chosen correctly.

Thus the boundary integral equation method is one of the class of "particular solution" methods.[14,15] Any approximate solution obeys the partial differential equation exactly, but only obeys the boundary conditions approximately. The advantage over the usual particular solution methods for Laplace's equation, as seen in Ref. 16, for example, is that the boundary integral particular solutions incorporate the exact boundary of the region and do not require a restricted region. They are more complicated to calculate, but are appropriate for the region.

Equation (2) may be used to obtain an integral equation for ϕ^* and ψ^*.

$$\pi\phi^*(t) = \fint_\Gamma \left[\psi^*(s)G - \phi^*(s)\frac{\partial G}{\partial n_s}\right] ds. \tag{3a}$$

Letting $\mathbf{R}$ be the vector from point t to point s, and R the length of $\mathbf{R}$, (3a) may be written as

$$\pi\phi^*(t) = \fint_\Gamma \left[\frac{\mathbf{n}_s \cdot \mathbf{R}}{R^2}\phi^*(s) - \ln(R)\psi^*(s)\right] ds \tag{3b}$$

This boundary integral equation has been used for many years for solving Laplace's equation.[5–9]

For example, if $\phi(s) = b_1(s)$ is given on all of Γ (Dirichlet problem), set $\phi^*(s) = \phi(s)$, and the above is then an integral equation for the unknown $\psi^*(s)$. Thus a two-dimensional partial differential equation has been reduced to a one-dimensional integral equation. An approximate solution may be obtained by expanding $\psi^*(s)$ in an appropriate set of basis functions, and taking a finite number of these.

$$\psi^*(s) = \sum_{j=1}^{N} a_j f_j(s).$$

The f's are piecewise constant functions in Ref. 6 and piecewise quadratic in Ref. 7. We discuss an appropriate set of f's later. The integral equation (3a) then becomes

$$\sum_{j=1}^{N} a_j \oint_\Gamma f_j(s) G \, ds = \oint_\Gamma b_1(s) \frac{\partial G}{\partial n_s} ds + \pi b_1(t).$$

If $M = N$ points t_i are chosen at which to make this equation hold exactly (collocation), a set of N linear equations for the N unknowns, a_j, is obtained. If M points t_i, $M > N$, are chosen, an over-determined set of linear equations is obtained for the a_j's. This reduces the sensitivity of the approximate solution to the exact choice of the t_i. The equations are

$$\sum_{j=1}^{N} A_{ij} a_j = r_i, \; j = 1,2,\ldots,M,$$

where

$$A_{ij} = \oint_\Gamma f_j(s) G(s,t_i) ds$$

$$r_i = \oint_\Gamma b_1(s) \frac{\partial G(s,t_i)}{\partial n_s} ds + \pi b_1(t_i).$$

These may be solved in a least-squares sense, say, by a standard subroutine.[17]

In addition to the obvious advantages of this formulation, there is a well-known disadvantage. The integral equation for $\psi^*(s)$ is a Fredholm integral equation of the first kind,[18] of the type

$$u(x) = \int_0^1 H(x,y) \nu(y) dy,$$

where u and H are known and ν is to be determined. This kind of integral equation is *ill-conditioned* (sometimes called *ill-posed*); it is difficult to obtain accurate solutions for ν.[19,20] The reason for the difficulty is easy

to see. Since ν appears only inside the integral, its high-frequency components are not well-determined; by the Riemann-Lebesgue lemma,

$$\lim_{n\to\infty} \int_0^1 H(x,y) \sin(ny)dy = 0,$$

if H is not too badly behaved. The difficulty numerically is that the matrix $\{A_{jk}\}$ is ill-conditioned. Small errors in calculating elements A_{jk} or r_j lead to much-magnified errors in the coefficients a_k. If a sequence of approximate solutions with increasing N is done, the larger matrices are increasingly ill-conditioned. The typical failure mode is that $\psi^*(s)$ does not converge as N increases, after a certain point; rather, spurious and unphysical oscillations in $\psi^*(s)$ are seen.

Various methods of ameliorating the difficulty have been suggested, such as regularization[21] and matrix singular-value decomposition.[19,20,22] Better yet is to derive a Fredholm integral equation of the second kind.

In the appendix, we derive the following identity for t any point at a smooth part of Γ.

$$\pi\psi(t) = -\!\!\!\!\!\!\int_\Gamma \left\{ \psi(s) \frac{\partial G}{\partial n_t} - [\phi(s) - \phi(t)] \frac{\partial^2 G}{\partial n_s \partial n_t} \right\} ds. \tag{4a}$$

For the Dirichlet problem, this identity leads to a Fredholm integral equation of the second kind for $\psi^*(s)$ and is not ill-conditioned. Apparently, but surprisingly, (4a) is new. The integral equation derived from (4a) may be written as

$$\pi\psi^*(t) = -\!\!\!\!\!\!\int_\Gamma \left\{ [\phi^*(s) - \phi^*(t)] \times \frac{2(\mathbf{n}_s \cdot \mathbf{R})(\mathbf{n}_t \cdot \mathbf{R}) - R^2 \mathbf{n}_s \cdot \mathbf{n}_t}{R^4} + \frac{\mathbf{n}_t \cdot \mathbf{R}}{R^2} \psi^*(s) \right\} ds. \tag{4b}$$

With two integral equations, one well-conditioned for ϕ^* and the other for ψ^*, problem (P1) can be reduced to a set of linear equations with a well-conditioned matrix. If fitting point t_j is on Γ_1, where $\phi(s)$ is specified, use (4). If t_j is on Γ_2, where $\psi(s)$ is specified, use (3). A coupled pair of linear integral equations results. Analogously to the Dirichlet problem discussed earlier, appropriate basis functions and fitting points can be chosen, and the problem reduced to a set of linear equations. Some of the complications will be covered in later sections of the paper.

For the Dirichlet problem, ϕ given everywhere on Γ, (4) cannot be used everywhere. Since (4) is independent of the zero of potential, (4) alone will lead to a singular matrix, of rank $N - 1$. Special methods may be used for dealing with rank-deficient matrices, or the other equation, (3), may be used at some fitting points.

2.1 Exterior two-dimensional problems

We now consider solving Laplace's equation in an infinite region, D, exterior to a finite boundary, Γ. To have a unique solution, it is insufficient to specify either $\phi(s)$ or $\psi(s)$ at each point of Γ. In addition, the behavior of $\Phi(x,y)$ far from Γ must be specified. Use standard polar coordinates, (r,θ), with $r = \sqrt{x^2 + y^2}$ and suppose

$$\lim_{r\to\infty} \Phi(x,y) = \frac{\Psi_\infty}{2\pi} \ln\frac{1}{r} + \Phi_\infty + O(1/r),$$

where Φ_∞ and Ψ_∞ are constants. If Ψ_∞ is specified, then a unique solution can be found.[12] Ψ_∞ is the negative of total flux extending to infinity.

The earlier equations apply with small changes. For example, (3a) must be replaced by

$$\pi\phi^*(t) = 2\pi\Phi_\infty^* + \int_\Gamma \left[\phi^*(s) \frac{\partial G}{\partial n_s} - \psi^*(s) G \right] ds,$$

and the unknown Φ_∞^* must also be found.

The user specifies Ψ_∞ as well as boundary conditions. The Laplace package calculates an approximate value for Φ_∞^* as well as for ϕ^* and ψ^* on Γ.

2.2 Three-dimensional axisymmetric problems

Most of the preceding two-dimensional analysis needs only minor changes for the three-dimensional axisymmetric problem. Unlike the two-dimensional problem, the same formulation is adequate for interior and exterior three-dimensional problems. We use standard cylindrical coordinates (r,θ,z). We wish to solve

$$\nabla^2\Phi(r,\theta,z) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} + \frac{\partial^2\Phi}{\partial z^2} = 0$$

in an axisymmetric region $\overline{D}$; $\overline{D}$ is formed as a figure of revolution by rotating a region D, with boundary Γ, about the z-axis. The boundary conditions must also be independent of θ.

For any fixed point $F = (x_F,y_F,z_F)$, the Green's function is

$$G(x,y,z;x_F,y_F,z_F) = \frac{1}{[(x-x_F)^2 + (y-y_F)^2 + (z-z_F)^2]^{1/2}} \equiv \frac{1}{R_3}$$

The integral equation corresponding to (3) is[13]

$$2\pi\phi^*(t) = \int_\Omega \left[\psi^*(s) G - \phi^*(s) \frac{\partial G}{\partial n_s} \right] d\Omega.$$

The integral is an area integral on the boundary, the surface of revolution.

Without loss of generality, let t be at $\theta = 0$. Let Γ be the intersection of Ω with any plane θ = constant. Express the area integral as an iterated integral over θ and s, arc length along Γ. Since ϕ^* and ψ^* are independent of θ, all the θ dependence is in G and $\partial G/\partial n_s$. R_3 may be expressed as

$$R_3^2 = R_m^2 - 2r_s r_t(1 + \cos\theta),$$

where

$$R_m^2 = (r_s + r_t)^2 + (z_s - z_t)^2.$$

With much manipulation, the θ integration may be performed, giving

$$2\pi\phi^*(t) = \oint_\Gamma \left\{ 4r_s K(m)\psi^*(s) + \left[\frac{4r_s \mathbf{n}_s \cdot \mathbf{R}_2}{R_m^2(1-m)} E(m) + 2\mathbf{n}_s \cdot \mathbf{e}_r [K(m) - E(m)] \right] \phi^*(s) \right\} \frac{ds}{R_m}, \quad (5)$$

where $\mathbf{e}_r$ and $\mathbf{e}_z$ are unit vectors in the $\theta = 0$ plane, and $\mathbf{R}_2$ is the vector in the $\theta = 0$ plane from t to s.

$$\mathbf{R}_2 = (r_s - r_1)\mathbf{e}_r + (z_s - z_t)\mathbf{e}_z$$

$$m = \frac{4r_s r_t}{R_m^2}.$$

K and E are the usual complete elliptic integrals.[23]

$$E(m) = \int_0^{\pi/2} (1 - m \sin^2 u)^{1/2} du$$

$$K(m) = \int_0^{\pi/2} (1 - m \sin^2 u)^{-1/2} du.$$

The integral equation corresponding to (4) is considerably more complicated.

$$2\pi\psi^*(t) = \oint_\Gamma \frac{4r_s}{R_m^3} \left\{ \left[\mathbf{n}_t \cdot \mathbf{R}_2 \frac{E}{1-m} - 2r_s \mathbf{n}_t \cdot \mathbf{e}_r \frac{K-E}{m} \right] \psi^*(s) + \left[(\mathbf{n}_s \cdot \mathbf{e}_r)(\mathbf{n}_t \cdot \mathbf{e}_r)(2E - K) - \mathbf{n}_s \cdot \mathbf{n}_t \frac{E}{1-m} + \frac{(\mathbf{n}_s \cdot \mathbf{R}_2)(\mathbf{n}_t \cdot \mathbf{R}_2)}{R_m^2(1-m)} \left(\frac{2(2-m)}{(1-m)} E - K \right) + \frac{2}{R_m^2} [(\mathbf{n}_s \cdot \mathbf{e}_r)(\mathbf{n}_t \cdot \mathbf{R}_2) r_t - (\mathbf{n}_t \cdot \mathbf{e}_r)(\mathbf{n}_s \cdot \mathbf{R}_2) r_s] \times \left(\frac{E}{1-m} + \frac{K-E}{m} \right) \right] [\phi^*(s) - \phi^*(t)] \right\} ds. \quad (6)$$

K and E have been used as abbreviations for $K(m)$ and $E(m)$.

2.3 Error estimates

If (x,y) is strictly inside D, the approximate potential (in two dimensions) obeys

$$2\pi\Phi^*(x,y) = \int_\Gamma \left[\psi^*(s)G - \phi^*(s) \frac{\partial G}{\partial n_s} \right] ds.$$

If (x,y) is on a smooth part of Γ,

$$\pi\Phi^*(x,y) = \fint_\Gamma \left[\psi^*(s)G - \phi^*(s) \frac{\partial G}{\partial n_s} \right] ds.$$

If (x,y) is at a vertex of Γ, the π is replaced by the interior angle of the vertex. Similarly, $\nabla\Phi^*$ inside D and $\partial\Phi^*/\partial n$ on Γ may be obtained by the analog of (4).

The function Φ^* as defined above exactly obeys Laplace's equation inside D. Therefore, by the maximum principle,[24] the maximum error in Φ^* occurs somewhere on Γ.

$$\left| \Phi^*(x,y) - \Phi(x,y) \right| \leq \max_s \left| \Phi^*(x_s,y_s) - \phi(s) \right|.$$

For the Dirichlet problem, a rigorous error bound is in principle possible by finding the largest discrepancy between Φ^* and the boundary condition ϕ. However, finding the error bound can be more expensive than solving the integral equation.

For mixed boundary conditions, a rigorous bound is in general impossible. The above bound is still correct, but is not useful, since the true Φ is not known on all of the boundary. For certain restricted regions, another rigorous error bound can be obtained.[25] For these restricted regions,

$$\left| \Phi^*(x,y) - \Phi(x,y) \right| \leq \max_{\Gamma_1} \left| \Phi^*(x_s,y_s) - \phi(s) \right| + R_D \max_{\Gamma_2} \left| \frac{\partial \Phi^*(x_s,y_s)}{\partial n_s} - \psi(s) \right|,$$

where R_D is the maximum perpendicular distance from any point of Γ_2 to any other point of Γ. This bound is in principle possible to compute, but is expensive in practice.

An error *estimate* is available at no extra cost in the Laplace package, because of the method of solution. The over-determined system of linear equations is solved in a least-squares sense, minimizing the total fitting error (TFE),

$$\left[\sum_{i=1}^{M} \sum_{j=1}^{N} (A_{ij}a_j - r_j)^2 \right]^{1/2},$$

and returning this error. For the implementation discussed in the next section, with $M \approx 3N/2$, numerical experiments indicate that the TFE is a reliable upper bound on the error in the potential on the boundary, and a substantial overestimate of the error away from the boundary.

III. IMPLEMENTATION

Section II was general and discussed mathematics; we now become more specific and discuss numerical analysis. We also discuss some of the myriad details necessary to make a computer program feasible.

3.1 Geometry

Section II considered regions of arbitrary shape. The current implementation of the Laplace package requires that Γ be composed of finite straight-line segments. This is in contrast to the usual practice in analysis, of requiring that Γ be a smooth curve everywhere. Many practical problems have corners in their geometries, so it is essential to be able to handle such boundaries. It is easier to analyze exact corners than "smooth" geometries with a very small radius of curvature rather than a corner. In the following, each of the straight-line segments is called a *side*.

3.2 Basis functions

In the previous section, the choice of the basis functions $f_k(s)$ was left arbitrary. However, the particular choice made strongly affects the accuracy and efficiency of the program. At least four factors should be considered.

(*i*) The basis functions should be able to model the behavior of $\phi(s)$ and $\psi(s)$ with only a few functions.

(*ii*) If enough basis functions are used, they should be able to approximate $\phi(s)$ and $\psi(s)$ arbitrarily well.

(*iii*) The basis functions should be a well-conditioned set, so that small errors in doing the integrals do not lead to large errors in the approximate solution.

(*iv*) The integrals of the basis functions times G, $\partial G/\partial n_s$, and $\partial^2 G/\partial n_s \partial n_t$ must be tractable, either analytically or numerically.

Historically, (*iv*) has been dominant. Symm[6] approximated curved boundaries by straight-line segments and used piecewise constant basis functions. Hayes[7] allowed boundaries to be straight-line segments or arcs of circles, and used piecewise quadratic basis functions. Blue[9] allowed straight-line boundaries and allowed piecewise polynomial basis functions. For all these choices, the integrals in (3) and (4) can be done

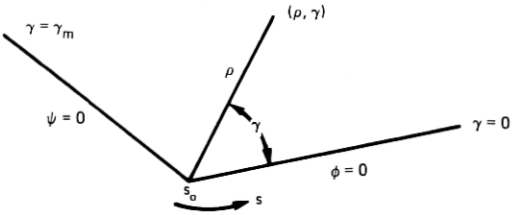

Fig. 4—Local polar coordinates used for eq. (7).

analytically. The above authors did not treat the axisymmetric problem, but the integrals in (5) and (6) are intractable analytically.

If the boundary has corners, $\psi(s)$ can be infinite at the corners, and piecewise polynomial basis functions will not be able to approximate $\psi(s)$ well. For example, in Fig. 4, suppose the boundary conditions are as shown, and the interior angle is γ_m. Choose polar coordinates (ρ,γ) centered at the vertex, with angle $\gamma = 0$ on the $\phi = 0$ side; let $s = s_0$ at the corner. Then for small ρ, Φ has an expansion (in two dimensions)[26]

$$\Phi(\rho,\gamma) = \sum_{n=1}^{\infty} C_n \rho^{\alpha_n} \sin(\alpha_n \gamma), \tag{7}$$

where

$$\alpha_n = \frac{(n - 1/2)\pi}{\gamma_m}.$$

Thus Φ is identically zero on the line $\gamma = 0$. On the line $\gamma = \gamma_m$, the normal derivative is identically zero.

On the line $\gamma = 0$, where $s_0 \geqslant s$, the normal derivative is

$$\psi(s) = \sum_{n=1}^{\infty} \alpha_n C_n (s - s_0)^{\alpha_n - 1}.$$

For the case $\gamma_m > \pi/2$, we have $\alpha_1 < 1$, and we expect $\psi(s)$ to be infinite at the corner, unless C_1 happens to be zero. For $\psi(s)$ to be approximated accurately with only a few basis functions, one of them should be $\alpha_1(s - s_0)^{\alpha_1 - 1}$ with the correct α_1.

Similarly, on the line $\gamma = \gamma_m$, where $s \leqslant s_0$, the potential is

$$\phi(s) = \sum_{n=1}^{\infty} C_n (s_0 - s)^{\alpha_n} (-1)^{n+1}.$$

Therefore a basis function $(s_0 - s)^{\alpha_1}$ is needed on the $\gamma = \gamma_m$ side. In fact, only a single unknown coefficient, C_1, need be introduced to deal with the worst part of $\phi(s)$ and $\psi(s)$ at s_0. It may also be desirable to include a few of the less singular basis functions. The Laplace package includes singular basis functions for which $\alpha < \alpha_{\max}$, with a default value $\alpha_{\max}$

$= 1$, and does not include any singular function whose α is within 0.1 of an integer.

Similar singular basis functions are used at corners where ϕ is specified on both sides and where ψ is specified on both sides. Since the expansion (7) is not necessarily convergent far from the vertex, the singular basis functions centered at a corner are used only on the two sides meeting at that corner.

For axisymmetric problems, the expansion (7) does not hold, but the exponent of the singularity is the same for off-axis points, since the singularity depends only on the highest order derivatives in the differential equation.[26] For singularities on the axis, the exponents are different,[27] and singular functions have not yet been implemented.

Additional "smooth" basis functions are also needed. A well-conditioned family of basis functions is B-splines. A brief description of some of their properties follows.[28,29] B-splines are defined on a line divided into intervals by *knots*. B-splines of order k are piecewise polynomials of degree $k - 1$. Each B-spline is nonnegative, has exactly one maximum, and has local support. The sum of B-splines at any point is identically one. In any interval, exactly k B-splines are nonzero; each B-spline is nonzero in at most k intervals. The B-splines on a line are uniquely determined by the knots, which may be multiple. At a knot with multiplicity m, a kth-order B-spline has $k - m - 1$ continuous derivatives. If $m = k - 1$, the B-spline is only continuous; if $m = 1$, the B-spline has $k - 2$ continuous derivatives.

The user chooses a k, the same for all sides, and the number of interior knots on each side. Mesh spacing proceeds according to the following rules. A vertex is called *singular* if its expansion, as in (7), has $\alpha_1 < 0.9$. If a singular basis function is used, the vertex is called *compensated*. If the two vertices delimiting a side are each either compensated or nonsingular, the interior knots on the side are spaced uniformly. Otherwise, the interior knots are spaced closer together near uncompensated singular vertices.

For a given mesh, higher-order B-splines are potentially more accurate, since the approximation error can be $O(h^k)$ [30], where h is the maximum mesh. However, the integrals for higher order splines are more difficult, and there are more unknown spline coefficients for higher k. Currently, the Laplace package restricts k to be 2, 3, or 4.

3.3 Boundary conditions

If $\phi(s)$ or $\psi(s)$ is specified as an arbitrary function, the integrals involving the boundary conditions require special methods. Instead, the Laplace package does a least-squares fit of the boundary condition to a B-spline. A separate fit is done on each side; the same order and mesh

are used as specified by the user for that side for the unknown $\psi^*(s)$ or $\phi^*(s)$.

For the Neumann problem—ψ specified on all of Γ—the problem is undetermined up to an additive constant in Φ. A solution exists for the interior problem only if $\int_\Gamma \psi(s)\, ds$ is exactly zero. The Laplace package currently will not solve the Neumann problem; ϕ must be specified on at least one side.

3.4 Integrals

With polynomial basis functions and boundaries composed of straight-line segments, the integrals in (3a) and (4a) can be done analytically. This can cause conditioning problems; B-splines are a well-conditioned basis only if calculated properly.[29] The integrals in (5) and (6) cannot be done analytically, even with polynomial basis functions. With singular basis functions like $(s - s_0)^\alpha$, none of the integrals can be done analytically unless α is special.

All the necessary integrals can be done accurately and efficiently by the numerical methods described in this section. We first consider (3a) and (4a), for any fixed t. For straight-line boundaries, the integral over Γ is divided up into a sum of integrals over the line segments. We consider only a single segment, and eliminate any subscript referring to the segment. On the segment, $\mathbf{n}_s$ is constant, and $\mathbf{R}$ may be written as

$$\mathbf{R} = R_\perp \mathbf{n}_s + (s - s_\perp)\mathbf{e}_s,$$

where $\mathbf{e}_s$ is a unit vector along the side. Also expand $\mathbf{n}_t$ as

$$\mathbf{n}_t = n_\perp \mathbf{n}_s + n_\parallel \mathbf{e}_s.$$

The portions of (3a) and (4a) from the segments are

$$\pi\phi^*(t) = \int\!\!\!\!\!\!-_{s_1}^{s_2} \left\{ \frac{R_\perp}{R_\perp^2 + (s - s_\perp)^2}\, \phi^*(s) - \tfrac{1}{2} \ln [R_\perp^2 + (s - s_\perp)^2] \psi^*(s) \right\} ds \quad (3c)$$

$$\pi\psi^*(t) = \int\!\!\!\!\!\!-_{s_1}^{s_2} \left\{ [\phi^*(s) - \phi^*(t)] \times \frac{2R_\perp [n_\perp R_\perp + n_\parallel (s - s_\perp)] - [R_\perp^2 + (s - s_\perp)^2] n_\perp}{[R_\perp^2 + (s - s_\perp)^2]^2} + \frac{n_\perp R_\perp + n_\parallel (s - s_\perp)}{R_\perp^2 + (s - s_\perp)^2} \psi^*(s) \right\} ds. \quad (4c)$$

We first consider the case where the point t is not on the segment in question. Then the Green's function parts of the integrals are not sin-

gular; either $R_\perp \neq 0$ or $s_\perp$ is not in the interval $[s_1,s_2]$. As an example, look at the integral with the logarithm in it, and look at one term of the expansion of $\psi^*(s)$, with the basis function $B_i(s)$. Further divide the segment into subintervals, between knots of the spline, so that over each subinterval $B_i(s)$ is a polynomial. Over each subinterval, the integrand is a polynomial times a nonsingular function. Gauss-Legendre quadrature is ideal for such integrands, if the order of the quadrature rule can be determined *a priori*. (An automatic quadrature method could be used, such as Refs. 31 or 32, but these are usually less efficient.) Computing the order of the quadrature rule necessary can be done using the results of numerical experimentation. If s_{j_1} and s_{j_2} are the ends of the subinterval, let $s_c = (s_{j_1} + s_{j_2})/2$ and $h = s_{j_2} - s_{j_1}$. The change of variable $u = 2(s - s_c)/h$ changes the term in question to

$$-\frac{h}{4}\int_{-1}^{1} [\ln (h^2/4) + \ln [a^2 + (u - b)^2]]B_i(s_c + hu/2)du,$$

where $a = 2R_\perp/h$ and $b = 2(s_\perp - s_c)/h$. Since the integral is over a single mesh interval of B_i, we expect the error to be no worse than the worst error in any of the kth-order B-splines with k-fold knots at -1 and 1, and no interior knots, since the latter B-splines vary more rapidly over the interval. Thus we look only at the errors in these k B-splines; call them $\overline{B}(u)$ to distinguish them.

Now consider the family of integrals

$$I_j(a,b,k) = \int_{-1}^{1} \ln [a^2 + (u - b)^2]\overline{B}_j(u)du.$$

Let $E_j(a,b,k,n)$ be the error in evaluating $I_j(a,b,k)$ by an n point Gauss-Legendre quadrature rule, and let

$$E(a,b,k,n) = \left[\sum_{j=1}^{k} E_j(a,b,k,n)^2\right]^{1/2}.$$

Numerical experiments show that in the (a,b) plane, the locus of constant $E(a,b,k,n)$ is approximately an ellipse. For given n and desired accuracy, ϵ, there is an ellipse with semi-axes $A(k,n,\epsilon)$ and $B(k,n,\epsilon)$ so that the error is satisfactory if a and b are outside the ellipse, or

$$\left[\frac{a}{A(k,n,\epsilon)}\right]^2 + \left[\frac{b}{B(k,n,\epsilon)}\right]^2 \geq 1.$$

For doing the integrals $I_j(a,b,k)$ to accuracy ϵ, the functions $A(k,n,\epsilon)$ and $B(k,n,\epsilon)$ are determined experimentally for a series of values of n. (The default values are $n = 4, 6, 8, 10, 12$, and 16, and $\epsilon = 10^{-6}$.) For any particular a and b, the smallest satisfactory n is used. If the largest n available is insufficient, then the interval is divided; this is seldom

necessary. In the Laplace package, $A(4,n,\epsilon)$ and $B(4,n,\epsilon)$ are used for $k \leqslant 4$.

The other integrals in (3a) and (4a) are done similarly, using numerically derived ellipses for B-spline basis functions. For singular basis functions, Gauss-Jacobi quadrature formulas are used; these are Gauss quadrature formulas on (0,1) with weight function $x^{\alpha-1}$. Different quadrature formulas are used for each of the unique α's used in singular basis functions. The same ellipses as calculated for B-splines are used; slightly smaller ellipses could be used, but the gain in efficiency is small.

The Gauss quadrature formulas are calculated portably by the method of Sack and Donovan,[33] using programs in the PORT library.[34]

The integrals of (5) and (6) are somewhat more complicated than those of (3a) and (4a), but are no harder numerically. The same ellipses are used.

If point t is on the line segment, then the Green's functions in the integrals have singularities. The integrals (3c) and (4c) simplify somewhat, since $\mathbf{n}_s = \mathbf{n}_t$, $\mathbf{n}_\parallel = 0$, $\mathbf{n}_\perp = 1$, and $R_\perp = 0$. The ϕ^* term in (3c) is identically zero; the ψ^* term is

$$-\tfrac{1}{2} \int_{s_1}^{s_2} \ln [(s-t)^2] \psi^*(s)\, ds.$$

The ψ^* term in (4c) is identically zero; the ϕ^* term is

$$-\!\!\!\!\!\!\int_{s_1}^{s_2} [\phi^*(s) - \phi^*(t)] \frac{ds}{(s-t)^2}.$$

Special care must be taken to get accurate approximations to these singular integrals.

First consider a B-spline basis function, $B_i(x)$, again dividing (s_1,s_2) into subintervals. If t is not in the subinterval in question, then the previous methods are adequate. (The Laplace package never takes t to be exactly at a knot.) For the logarithmic integral, the subinterval including t is, for some positive δ_1 and δ_2,

$$\begin{aligned}
&-\tfrac{1}{2} \int_{t-\delta_1}^{t+\delta_2} \ln [(s-t)^2] B_i(s)\, ds \\
&\quad = -\int_0^{\delta_1} \ln (u) B_i(t-u) du - \int_0^{\delta_2} \ln (u) B_i(t+u) du \\
&\quad = -\delta_1 \int_0^1 \ln (\nu) B_i(t - \nu\delta_1) d\nu - \ln (\delta_1) \int_0^{\delta_1} B_i(t-u) du \\
&\qquad - \delta_2 \int_0^1 \ln (\nu) B_i(t + \nu\delta_2) d\nu - \ln (\delta_2) \int_0^{\delta_2} B_i(t+u) du.
\end{aligned}$$

The integrals with ln (ν) are done by Gauss quadrature with weight function ln (ν); the others are done by Gauss-Legendre quadrature. The Gauss quadrature formulas with logarithmic weight function are also calculated portably by the method of Ref. 33.

The Cauchy principal-value integral, for the subinterval including t, is

$$-\oint_{t-\delta_1}^{t+\delta_1} \frac{B_i(s) - B_i(t)}{(s-t)^2}\,ds$$

$$= -B'_i(t)\oint_{t-\delta_1}^{t+\delta_1} \frac{ds}{s-t} - \int_{t-\delta_1}^{t+\delta_2} \frac{B_i(s) - B_i(t) - (s-t)B'_i(t)}{(s-t)^2}\,ds.$$

The first integral is done analytically. The second has no singularity at $s = t$ and is done analytically as

$$-\int_{t-\delta_1}^{t+\delta_2} \left[\frac{1}{2}B_i''(t) + \frac{1}{6}(s-t)B_i'''(t) + \ldots\right]ds.$$

This is adequate for low-order B-splines. For high-order B-splines, more care would be necessary.

Now consider integrals with singular basis functions and with t on the same segment as s. If $\psi(s)$ is given on the segment, $\phi^*(s)$ may have $(s - s_1)^\alpha$ or $(s_2 - s)^\alpha$ terms; however, if $\psi(s)$ is given, (3) is always used for t on the side, and the ϕ^* terms vanish because $R_\perp = 0$. If $\phi(s)$ is given on the segment, $\psi^*(s)$ may have $(s - s_1)^{\alpha-1}$ or $(s_2 - s)^{\alpha-1}$ terms; however, if $\phi(s)$ is given, (4) is almost always used, and the ψ^* terms vanish because $R_\perp = 0$. The exception, when $\phi(s)$ is given on a segment and (3) is used, occurs only for the Dirichlet problem, ϕ given on all of Γ. Then (3) is used at the central fitting point of each side, and we need integrals of the form

$$\pm\tfrac{1}{2}\alpha\int_{s_1}^{s_2} \ln\,[(s-t)^2](s-s_1)^{\alpha-1}ds.$$

As much as possible of the integral

$$\int_{s_1}^{t} \ln\,(t-s)(s-s_1)^{\alpha-1}ds,$$

starting from s_1, is done using Gauss-Jacobi quadratures. The remainder has only a logarithmic singularity. It and the integral form t to s_2 are done by Gauss quadrature with a logarithmic weight function, as described earlier in this section.

3.5 Complete elliptic integrals

The complete elliptic integrals $K(m)$ and $E(m)$ are necessary for the axisymmetric problem. Suitable expansions are[35]

$$K(m) = P_K(1 - m) - Q_k(1 - m) \ln (1 - m)$$

$$E(m) = P_E(1 - m) - Q_E(1 - m) \ln (1 - m).$$

Polynomial approximations for the Ps and Qs are given in Ref. 35. The argument $(1 - m)$ is used instead of m to avoid excessive error as $m \to 1$, i.e., as $s \to t$ in (5) and (6).

The combination $D(m) = [K(m) - E(m)]/m$ is also needed. As $m \to 0$, $D(m) \to \pi/4$. For $D(m)$, another approximation of the above type was generated.

3.6 Fitting points

At least N fitting points are needed to determine the N unknown coefficients of the basis functions. The work to calculate the matrix is proportional to the number of points used. If more than N points are used, the sensitivity of the solution to the placement of the points is diminished, as is the amplification of any small errors in calculating matrix elements. In the Laplace package, approximately f times N fitting points are used; the default value of f is 1.5. In the subinterval between each pair of knots, the number of fitting points is f times the number of unknowns associated with the subinterval, rounded up. The fitting points are uniformly spaced within each subinterval.

3.7 Scaling, constraints, and matrix solution

Each row of the matrix corresponds to applying either (3) or (4) at one fitting point, t_i. To keep the solution approximately independent of the scaling of the region, each row corresponding to (4) is multiplied by the length of the side containing t_i.

For an interior problem, $\int \psi^*(s)\, ds = 0$. For an exterior two-dimensional problem, $\int \psi^*(s)\, ds = \Psi_\infty$. Either restriction may be written as a linear equality constraint on the unknown coefficients. When the matrix equations are solved by QR factorization, such linear constraints can easily be enforced using a method described by Lawson and Hanson.[36]

3.8 Portability

A portable stack allocation mechanism[34] is used for all temporary storage. The program is written in EFL.[11] The output of the EFL compiler is portable Fortran.

Two parts of the program are not portable. For $\epsilon \neq 10^{-6}$, new ellipses are necessary. The approximations to the complete elliptic integrals are accurate to about 10^{-8}.

IV. POSSIBLE EXTENSIONS

In this section, we discuss several extensions to the Laplace package which could be implemented if there were sufficient incentive, and the difficulties involved with each. Combinations of the individual extensions pose further difficulties, but will not be discussed.

4.1 Higher-order B-splines and higher-accuracy integrals

B-splines of order higher than 4 are useful if very high accuracy solutions are desired. The only change necessary to allow higher-order B-splines or higher-accuracy integrals is to change the ellipse semi-axes. This feature was not included in the Laplace package, since calculating the ellipses portably for any specified accuracy and B-spline order requires too much code. Alternate methods for doing integrals to any specified accuracy are under consideration.

4.2 Singular basis functions for axisymmetric problems

At a vertex away from the axis of revolution, an expansion similar to (7) will hold; the exponents $\{\alpha_n\}$ are the same as for the two-dimensional problem with the same shape as the cross section of the figure of revolution. At a vertex on the axis of revolution, the exponents are different; on-axis singular functions have not been implemented.

4.3 General linear boundary conditions

In some applications, it is desirable to solve Laplace's equation with the general linear boundary conditions on Γ

$$a(s)\phi(s) + b(s)\psi(s) = c(s),$$

with a and b simultaneously nonzero. Then (3a), say, would become

$$\pi\phi^*(t) = \oint_\Gamma \left\{ \left[\frac{\mathbf{n}_s \cdot \mathbf{R}}{R^2} - \frac{a(s)}{b(s)} \ln\left(\frac{1}{R}\right) \right] \phi^*(s) + \ln\left(\frac{1}{R}\right) \frac{c(s)}{b(s)} \right\} ds.$$

The difficulty here is in choosing a method for accurately evaluating the integrals involving a/b and c/b, unless a/b and c/b are restricted drastically, say, to being constants on each of the boundary line segments.

4.4 Curved boundaries

Many applications have part or all of the boundary as a smooth curve, which the user might not wish to approximate by straight-line segments. In principle, all that is needed to allow Γ to be any smooth curve is a parameterization of x_s, y_s, and $\mathbf{n}_s$ as a function of s. Again, the difficulty is in doing the integrals accurately and efficiently. The ellipse method would not be directly applicable. In addition, some of the integrals which

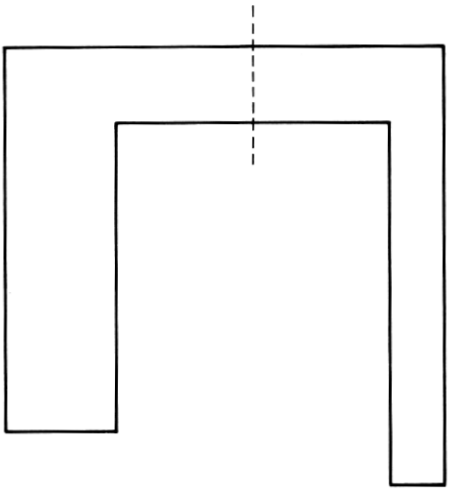

Fig. 5—A region which could be handled more easily by breaking it into two regions with an interface.

vanished identically for straight-line boundaries would not vanish. For example, the ϕ^* term of (3b) for s and t on the same segment vanishes if the segment is a straight line, because $\mathbf{n}_s \cdot \mathbf{R}$ is identically zero. If the line segment is curved, $\mathbf{n}_s \cdot \mathbf{R}/R^2$ in general has a finite limit as $s \rightarrow t$, and this term needs to be kept.

4.5 Interfaces

In other applications, there may be interfaces. A common problem is $\nabla^2 \Phi_1 = 0$ in region D_1 with boundary Γ_1, $\nabla^2 \Phi_2 = 0$ in region D_2 with boundary Γ_2, and interface conditions on the common portions of Γ_1 and Γ_2. Typical interface conditions are $\phi_1 = \phi_2$ and $\kappa_1 \psi_1 = \kappa_2 \psi_2$, where κ_1 and κ_2 are given constants.

Implementing this extension would require a significant change in data structure, but otherwise would be easy. No new types of integrals would arise. The singular basis functions at corners which are also points on the common boundary depend on κ_1 and κ_2 as well as the angles.[37]

This extension would also be useful for some single-region problems. A typical example is Laplace's equation inside a U-shaped region, Fig. 5. This could be broken artificially into two regions as shown, with interface conditions $\phi_1 = \phi_2$ and $\psi_1 = \psi_2$. The full region requires approximately $3\,N^2$ integrals, if N is the number of unknowns. The two half-size regions would each have $N/2$ unknowns, plus a few extra for the boundary values on the dotted line. Each region would require somewhat more than $3(N/2)^2$ integrals, so that the total work would be somewhat more than half.

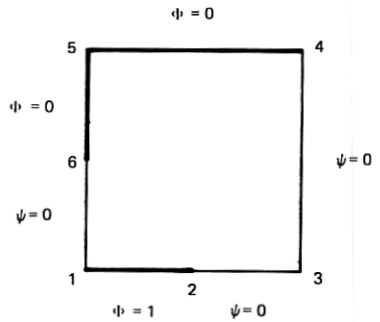

Fig. 6—Geometry for a sample problem.

V. AN EXAMPLE

Figure 6 gives the geometry and the boundary conditions for a sample problem. The boundary conditions are $\psi = 0$ on the light sides, $\phi = 1$ on the bottom dark side, and $\phi = 0$ on the top (L-shaped) dark side. This problem was solved approximately with third-order and fourth-order B-splines, and with various numbers of interior knots. Each side had the same number of interior knots. Some of the information is summarized in Table I. N is the number of basis functions. The running time is given in seconds for a Honeywell 6070 computer. TFE is the total fitting error, as defined in Section II. $\int \psi ds$ is over the side from 1 to 2. The next column gives ϕ at vertex 3. The approximate Φ at $(\frac{1}{2},\frac{1}{2})$ is the final column; vertex 1 is at (0,0) and vertex 3 is at (2,2). The time goes approximately as N^2; most of the work is in calculating elements of the matrix. Solving the matrix takes time proportional to N^3, but the proportionality constant is smaller than that of the N^2 term. Figure 7 is a log-log plot of TFE against N; TFE seems to be converging as N^{-3} for third-order splines and as N^{-4} for fourth-order splines. These rates of convergence are the optimum rates for approximating smooth functions by B-splines,[30] it is of interest to see them apparently applying for nonsmooth functions. The

Table I

kord	nknots	N	time	TFE	$\int \psi\, ds$	ϕ at 3	$\Phi(\frac{1}{2},\frac{1}{2})$
3	0	15	1.19	0.1067	0.997242	0.5482	0.6189
3	1	21	1.98	0.0255	1.000287	0.5069	0.6196
3	2	27	3.21	0.0231	0.999932	0.5011	0.6193
3	3	33	4.91	0.0123	0.999951	0.4999	0.6192
3	4	39	7.09	0.0080	0.999965	0.4997	0.6192
4	0	21	1.85	0.0235	0.999838	0.5041	0.6192
4	1	27	2.89	0.0135	0.999958	0.4997	0.6194
4	2	33	4.58	0.0066	0.999956	0.4987	0.6193
4	3	39	6.52	0.0034	0.999961	0.4995	0.6192
4	4	45	9.29	0.0024	0.999968	0.4995	0.6193

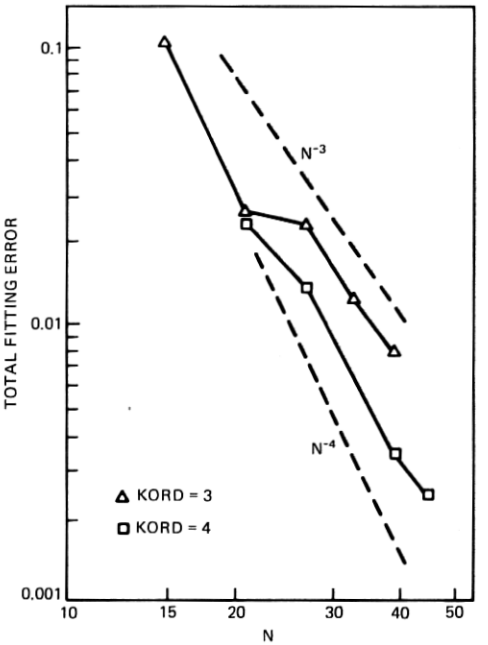

Fig. 7—Total fitting error (TFE) vs the number of basis functions, for third-order and fourth-order splines. Lines proportional to N^{-3} and to N^{-4} are shown for comparison.

last three columns appear to have converged to the accuracy allowed by the finite precision of the calculations. Matrix elements are calculated to a relative precision of about 10^{-6}, and the matrix has a condition number on the order of a few hundred, so accuracy of a few parts in 10^4 is all that can be expected for boundary values. $\int \psi(s)\, ds$ can be more accurate, since the integration can average out the boundary errors.

For these examples, the same number of knots was used on each side. Other examples may require differing numbers of knots on different sides. The intuition of the user is valuable in deciding on the number of knots per side.

APPENDIX

Derivation of Integral Equation (4)

Equation (4) can be derived in various ways. We use a derivation modeled on the derivation of (3) as sketched in Ref. 13. Start with Green's identity in two dimensions.

$$\int \int_D (u\nabla^2 v - v\nabla^2 u)\, dA = \int_\Gamma \left(u \frac{\partial v}{\partial n_s} - v \frac{\partial u}{\partial n_s} \right) ds.$$

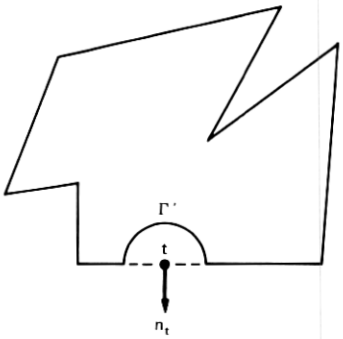

Fig. 8—Integral equation (4).

This identity is usually stated to hold for u and v which are C^2 inside D and C^1 in $D + \Gamma$, but is more generally true. For example, the condition on u can be weakened to include u's which have corner singularities as discussed in the body of the paper. The region D need not be simply-connected.

Pick any fixed point (x_t,y_t) at arc length t on Γ, at a smooth part of Γ. Let $\mathbf{n}_t$ be the outward-pointing normal at t. Choose

$$u(x,y) = \Phi(x,y) - \Phi(x_t,y_t)$$

$$v(x,y) = \mathbf{n}_t \cdot \nabla G(x,y;x_t,y_t),$$

and apply Green's identity to the region D', which is D minus a sector of a circle, with radius ϵ, centered at t (Fig. 8). Let Γ' be the circle sector. In D', $\nabla^2 u = 0$ and $\nabla^2 v = 0$, so the area integral is zero.

Consider the Γ' integral, and use polar coordinates (r,θ) centered at t. Let $\mathbf{e}_r$ be the unit vector at (r,θ) pointing away from the point t. On Γ', $\mathbf{n}_s = -\mathbf{e}_r$,

$$v = -\mathbf{n}_t \cdot \mathbf{e}_r/\epsilon,$$

$$\partial v/\partial n_s = -\mathbf{n}_t \cdot \mathbf{e}_r/\epsilon^2.$$

Expand $\Phi(x,y)$ about (x_t,y_t). For (x,y) on Γ',

$$\Phi(x,y) = \Phi(x,y_t) + \epsilon \mathbf{e}_r \cdot \nabla\Phi(x_t,y_t) + O(\epsilon^2),$$

$$\frac{\partial \Phi}{\partial n}(x,y) = -\frac{\partial \Phi}{\partial r} = -\mathbf{e}_r \cdot \nabla\Phi(x_t,y_t) + O(\epsilon),$$

where $\nabla\Phi(x_t,y_t)$ is an abbreviation for $\nabla\Phi(x,y)|_{x_t,y_t}$. The integrals over Γ' may be evaluated explicitly in the limit as $\epsilon \to 0$.

$$\lim_{\epsilon\to 0}\int_\Gamma u\frac{\partial v}{\partial n_s}\,ds = \lim_{\epsilon\to 0}\int_0^\pi [\epsilon \mathbf{e}_r\cdot\nabla\Phi(x_t,y_t)+O(\epsilon^2)][-\mathbf{n}_t\cdot\mathbf{e}_r/\epsilon^2]\epsilon\,d\theta$$

$$= -\lim_{\epsilon\to 0}\int_0^\pi [\mathbf{e}_r\cdot\nabla\Phi(x_t,y_t)+O(\epsilon)][\mathbf{n}_t\cdot\mathbf{e}_r]\,d\theta$$

$$= -\frac{\pi}{2}\,\mathbf{n}_t\cdot\nabla\Phi(x_t,y_t) = -\frac{\pi}{2}\,\psi(t).$$

In performing the integral, we used the identity

$$\int_0^\pi (\mathbf{a}\cdot\mathbf{e}_r)(\mathbf{b}\cdot\mathbf{e}_r)\,d\theta = \frac{\pi}{2}\,\mathbf{a}\cdot\mathbf{b},$$

true for constant vectors **a** and **b.** The other integral is evaluated similarly.

$$\lim_{\epsilon\to 0}\int_\Gamma\left(-\nu\frac{\partial u}{\partial n_s}\right)ds$$

$$= \lim_{\epsilon\to 0}\int_0^\pi\left[\frac{\mathbf{n}_t\cdot\mathbf{e}_r}{\epsilon}\right][-\mathbf{e}_r\cdot\nabla\Phi(x_t,y_t)+O(\epsilon)]\epsilon\,d\theta$$

$$= -\frac{\pi}{2}\,\psi(t).$$

Thus the integral over Γ' gives $-\pi\psi(t)$, in the limit $\epsilon\to 0$. Again in the limit $\epsilon\to 0$, the integral over the remainder of Γ becomes a Cauchy principal-value integral, and (4) is obtained. The argument depends only on the most singular terms in the Green's function, and so is easily generalized to the axisymmetric case.

REFERENCES

1. F. Dorr, "The Direct Solution of the Discrete Poisson Equation on a Rectangle," SIAM Rev., *12* (1970), pp. 248–263.
2. B. L. Buzbee, G. H. Golub, and C. W. Neilson, "On Direct Methods for Solving Poisson's Equation," SIAM J. Numer. Anal., *7* (1970), pp. 627–656.
3. O. D. Kellogg, *Foundations of Potential Theory,* New York: Dover, 1953 (reprint of original 1929 edition).
4. N. I. Muskhelishvili, *Singular Integral Equations,* P. Noordhoff, Gröningen, Holland, 1953.
5. M. A. Jaswon, "Integral Equation Methods in Potential Theory. I," Proc. Roy. Soc. London, *A275* (1963), pp. 23–32.
6. G. T. Symm, "Integral Equation Methods in Potential Theory. II," Proc. Roy. Soc. London, *A275* (1963), pp. 33–46.
7. J. K. Hayes, "The LAPLACE FORTRAN Code," Los Alamos Scientific Laboratory Report LASL-4004, October, 1968.
8. R. F. Harrington, *Field Computation by Moment Methods,* New York: MacMillan, 1968.
9. J. L. Blue, "On Finding the Admittance Matrix of a Thin-Film Network by Solving the Reduced Wave Equation in Two Dimensions," J. Comp. Phys., *7* (1971), pp. 327–345.
10. J. L. Blue, "Boundary Integral Solutions of Laplace's Equation," Bell Laboratories Computing Science Technical Report No. 60, April, 1977.
11. S. I. Feldman, private communication.

12. G. Hsiao and R. C. MacCamy, "Solution of Boundary Value Problems by Integral Equations of the First Kind," SIAM Rev., *15* (1973), pp. 687–705.
13. R. Courant and D. Hilbert, *Methods of Mathematical Physics,* Vol. 2, New York: Interscience, 1962.
14. S. Bergman, *Integral Operators and Partial Differential Equations,* Ergebnisse der Mathematic und Ihrer Grenzgebiete, Neue Folge, Heft 23, 1961.
15. I. N. Vekua, *New Methods for Solving Elliptic Equations,* Amsterdam: North-Holland Publishing Company, 1967.
16. J. R. Cannon, "The Numerical Solution of the Dirichlet Problem for Laplace's Equation by Linear Programming," SIAM J. Appl. Math., *12* (1964), pp. 233–237.
17. P. Businger and G. H. Golub, "Linear Least Squares Solutions by Householder Transformations," Num. Math., *7* (1965), pp. 269–276.
18. J. A. Cochran, *Analysis of Linear Integral Equations,* New York: McGraw-Hill, 1972.
19. R. J. Hanson, "A Numerical Method for Solving Fredholm Integral Equations of the First Kind Using Singular Values," SIAM J. Numer. Anal., *8* (1971), pp. 616–622.
20. J. M. Varah, "On the Numerical Solution of Ill-Conditioned Linear Systems with Applications to Ill-Posed Problems," SIAM J. Numer. Anal., *10* (1973), pp. 257–267.
21. A. N. Tikhonov, "Solution of Nonlinear Integral Equations of the First Kind," Soviet Math. Dokl., *5* (1964), pp. 835–838.
22. C. L. Lawson, "Applications of Singular Value Analysis," *Mathematical Software,* ed. J. Rice, New York: Academic Press, 1971.
23. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions,* New York: Dover, 1965.
24. M. H. Protter and H. F. Weinberger, *Maximum Principles in Differential Equations,* Englewood Cliffs: Prentice-Hall, 1967.
25. J. D. P. Donnelly, "Eigenvalues of Membranes with Reentrant Corners," SIAM J. Numer. Anal., *6* (1969), pp. 47–61.
26. R. S. Lehman, "Developments at an Analytic Corner of Solutions of Elliptic Partial Differential Equations," J. Math. and Mech. *8* (1959), pp. 727–760.
27. J. A. Morrison, "Charge Singularity at the Vertex of a Slender Cone of General Cross-Section," SIAM J. Appl. Math. *33* (1977), pp. 127–132.
28. H. B. Curry and I. J. Schoenberg, "On Polya Frequency Functions IV: The Fundamental Spline Functions and their Limits," J. of Anal. and Math., *17* (1966), pp. 71–107.
29. C. deBoor, "On Calculating with B-Splines," J. Approx. Th., *6* (1972), pp. 50–62.
30. C. deBoor, "On Uniform Approximation by Splines," J. Approx. Th., *1* (1968), pp. 219–235.
31. J. L. Blue, "Automatic Numerical Quadrature," B.S.T.J., *56,* No. 9 (November 1977), pp. 1651–1678.
32. T. N. L. Patterson, Algorithm 68, "Algorithm for Automatic Numerical Integration over a Finite Interval," Comm. ACM, *16* (1973), pp. 696–699.
33. R. A. Sack and A. F. Donovan, "An Algorithm for Gaussian Quadrature Given Modified Moments," Num. Math., *18* (1972), pp. 465–478.
34. P. A. Fox, A. D. Hall, and N. L. Schryer, "The PORT Mathematical Subroutine Library," ACM Trans. Math. Software, *4* (1978), pp. 104–126.
35. J. F. Hart, et al., *Computer Approximations,* New York: John Wiley, 1968.
36. C. L. Lawson and R. J. Hanson, *Solving Least Squares Problems,* Englewood Cliffs: Prentice-Hall, 1974, Chapter 20.
37. J. A. Lewis and J. McKenna, "The Field of a Line Charge Near the Tip of a Dielectric Wedge," B.S.T.J., *55,* No. 3 (March 1976), pp. 335–342.