JOURNAL OF COMPUTATIONAL PHYSICS 100, 236–245 (1992)

The Rapid Evaluation of Volume Integrals of Potential Theory on General Regions

ANITA MAYO

IBM Research Division, T. J. Watson Research Divison, Yorktown Heights, New York 10598

Received May 30, 1989; revised October 30, 1990

We present a new method for the rapid, high order accurate evaluation of certain volume integrals in potential theory on general irregular regions. The kernels of the integrals are either a fundamental solution, or a linear combination of the derivatives of a fundamental solution of a second-order linear elliptic differential equation. Instead of using a standard quadrature formula or the exact evaluation of any integral, the methods rely on rapid methods of solving the differential equation which the kernel is the solution of. Therefore, the number of operations needed to evaluate the volume integral is essentially equal to the number of operations needed to solve the differential equation on a rectangular region with a regular grid, and the method requires no evaluation of the kernel.

1. INTRODUCTION

In this paper we present a new, high order accurate method for the rapid evaluation of certain volume integrals in potential theory on general regions. The kernels of the integrals are a fundamental solution, or a linear combination of the derivatives of a fundamental solution of some second-order linear elliptic differential equation. What is different and important about these methods is that they avoid the use of any standard quadrature formula or the exact evaluation of any integral. Instead, they rely on rapid methods of solving the differential equation of which the kernel is the solution. In fact, the number of operations needed to evaluate the volume integral is essentially equal to the number of operations neded to solve the differential equation on a regular rectangular grid. In particular, one can evaluate integrals whose kernels are the Green function for the Poisson equation by using Fourier methods on a rectangular grid, or a fast Poisson solver. Furthermore, the method requires no evaluation of the kernel. Before applying the Poisson solver one only needs to compute special correction terms to the right-hand side of the Poisson equation at mesh points near the boundary of the irregular region, and these correction terms can be obtained by local calculations. (We note that is is not possible to evaluate these integrals by straightforward use of Poisson solvers, since they have discontinuities in their second derivatives across the region of integration.) The method we present can also be thought of as a way of solving elliptic differential equations whose solutions and gradients are continuous, but which have discontinuities in their second derivatives across some irregular boundary.

The ability to evaluate these integrals rapidly is important when integral equation methods are used for solving inhomogeneous differential equations. This is because a particular solution of the differential equation is given by the volume integral of the product of the fundamental solution of the differential equation and the inhomogeneous term. Once the volume integral has been evaluated, the problem is reduced to a homogeneous boundary value problem, which in turn reduces to a surface integral equation. Consider, for example, the problem $\Delta u = f$ on a two-dimensional region D, with Dirichlet boundary data $u = g$ prescribed on ∂D. The solution u can be expressed as the sum of the volume integral $v(x, y) = (1/2\pi) \int_D \int f \log r \, dV$ and a harmonic function w with Dirichlet boundary data $g - v$. The function w can be expressed as the integral of a double layer density function, $(1/2\pi) \int_{\partial D} \mu(s) (\partial \log r/\partial n_s) \, ds$, where μ is the solution of the following integral equation on ∂D:

$$u(t) + \frac{1}{\pi} \int_{\partial D} \mu(s) \frac{\partial \log r(s, t)}{\partial n_s} \, ds = g(t) - v(t).$$

See [10]. Similar formulations hold when Neumann data is given.

We note that integral equation methods for solving elliptic differential equations have become increasingly popular, in part due to the very effective methods for solving certain integral equations developed by Rokhlin [11] and others. We furthermore note that our ability to evaluate these volume integrals may allow us to solve other differential equations such as $\nabla \cdot a(x, y, u) \nabla u = f$, which are not normally solved using integral equation methods. (See [12] and Section 3.)

0021-9991/92 $5.00

These volume integrals also arise in other contexts. In particular, these integrals are needed when applying the Biot Savart law to evaluate the magnetic field induced by a conducting wire. This law says that the field B induced by a conducting wire is the curl of the volume integral of the product of the fundamental solution of the Poisson equation and the current density J:

$$B(x, y, z) = \nabla x \iiint_D J * \frac{1}{4\pi R}\, dx'\, dy'\, dz'$$

$$= \frac{1}{4\pi} \iiint_D J * \nabla\left(\frac{1}{R}\right) dV, \tag{1.1}$$

where

$$R = \sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}.$$

Therefore, each of the three components of the field is equal to the sum of integrals whose integrands are comprised of products of derivatives of the fundamental solution with components of the current density. For example,

$$B_x = \iiint_D (G_y I_z - G_z I_y)\, dV,$$

where

$$G = 1/4\pi R.$$

It is seldom possible to evaluate these integrals analytically when the geometry is complicated. Even if an exact formula is known, it can be expensive to evaluate. For example, the field due to a sequence of circular current loops is an expression which involves sums of elliptic functions [5].

The most commonly used method of evaluating the integrals is by direct application of some quadrature formula. See, for example, [1]. Unfortunately, this can be very expensive. In particular, a total of $O(n^6)$ operations would be required to evaluate the field by computing an integral at every point of an n by n grid, since the evaluation of each integral requires $O(n^3)$ operations, where n is the number of quadrature points in each direction. Even if the field were only needed at $O(n^2)$ points, $O(n^5)$ operations would be required. This is in contrast to $O(n^3 \log n)$ operations required by our method. We also note that while the asymptotic operation count for direct evaluation is smaller for two-dimensional integrals than for three-dimensional integrals, the kernel, $\log r$, is expensive to evaluate.

There is, however, an even more serious difficulty with the straightforward use of quadrature formulas. The problem is that the kernels are unbounded as their arguments approach 0, that is, as the point at which the integral is being evaluated nears a point of integration. It is therefore very difficult to compute these integrals with any degree of accuracy at points in, or near, the domain of integration.

In our method we overcome these problems. The region D over which the integral is to be evaluated, and the points at which the solution is needed, are embedded in some larger rectangular domain. On this larger region we use a rapid method of solving the related differential equation. For example, to evaluate the integral in (1.1) we embed the region of integration D in a larger region for which there is a fast Poisson solver, and to evaluate an integral whose kernel is a fundamental solution for the Helmholtz operator, $(1/4\pi)(e^{ikr}/r)$, we embed the region in a region for which there is a fast solver for the three-dimensional Helmholtz equation.

This method is similar to the method we developed in [9] for solving Laplace's equation on an irregular region. There the problem was reduced to evaluating certain surface integrals. The main idea of our method is the following. Let $U(x, y, z)$ be the function (integral) we wish to compute. Given a discretization L_h of the differential operator, we compute an approximation to $L_h U$ at all points on the mesh of the embedding region. We then apply an operator that inverts L_h to obtain an approximation to U. To compute $L_h U$ at points inside or outside the region of integration which have all of their neighbors on the same side of the boundary we use the fact that, up to truncation error, $L_h U$ is equal to LU which is known exactly. (It is of course equal to the value of the function with which the kernel is convolved.) However, because the integrals we compute necessarily have discontinuities in some of their derivatives at the edge of the domain of integration, we must compute special correction terms at certain mesh points near the boundary. It turns out that these correction terms can be computed in terms of the discontinuities in the derivatives of the integral and how far the mesh points are from the boundary. We show how to compute these discontinuities and how to use them to compute approximations to $L_h U$.

The organization of this paper is as follows. In Section 2 of this paper we show how to compute the integrals whose kernels are a fundamental solution of, or the derivative of, the fundamental solution of the Laplacian, and in Section 3 we discuss certain extensions of the method to the evaluation of other integrals. In Section 4 we provide results of numerical experiments. In particular, we compare our second- and fourth-order accurate methods with straightforward use of Poisson solvers without corrections at the boundaries.

2. THE EVALUATION OF INTEGRALS WHOSE KERNELS SATISFY LAPLACE'S EQUATION

In this section we show how to evaluate integrals whose kernels are any fundamental solution of the Laplacian or

one of its derivatives. To simplify the discussion we first show how to evaluate a second-order accurate approximation of an integral whose kernel is the fundamental solution of the Laplacian in the plane:

$$U(x, y) = 1/2\pi \iint_D f(x', y') \log r(x, y, x', y')\, dx'\, dy'. \quad (2.1)$$

In order to compute an approximation to this integral we first embed the region of integration D in some larger rectangular region R on which there is a uniform mesh.

We evaluate $U(x, y)$ by computing an approximation to its discrete Laplacian, $\Delta_h U$, at all the mesh points of R. Once we have done this, we apply a fast Poisson solver. We note that a Poisson solver is merely an algorithm for inverting the discrete Laplacian. Therefore, if we provide the discrete Laplacian of a function at every mesh point and apply the fast solver, then we will have an approximation to the original function, whether or not is is smooth.

It is easy to see how to compute an approximation to the five-point discrete Laplacian of U at points which have all their neighboring mesh points on the same side of ∂D. We use the fact that at points of R which are inside D,

$$\Delta U = f, \quad (2.2a)$$

and at points which are outside D,

$$\Delta U = 0. \quad (2.2b)$$

Therefore, at mesh points (i, j) inside D which have their four neighboring mesh points $(i+1, j)$, $(i-1, j)$, $(i, j+1)$, and $(i, j-1)$ also inside D we can approximate the discrete Laplacian of U by the value of f at that point, and at outside points which have all of their neighbors outside D, we approximate it by 0. That is, we set

$$\Delta_h U(i, j) = f(i, j)$$

at points inside D whose neighbors are all inside D, and at points outside D, with no neighbors inside D, we set

$$\Delta_h U(i, j) = 0.$$

Since U is not a smooth function, we cannot use either formula at points near ∂D. (We can easily see that U is not smooth at the boundary because its Laplacian is discontinuous there.) Therefore, at such points the values of the discrete Laplacian are not well approximated by the values of the exact Laplacian.

In this section we show how to compute an approximation to the discrete Laplacian of U at these other irregular mesh points, that is the set of points B which have one or more of their neighbors on the other side of ∂D.

It turns out that to be able to compute such an approximation it is sufficient to known what the discontinuities in U and its derivatives in the coordinate directions are at the boundary of D. We note that the discrete Laplacian can be derived by using a Taylor series expansion. Such an expansion is not valid when there are discontinuities in derivatives, but if the discontinuities in derivatives are known, then they may be used to compute correction terms to the Taylor series. One can thereby attain an accurate approximation to the difference operator applied to the integral. In this section we first show how to compute the discontinuities in U, and then we show how to use them to evaluate the discrete Laplacian of U.

To evaluate the discontinuities in U we use (2.2) and the fact U and its normal derivative are continuous across ∂D [7]. For a given function f defined on R which is discontinuous on $\partial D = (x(t), y(t))$ let $[f(p)]$ denote the discontinuity in f at a point p on ∂D. That is, let

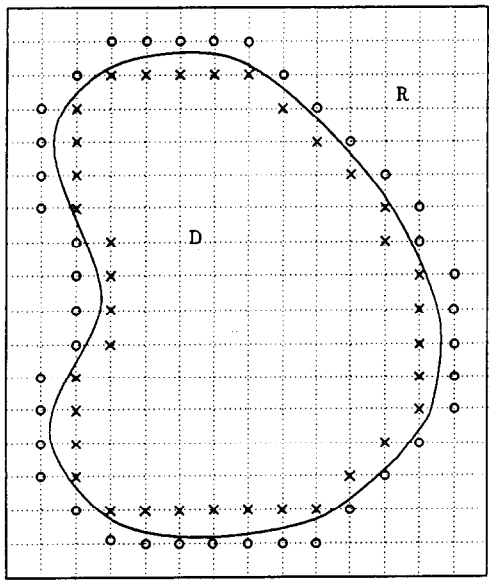
$$[f(p)] = \lim_{\substack{p' \to p \\ p' \in D}} f(p') - \lim_{\substack{p'' \to p \\ p'' \notin D}} f(p'').$$

We assume that $x(t)$ and $y(t)$ have three continuous derivatives. Since an integral of the form (2.1) and its normal derivative are continuous across ∂D,

$$[U(p)] = 0 \quad (2.3)$$

and

$$[U_n(p)] = \dot{y}(t)[U_x(p)] - \dot{x}(t)[U_y(p)] = 0. \quad (2.4)$$



B consists of × and o

FIGURE 1

By differentiating (2.3) in the tangential direction t, we see that

$$[U_t(p)] = \dot{x}(t)[U_x(p)] + \dot{y}(t)[U_y(p)] = 0. \quad (2.5)$$

Equations (2.4) and (2.5) imply that at all points, $p \in \partial D$,

$$[U_x] = 0 \quad (2.6a)$$

and

$$[U_y] = 0. \quad (2.6b)$$

By (2.2) there must be discontinuities in the second derivatives of U. We differentiate (2.4) and (2.5) in the tangential direction and use (2.6) to obtain

$$\dot{x}(t)^2\,[U_{xx}] + \dot{y}(t)^2\,[U_{yy}] + 2\dot{x}(t)\,\dot{y}(t)[U_{xy}] = 0 \quad (2.7)$$

$$\dot{x}(t)\,\dot{y}(t)[U_{xx}] - \dot{x}(t)\,\dot{y}(t)[U_{yy}] + (\dot{y}^2(t) - \dot{x}^2(t))[U_{xy}] = 0. \quad (2.8)$$

By (2.2) we see

$$[U_{xx}] + [U_{yy}] = f. \quad (2.9)$$

Equations (2.7), (2.8), and (2.9) form a three by three linear system of equations that can be used to solve for $[U_{xx}]$, $[U_{yy}]$, and $[U_{xy}]$ at any point on the boundary of D. The determinant of the system, $(\dot{x}(t)^2 + \dot{y}(t)^2)^2$, is nonzero at all points, and, therefore, the equations have a unique solution.

We use similar methods to evaluate discontinuities in the third derivatives of U. There are four such derivatives, U_{xxx}, U_{xxy}, U_{xyy}, and U_{yyy}. To determine the discontinuities in these derivatives we differentiate Eq. (2.6) and (2.7) in the tangential t direction and we differentiate (2.9) in both the normal and tangential directions; that is, we use the four equations $[U_{ntt}] = 0$, $[U_{ttt}] = 0$, $[(\Delta U)_t] = f_t$, and $[(\Delta U)_n] = f_n$. We can continue using this method to compute discontinuities in higher order derivatives.

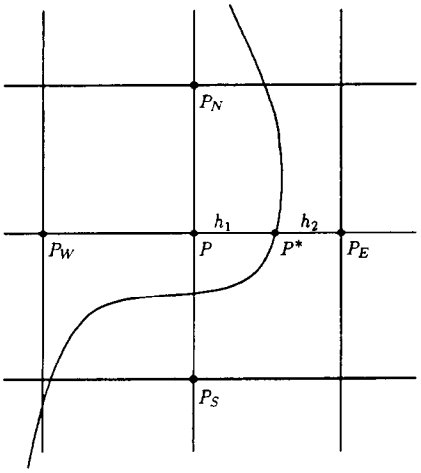


FIGURE 2

We now show how to use these discontinuities to determine the discrete Laplacian at the irregular mesh points. Let B denote the set of such points, and let $U(p) = u(p)$ for p in D, and let $U(p) = \tilde{u}(p)$ for p in $R - D$. To see how to compute $\Delta_h U$ at points of B suppose, for example, that a point p is inside the region, but its neighbor to the right p_E is not. Let p^* be the point where the line between p and p_E, and intersects ∂D, let h_1 be the distance between p and p^*, and let $h_2 = h - h_1$. See Fig. 2.

By manipulating the Taylor series at p and p_E, both evaluated at p^*, we can derive the following expression for $\tilde{u}(p_E) - u(p)$ (for details see [9]),

$$\begin{aligned}\tilde{u}(p_E) - u(p) &= (\tilde{u}(p^*) - u(p^*)) + h_2(\tilde{u}_x(p^*) - u_x(p^*)) \\ &\quad + \tfrac{1}{2}h_2^2(\tilde{u}_{xx}(p^*) - u_{xx}(p^*)) \\ &\quad + \tfrac{1}{6}h_2^3(\tilde{u}_{xxx}(p^*) - u_{xxx}(p^*)) \\ &\quad + hu_x(p) + \tfrac{1}{2}h^2u_{xx}(p) + \tfrac{1}{3}h^3u_{xxx}(p) \\ &= \{\text{known quantities}\} + hu_x(p) \\ &\quad + \tfrac{1}{2}h^2u_{xx}(p) + O(h^3), \end{aligned} \quad (2.10)$$

where the known quantities can be computed in terms of derivatives of f and the boundary curve, and the distances of the irregular mesh points from the boundary.

Now let p_w be the mesh point to the left of p. If p_w is in D then

$$U(p_W) - U(p) = -hu_x(p) + \frac{h^2}{2}u_{xx}(p) + O(h^3).$$

If not,

$$U(p_W) - U(p) = \{\text{known quantities}\} - hu_x(p) + \frac{h^2}{2}u_{xx}(p) + O(h^3).$$

In any case,

$$U(p_E) - 2U(p) + U(p_W) = \{\text{known quantities}\} + h^2u_{xx} + O(h^3).$$

Let p_N be the point above p, and let p_S be the point below p. By the same arguments as above we have

$$U(p_N) - 2U(p) + U(p_S) = \{\text{known quantities}\} + h^2u_{yy} + O(h^3).$$

It follows that $h^2\Delta_h U(p) = \{\text{known quantities}\} + O(h^3)$, since $u_{xx} + u_{yy} = 0$.

We note that we can also retain fourth-order Taylor series terms in our derivation. For example, (2.10) can be replaced by

$$\begin{aligned}\tilde{u}(p_E) - u(p) = {} & (\tilde{u}(p^*) - u(p^*)) + h_2(\tilde{u}_x(p^*) - u_x(p^*)) \\ & + \tfrac{1}{2}h_2^2(\tilde{u}_{xx}(p^*) - u_{xx}(p^*)) \\ & + \tfrac{1}{6}h_2^3(\tilde{u}_{xxx}(p^*) - u_{xxx}(p^*)) + hu_x(p) \\ & + \tfrac{1}{2}h^2u_{xx}(p) + \tfrac{1}{3}h^3u_{xxx}(p) + O(h^4). \qquad (2.11)\end{aligned}$$

By so doing we instead obtain a fourth-order accurate approximation to $h^2\Delta_h U(p)$ at points of B.

If the boundary data, and therefore the solution u are sufficiently regular, this guarantees the accuracy of the approximation to U that we obtain after applying a fast Poisson solver.

For mesh points $(x_i, y_i) \in B$ define the mesh function m_{ij} to be the value of the extra terms in the discrete Laplacian we obtain by our procedure using f and its derivatives.

We define U_{ij} to be the solution of the following equations:

$$\Delta_h U_{ij} = \begin{cases} f_{ij} & (i,j) \in D - B \\ f_{ij} + m_{ij} & (i,j) \in B \cap D \\ m_{ij} & (i,j) \in B \cap D^c \\ 0 & (i,j) \in R - D - B. \end{cases}$$

If the values of $m_{i,j}$ are third-order accurate, then by applying a second-order accurate Poisson solver we obtain a second-order accurate approximation $U_{i,j}$ to U; see [8, 9].

We can use the method we have just described to compute a fourth-order accurate approximation to U. In particular, if values of Δf are known we can use the following fourth-order accurate nine-point stencil [3]:

$$\begin{aligned}\Delta_h^9 U &= 1/(6h^2)\begin{bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{bmatrix} U \\ &= f + h^2\,\Delta f + O(h^4).\end{aligned}$$

This stencil is a linear combination of two second-order accurate stencils,

$$\Delta_h^9 = \tfrac{2}{3}\Delta_h + \tfrac{1}{3}\Delta_h^x,$$

where

$$\Delta_h^x = \frac{1}{2h^2}\begin{bmatrix} 1 & & 1 \\ & -4 & \\ 1 & & 1 \end{bmatrix}.$$

We have already shown how to approximate $\Delta_h U$, so it only remains to see how to approximate $\Delta_h^x U$. In order to compute this stencil we need to know the discontinuities in U and in its s and t derivatives, where $s = (x+y)/\sqrt{2}$ and $t = (x-y)/\sqrt{2}$. The discontinuities can, of course, be computed in terms of the discontinuities in the x and y directions by using the chain rule. For example, if p^* is on ∂D, then

$$u_s(p^*) - \tilde{u}_s(p^*) = \frac{[u_x(p^*) - \tilde{u}_x(p^*)]}{\sqrt{2}} + \frac{[u_y(p^*) - \tilde{u}_y(p^*)]}{\sqrt{2}}.$$

Once we know these discontinuities we may, in the same way as before, use them to compute a high order accurate approximation to $\Delta_h^x U$ and thereby $\Delta_h^9 U$. After applying a fourth-order accurate Poisson solver we obtain a fourth-order accurate approximation to U.

We can in the same way compute highly accurate approximations to three-dimensional integrals of the form

$$U = \frac{1}{4\pi}\iiint_D f(x', y', z')\frac{1}{r}\,dV'. \qquad (2.12)$$

Since we again have

$$\Delta U = \begin{cases} f & \text{inside } D \\ 0 & \text{outside } D, \end{cases}$$

the problem again reduces to evaluating the discontinuities in the derivatives of U at the boundary of the region of integration. In order to do this we can use essentially the same method as in the two-dimensional case. Again we note that there are no discontinuities in either the tangential derivatives or in the normal derivative of U. This again implies that there are no discontinuities in any of the first derivatives of U, i.e.,

$$[U_x] = [U_y] = [U_z] = 0.$$

Suppose the boundary surface ∂D is given by $(x(s,t), y(s,t), z(s,t))$, where s and t are two real parameters. To determine discontinuities in the six second derivatives of U we use the six equations

$$\begin{aligned}&[U_{ss}] = 0, \quad [U_{st}] = 0, \quad [U_{tt}] = 0, \\ &[U_{ns}] = 0, \quad [U_{nt}] = 0, \\ &[U_{xx}] + [U_{yy}] + [U_{zz}] = f.\end{aligned}$$

This system has a unique solution. Once determined, these discontinuity terms, and the discontinuities in the higher order derivatives can be used to compute approximations to the three-dimensional discrete Laplacian of U. By applying a three-dimensional fast Poisson solver, we obtain an approximation to U.

Before applying a Poisson solver we must, of course, supply appropriate boundary conditions. If we only need a particular solution of Poisson's equation, then there is no difficulty, since the discontinuities in the derivatives of the integral, and therefore the discrete Laplacian, will be the same, independent of which fundamental solution of the Laplacian is used as the kernel. The integral we obtain an approximation to is the one associated with the same boundary conditions as the fast Poisson solver we use. For example, if we use a doubly periodic Poisson solver, then we obtain an approximation to the integral whose kernel is the doubly periodic Green function for the Laplacian. If we need an integral with a specific kernel, then we use the corresponding Poisson solver.

A more difficult problem arises when we need to solve an exterior problem. In that case we can use a method originally developed by Hockney [2], and later improved by James [6], where one calculates the boundary potential by finding a set of correction charges on the boundary of the embedding region and then convolves them with a suitable Green function. This method, however, is more expensive than the others, since it requires the application of two Poisson solvers.

We now show how to evaluate integrals whose kernels are derivatives, or a linear combination of the derivatives of the fundamental solution of some elliptic differential equation. Consider, for example, an integral whose kernel is the gradient of a fundamental solution G for the Laplacian,

$$W(p) = \iiint_D M(p') \cdot \nabla_p G(p, p')\, dV',$$

where M is a smooth vector field, $p = (x, y, z)$, and $p' = (x, y', z')$. By noting that

$$\nabla_p G = -\nabla_{p'} G$$

and using the divergence theorem, we see that

$$W(p) = \iiint_D \nabla_{p'} \cdot M(p')\, G(p, p')\, dV' + \iint_{\partial D} M \cdot n \frac{\partial G}{\partial n}\, dS. \tag{2.13}$$

Since the second integral in the above equation is harmonic, $\Delta W = \nabla \cdot M$ in D and $\Delta W = 0$ outside.

To evaluate discontinuities in derivatives of volume integrals with differentiated kernels we use the fact that those integrals are derivatives of integrals with undifferentiated kernels. For example, suppose

$$V(p) = \iiint_D f(p')\, G_x(p, p')\, dV'.$$

We use the fact that $V(x, y, z) = U_x(x, y, z)$, where

$$U(p) = \iiint_D f(p')\, G(p, p')\, dV'.$$

Since we know how to compute the discontinuities in the derivatives of U, we can, of course, compute the discontinuities in the derivatives of $V = U_x$. As before, once we know the discontinuity terms we can use them to approximate the discrete Laplacian of V.

3. EXTENSIONS

This method can also be used to evaluate other integrals which are not solutions of the Poisson equation. For example, consider a nonlinear interface problem of the form

$$\nabla \cdot a(x, y, u) \nabla u = 0, \tag{3.1}$$

where $a(x, y, u)$ is positive definite in some bounded region D and equal to a constant a_0 in the unbounded region outside D. Such problems arise in magnetostatics where u denotes the total scalar potential function, that is, the function whose gradient is equal to the H field, $a(x, y, u)$ is the permeability of the material in region D, and a_0 is the permeability of free space. Suppose there is a current source in the unbounded region whose potential function is ϕ_a. Then, by using the fact that u and $a(x, y, u)(\partial u/\partial n)$ are continuous across ∂D and the divergence theorem (see [12]), one can show that on ∂D the solution u satisfies the integral equation,

$$u(z) - \frac{1}{\pi(\bar{a}(z)+1)}\left[\int_{\partial D} (\bar{a}(\zeta) - 1)\, u(\zeta) \frac{\partial \log r}{\partial n_s}\, ds + \int_D \int u \nabla a \cdot \nabla \log r\, dv\right] = \frac{2}{\bar{a}(z)+1} \phi_a(z), \tag{3.2}$$

where $\bar{a}(x, y) = a(x, y)/a_0$, and inside D, u satisfies the equation

$$u(z) = \frac{1}{\bar{a}(z)}\left[\phi_a(z) - \frac{1}{2\pi}\int_{\partial D} (\bar{a}(\zeta) - 1)\, u(\zeta) \times \frac{\partial \log r}{\partial n_s}\, ds + \frac{1}{2\pi}\int_D \int u \nabla \bar{a} \cdot \nabla \log r\, dV\right]. \tag{3.3}$$

The volume integrals occurring in (3.2) and (3.3) are of the form (2.1) and can therefore be evaluated by the method described in Section 2, if an estimate for u is available. Rapid methods for evaluating this integral could therefore be used in an iterative method for solving (3.1).

TABLE I

$n = 33$

Rms error = 0.3152E-03
Max. abs. error = 0.1018E-02 at 0.72, 0.50
Max. rel. error = 0.6696E-03 at 0.72, 0.50

$n = 65$

Rms error = 0.7468E-04
Max. abs. error = 0.2193E-03 at 0.34, 0.66
Max. rel. error = 0.1502E-03 at 0.33, 0.33

$n = 129$

Rms error = 0.1861E-04
Max. abs. error = 0.5244E-04 at 0.66, 0.66
Max. rel. error = 0.3564E-04 at 0.33, 0.66

TABLE III

$n = 33$

Rms error = 0.2598E-01
Max. abs. error = 0.6373E-01 at 0.50, 0.66
Max. rel. error = 0.3433E-01 at 0.50, 0.66

$n = 65$

Rms error = 0.7176E-02
Max. abs. error = 0.1828E-01 at 0.64, 0.55
Max. rel. error = 0.9576E-02 at 0.64, 0.55

$n = 129$

Rms error = 0.2514E-02
Max. abs. error = 0.6783E-02 at 0.63, 0.57
Max. rel. error = 0.3579E-02 at 0.63, 0.57

We can also evaluate integrals whose kernels G are the fundamental solution of other second-order self-adjoint linear elliptic differential operators L, when efficient methods are available for inverting the differential operator on a larger region. For example, we can evaluate integrals whose kernels are Hankel functions of the first kind by embedding the region of integration in a region for which there is a two-dimensional Helmholtz solver. The reason we can do this is because the fundamental solutions of these types of equations have the same types of singularities as the fundamental solutions of the Poisson equation [10]. Therefore, the integrals will have the same kind of computable discontinuities across the boundary of the region of integration. The integrals will also satisfy an inhomogeneous differential equation inside the region and the homogeneous equation outside. That is, an integral of the form

$$W = \iiint_D f^* G \, dV$$

will satisfy $LW = f$ inside D and $LW = 0$ outside D. This means that we can again compute an approximation to a discrete difference operator L_h applied to the integral W, invert the difference operator L_h, and obtain an approximation to the integral.

4. RESULTS OF NUMERICAL EXPERIMENTS

In this section we present results of numerical experiments. We tested this method on two problems for which we could evaluate the integrals analytically, both inside and outside the domain of integration. As our first test problem we evaluated the integral

$$U(x, y) = \frac{1}{4\pi} \iint f(x', y') \log[(x - x')^2 + (y - y')] \, dV'$$

with $f(x, y) = 5$. The domain of integration was the disk of radius $r_0 = 0.2$ centered at (0.5, 0.5), $D = (x - 0.5)^2 +$

TABLE II

$n = 33$

Rms error = 0.5508E-03
Max. abs. error = 0.1316E-02 at 0.34, 0.41
Max. rel. error = 0.7729E-03 at 0.34, 0.41

$n = 65$

Rms error = 0.1905E-08
Max. abs. error = 0.7384E-08 at 0.33, 0.42
Max. rel. error = 0.4449E-08 at 0.42, 0.31

$n = 129$

Rms. error = 0.1339E-10
Max. abs. error = 0.7138E-10 at 0.43, 0.32
Max. rel. error = 0.4364E-10 at 0.42, 0.32

TABLE IV

$n = 33$

Rms error = 0.2571E-01
Max. abs. error = 0.6301E-01 at 0.34, 0.50
Max. rel. error = 0.3394E-01 at 0.34, 0.50

$n = 65$

Rms error = 0.7264E-02
Max. abs. error = 0.1890E-01 at 0.45, 0.36
Max. rel. error = 0.9902E-02 at 0.45, 0.36

$n = 129$

Rms error = 0.2495E-02
Max. abs. error = 0.6836E-02 at 0.43, 0.37
Max. rel. error = 0.3607E-02 at 0.43, 0.37

TABLE V

$n = 33$

Rms error = 0.3514E-02
Max. abs. error = 0.1384E-01 at 0.31, 0.50

$n = 65$

Rms error = 0.8122E-03
Max. abs. error = 0.2732E-02 at 0.67, 0.63

$n = 129$

Rms error = 0.2036E-03
Max. abs. error = 0.6895E-03 at 0.44, 0.70

TABLE VI

$n = 33$

Rms error = 0.9743E-05
Max. abs. error = 0.1285E-04 at 0.34, 0.38

$n = 65$

Rms error = 0.3216E-07
Max. abs. error = 0.2015E-06 at 0.59, 0.34

$n = 129$

Rms error = 0.4020E-09
Max. abs. error = 0.2402E-08 at 0.32, 0.44

$(y-0.5)^2 < 0.04$. For this region the values of the integral are given by

$$U(r) = 0.5\frac{r^2}{r_0^2} - 0.5 + \log r_0 \quad \text{for } r < r_0$$

and

$$U(r) = \log r \qquad \text{for} \quad r \geqslant r_0,$$

where $r = \sqrt{(x-0.5)^2 + (y-0.5)^2}$. We embedded D in the unit square and gave exact values of the integral at the edge of the embedding region. The computations were done in double precision on an IBM 3090 machine. The running time was essentialyy equal to the time needed to invert the discrete Laplacians.

In Table I we present the results of calculations using the second-order accurate method, and in Table II we present results of using the fourth-order accurate method. Here n

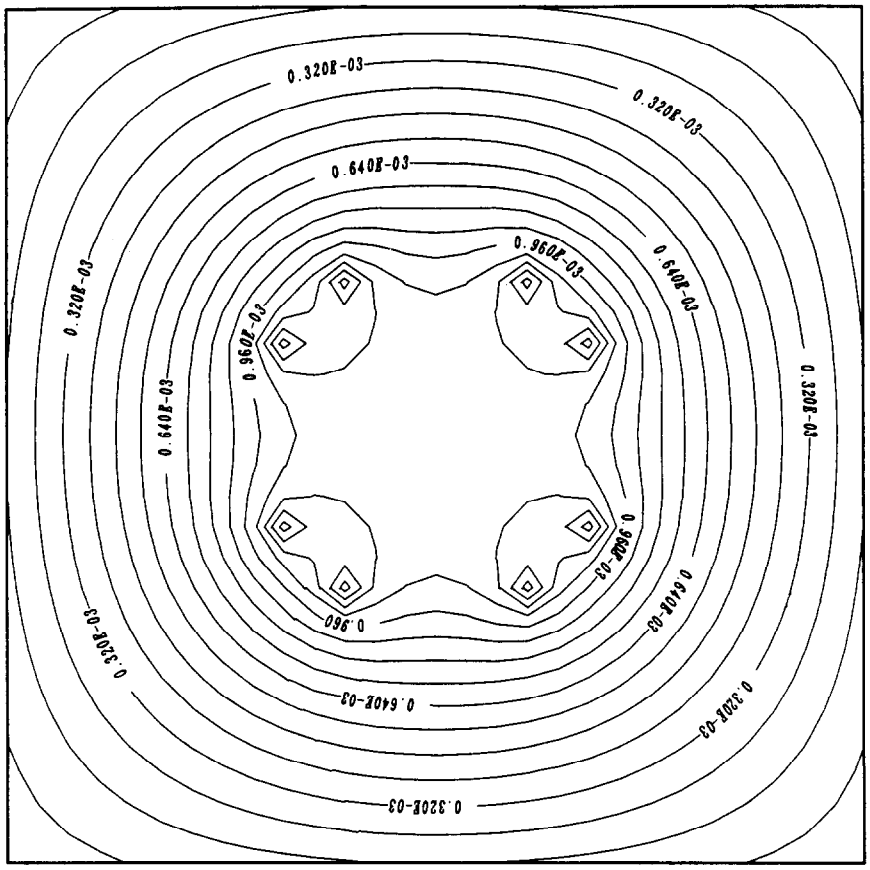


FIGURE 3

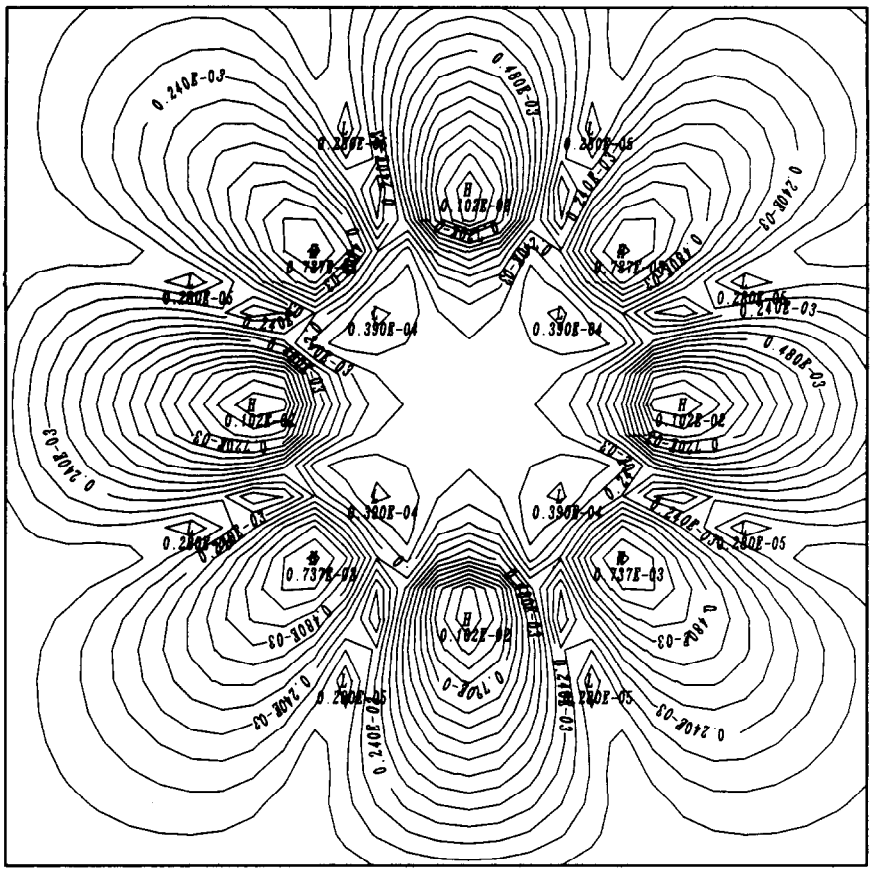


FIGURE 4

denotes the number of mesh points in each direction across the square. These numbers show that the methods do achieve the predicted levels of accuracy.

In Fig. 3 the errors we obtained in computing the integral U by the second-order accurate method on a 33 by 33 grid are graphed, and in Fig. 4 the errors obtained by the fourth-order accurate method are graphed.

We also did calculations where we did not add the proper correction terms to the right-hand sides of the equations at mesh points near boundaries of the regions of integration before applying the solvers. That is, we set the discrete Laplacian of U equal to f at points inside D and equal to 0 at points outside. Results of applying a second-order accute Poisson solver are given in Table III and results of applying a fourth-accurate solver are given in Table IV. These errors show that if we do not make corrections at the boundary, then we cannot expect even second-order accurate convergence.

We also computed the x derivative of the integral in the previous example. In this case the values of the integral V are given by $V(r) = (x-0.5)/r_0^2$ for $r < r_0$, and $V(r) = (x-0.5)/r^2$ for $r > r_0$. Results of calculations by the second-order accurate method are given in Table V and results of fourth-order accurate calculations are given in Table VI.

We again achieved the predicted rates of convergence, although the errors were larger in magnitude. The larger errors obtained when computing the derivative function are not the results of numerical differentiation, but are due to the fact that the discrete Laplacian of the exterior function has a larger truncation error. That is, the derivatives of $(x-0.5)/r^2$ are larger than those of $\log r$.

CONCLUSIONS

We have presented a rapid numerical method for the evaluation of certain volume integrals in potential theory. In particular, we have shown that second- and fourth-order acute approximations are easily obtained. We have also suggested how these methods might be used in other contexts.

ACKNOWLEDGMENT

The author is grateful for critical reading of this paper by Leslie Greengard, Jonathan Goodman, and Olof Widlund.

REFERENCES

1. K. Atkinson, *J. Num. Anal.* **5**, 319 (1985).
2. R. Hockney, *Methods in Computational Phys.* Vol. 9 (Academic Press, New York, 1970), p. 135.
3. E. Houstics and T. Papatheodorou, "Comparison of Fast Direct Methods for Elliptic Problems," in Advances in Computer Methods for Partial Differential Equations, IMACS, Lehigh, 1977.
4. E. Isaacson and H. Keller, *Analysis of Numerical Methods* (Wiley, New York, 1966).
5. J. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975).
6. R. James, *J. Comput. Phys.* **25**, 71 (1977).
7. O. Kellogg, *Foundations of Potential Theory* (Dover, New York, 1953).
8. A. Mayo, *SIAM J. Sci. Stat. Comput.* **6**, 144 (1985).
9. A. Mayo, *SIAM J. Num. Anal.* **21**, 285 (1984).
10. S. Mikhlin, *Linear Equations of Mathematical Physics* (Holt, Rinehart & Winston, New York, 1967).
11. V. Rokhlin, *J. Comput. Phys.* **60**, 187 (1985).
12. J. Simpkin and E. Trowbridge, *Int. J. Num. Methods* **14**, 423 (1979).