JOURNAL OF COMPUTATIONAL PHYSICS 47, 281–290 (1982)

Regional Monte Carlo Solution of Elliptic Partial Differential Equations*†

THOMAS E. BOOTH

Los Alamos National Laboratory, Los Alamos, N. M. 87545

Received July 15, 1981; revised March 31, 1982

A continuous random walk procedure for solving some elliptic partial differential equations at a single point is generalized to estimate the solution everywhere. The Monte Carlo method described here is exact (except at the boundary) in the sense that the only error is the statistical sampling error that tends to zero as the sample size increases. A method to estimate the error introduced at the boundary is provided so that the boundary error can always be made less than the statistical error.

INTRODUCTION

Monte Carlo methods have been suggested [1, 2] for solving elliptic partial differential equations at a single point. The theory described in [1] can be generalized to estimate the solution everywhere.

We shall show how to solve some partial diferential equations of the form

$$u_{xx} + u_{yy} - \alpha^2 u = 0, \qquad \alpha^2 \text{ const.} \tag{1}$$

This is an important class of partial differential equations because any elliptic partial differential equation with constant coefficients can be reduced, by suitable transformations [3] to the canonical form of Eq. (1).

DIRICHLET PROBLEM IN POLAR COORDINATES

We shall consider solving Eq. (1) with u specified on the boundary. A separation of variables in polar coordinates yields [1]

$$u(r, \theta) = \tfrac{1}{2} a_0 I_0(\alpha r) + \sum_{n=1}^{\infty} I_n(\alpha r)(a_n \cos n\theta + b_n \sin n\theta), \tag{2}$$

† This work was performed under the auspices of the U.S. Department of Energy.

0021-9991/82/080281-10$02.00/0

where the I_n are the modified Bessel functions. The expansion coefficients are obtained in the usual manner by integrating with $\cos n\theta$ and $\sin n\theta$ to give

$$a_n = \frac{2}{I_n(\alpha r)} \frac{1}{2\pi} \int_{-\pi}^{\pi} u(r, \theta) \cos n\theta \, d\theta, \tag{3}$$

$$b_n = \frac{2}{I_n(\alpha r)} \frac{1}{2\pi} \int_{-\pi}^{\pi} u(r, \theta) \sin n\theta \, d\theta. \tag{4}$$

These coefficients may be estimated, however, by sampling θ_i uniformly on $[0, 2\pi]$ and using

$$\hat{a}_n = \frac{2}{I_n(\alpha r)} \frac{1}{M} \sum_{i=1}^{M} u(r, \theta_i) \cos n\theta_i, \tag{5}$$

$$\hat{b}_n = \frac{2}{I_n(\alpha r)} \frac{1}{M} \sum_{i=1}^{M} u(r, \theta_i) \sin n\theta_i. \tag{6}$$

Now if we wish to solve Eq. (1) in the vicinity of a point P_0 (see Fig. 1) we draw the largest circle (with center at P_0) that lies entirely within D and proceed to sample the θ_i of Eqs. (5) and (6). We do not know $u(r, \theta_i)$, and so we use the single point theory [1] to get a one-particle estimate $\hat{u}(r, \theta_i)$ and then use

$$\hat{\hat{a}}_n = \frac{2}{I_n(\alpha r)} \frac{1}{M} \sum_{i=1}^{M} \hat{u}(r, \theta_i) \cos n\theta_i, \tag{7}$$

$$\hat{\hat{b}} = \frac{2}{I_n(\alpha r)} \frac{1}{M} \sum_{i=1}^{M} \hat{u}(r, \theta_i) \sin n\theta_i. \tag{8}$$

Thus, the solution *at any point* inside D (the solution may be extented for $\rho > r$ because all the derivatives exist) may be estimated by:

$$\hat{u}(\rho, \phi) = \tfrac{1}{2}\hat{\hat{a}}_0 I_0(\alpha\rho) + \sum_{n=1}^{N} I_n(\alpha\rho)(\hat{\hat{a}}_n \cos(n\phi) + \hat{\hat{b}}_n \sin(n\phi)). \tag{9}$$

Note that N has replaced infinity as the upper limit on the sum. The reasons for this replacement are twofold. First, as a practical matter, we simply cannot sum an

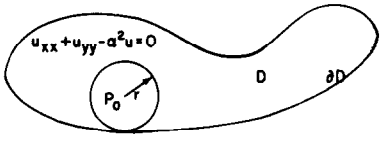


FIGURE 1

infinite number of terms; and second, there are mathematical difficulties for $\rho \geqslant r$ as N approaches infinity.

The mathematical difficulties arise from the $1/I_n(\alpha r)$ of Eqs. (7) and (8) that is multiplied by the $I_n(\alpha\rho)$ of Eq. (9) to give the ratio $R_n = I_n(\alpha\rho)/I_n(\alpha r)$. Recalling that

$$I_n(z) = (1/n!)(z/2)^n[1 + (z/2)^2/(1!(n+1)) + (z/2)^4/(2!(n+1)(n+2)) + \cdots], \quad (10)$$

we see that $R_n \to \infty$ as $n \to \infty$ as long as $\rho < r$. Thus for $\rho < r$ (and α real) errors in estimating (see Eqs. (3) and (4))

$$C_n = \int_{-\pi}^{\pi} u(r, \theta) \cos n\theta \, d\theta$$

and

$$S_n = \int_{-\pi}^{\pi} u(r, \theta) \sin n\theta \, d\theta$$

become progressively less important to $\hat{u}$ as $n \to \infty$. For $\rho > r$, $R_n \to \infty$ as $n \to \infty$, and thus any statistical errors are magnified. For any finite m, we can make the statistical estimation good enough (by increasing the number of samples) so that the error in the mth term is arbitrarily small. Consider the term $\hat{A}_m = I_m(\hat{\hat{a}}\rho)\, a_m \cos m\theta$ of Eq. (9). Let e_m be the error in $\hat{\hat{a}}_m$; then the error in $\hat{A}_m$ is $E_m = e_m |I_m(\alpha\rho) \cos m\theta|$. In a bounded domain, however, $|I_m(\alpha\rho) \cos m\theta|$ can be bounded by some number B_m and thus $E_m < B_m e_m$. Furthermore, the central limit theorem guarantees that e_m decreases as $M^{-1/2}$ ($M =$ the number of samples), so that $E_m < B_m e_m$ will also decrease as $M^{-1/2}$.

As a practical matter, one should not extend the solution outside the circle without checking to see if $\hat{u}$ matches the boundary conditions reasonably well. The estimated solution $\hat{u}$ must satisfy Eq. (1) because of the manner in which it is defined. If $\hat{u}$ also matches the boundary conditions, then $\hat{u}$ is the solution we seek.

Convergence of the Estimates for a_n and b_n

In [1] it was shown that the estimate for a_0 converged for real α. To prove that the estimates for a_n and b_n converge, one need only replace the u of [1, Eq. (24)] with $u \cos n\theta_0$ and $u \sin n\theta_0$, where θ_0 is the angle selected when departing the initial point P_0.

An Iterative Monte Carlo Approach

Using the superposition principle, we may write the solution to Eq. (1) as

$$u(r, \theta) = f(r, \theta) + g(r, \theta), \quad (11)$$

where f is any function that satisfies Eq. (1). In this case, g must also satisfy Eq. (1) subject to the boundary condition that g on the boundary be equal to u on the

boundary minus f on the boundary. If f is approximately equal to u then the boundary values of g will be small, leading to a small absolute error when estimating g by the Monte Carlo method described here. In other words, we shall solve for g, the (residual) difference between the true solution u and the best estimate of u, which we shall call f. We know (from Eq. (9)) that choosing $f = f^0(r, \theta) = \hat{u}(r, \theta)$ will ensure that f satisfies Eq. (1), because $\hat{u}(r, \theta)$ is always a sum of functions that individually satisfy Eq. (1). Furthermore, choosing

$$f^{n+1}(r, \theta) = f^n(r, \theta) + \hat{g}^n(r, \theta) \tag{12}$$

also guarantees that f^{n+1} satisfies Eq. (1) by induction on n, because f^0 and all the $\hat{g}^n$ satisfy Eq. (1). Thus we estimate

$$\hat{u}^n(r, \theta) = f^n(r, \theta) + \hat{g}^n(r, \theta) \tag{13}$$

and then choose $f^{n+1} = \hat{u}^n$ for the next iteration.

Example. Consider solving Eq. (1) in a rectangle of dimensions $\pi/2$ by 1 subject to the boundary conditions in Fig.2. The solution to this problem is $u(x, y) = \sin x$ because $\sin x$ both satisfies Eq. (1) and meets the boundary conditions. Now take a circle of radius 0.5 centered on $(0.2\pi, 0.5)$ and estimate the solution using the iterative Monte Carlo method described earlier. In particular, suppose we wish u at $x_1 = 0.2\pi + 0.4$, $y_1 = 0.5$.

The approximate solution was taken to be $(J_n(r) = I_n(ir))$ (i.e., $\alpha = i$ in Eq. (1)

$$\hat{u}(r, \theta) = \tfrac{1}{2}\hat{\hat{a}}_0 J_0(r) + \sum_{n=1}^{8} J_n(r)(\hat{\hat{a}}_n \cos n\theta + \hat{\hat{b}}_n \sin n\theta), \tag{14}$$

where the coefficients were taken to be zero until the estimate was at least three times the standard deviation of the estimate. Furthermore, the sample size on each iteration was doubled if the estimated error in $\hat{u}(x_1 = 0.2\pi + 0.4, y_1 = 0.5)$ was more than 0.7 times the estimated error on the previous iteration, otherwise the sample size was taken to be the same size as on the previous iteration.

Table I shows how the error in $\hat{u}(x_1, y_1)$ decreases with the number of iterations and Table II compares the estimated coefficients after 29 iterations with the true values obtained by using Eqs. (3) and (4) with the true solution and Bessel's Integral

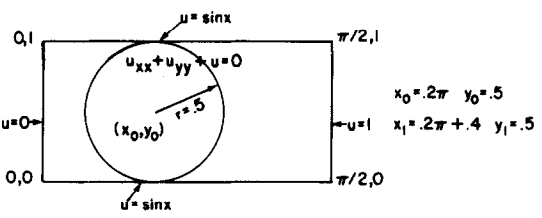


FIGURE 2

TABLE I

Iteration	Number samples	Total samples	$\hat{u}(x_1, y_1)$	$\sigma_{\hat{u}}$ (error)	Last nonzero COEFF	$u(x_1, y_1) - \hat{u}(x_1, y_1)$
1	100	100	0.80428	8.1E − 2	—	5.2E − 2
2	200	300	0.87097	1.0E − 2	A(1)	−1.5E − 2
3	200	500	0.85455	2.6E − 3	A(2)	1.9E − 3
4	200	700	0.85640	4.6E − 4	A(3)	3.3E − 5
5	200	900	0.85565	1.4E − 4	A(3)	7.9E − 4
6	200	1100	0.85633	1.8E − 4	A(3)	1.0E − 4
7	400	1500	0.85645	9.7E − 5	A(3)	−2.0E − 5
8	400	1900	0.85651	7.8E − 5	A(3)	−7.7E − 5
9	800	2700	0.85642	1.1E − 5	A(4)	8.5E − 6
10	800	3500	0.85643	4.8E − 6	A(4)	3.9E − 6
11	800	4300	0.85643	8.5E − 7	A(5)	1.9E − 7
12	800	5100	0.85643	4.1E − 7	A(5)	−2.4E − 7
13	800	5900	0.85643	5.6E − 7	A(5)	−1.1E − 6
14	1600	7500	0.85643	3.5E − 7	A(5)	1.6E − 6
15	1600	9100	0.85643	2.1E − 7	A(5)	8.5E − 7
16	1600	10,700	0.85643	1.3E − 7	A(6)	2.7E − 7
17	1600	12,300	0.85643	9.9E − 8	A(6)	1.8E − 8
18	3200	15,500	0.85643	6.4E − 8	A(6)	−2.2E − 7
19	3200	18,700	0.85643	7.9E − 8	A(6)	2.2E − 7
20	6400	25,100	0.85643	1.7E − 8	A(6)	−2.0E − 8
21	6400	31,500	0.85643	1.9E − 8	A(6)	−2.1E − 8
22	12,800	44,300	0.85643	1.5E − 8	A(6)	−5.4E − 8
23	25,600	69,900	0.85643	6.7E − 9	A(6)	7.2E − 9
24	25,600	95,500	0.85643	5.9E − 9	A(7)	−4.0E − 9
25	51,200	146,700	0.85643	5.0E − 10	A(7)	8.6E − 10
26	51,200	197,900	0.85643	2.8E − 10	A(7)	−5.7E − 10
27	51,200	249,100	0.85643	1.2E − 10	A(8)	1.8E − 10
28	51,200	300,300	0.85643	5.8E − 11	A(8)	2.4E − 11
29	51,200	351,500	0.85643	2.1E − 11	A(8)	5.9E − 12

Note. Mean time per sample is independent of the iteration index.

[5]. Recall that the estimated coefficients were taken to be zero unless the estimate was at least three times the standard deviation of the estimate. The mean time per sample is independent of the iteration number.

Comments on the Boundary Error

As noted in [1] there is an error made at the last step of the random walk unless there is a nonzero probability of actually sampling the boundary points. For special geometries, one may choose to sample points on shapes other than the circle discussed here so that there is a nonzero probability of sampling the boundary. In

TABLE II

Comparison After 29 Iterations (all $b_n = \hat{b}_n = 0$)

	True a_n	Estimated $\hat{a}_n$	σ_{a_n}	1σ error $\sigma_{b_n}(\hat{b}_n = 0 \text{ all } n)$
$n=0$	1.17557050	1.17557050	1.9E − 11	
1	1.61803399	1.61803399	6.7E − 11	1.6E − 11
2	−1.17557050	−1.17557050	4.4E − 10	1.9E − 11
3	−1.61803399	−1.61803399	5.0E − 9	2.0E − 11
4	1.17557050	1.17557050	8.1E − 8	2.0E − 11
5	1.61803399	1.61803407	1.6E − 6	2.1E − 11
6	−1.17557050	−1.17561773	3.9E − 5	2.1E − 11
7	−1.61803399	−1.61900777	1.1E − 3	2.1E − 11
8	1.17557050	1.11109851	3.4E − 2	2.1E − 11

other words, a shape can be chosen such that the boundary and a portion of the shape coincide for some nonzero length [1].

In general, however, the random walks must terminate not on the boundary but within some ε of the boundary because the circle (or other shape) that we are sampling only coincides with the boundary at a finite number of points. Thus, a small error is introduced when we take the value at the end of the random walk to be the boundary value. This boundary error can be easily estimated during the Monte Carlo solution and ε can be adjusted on each iteration to ensure that the boundary error always remains less than the statistical error.

To estimate the boundary error we occasionally (say, on every tenth sample) require the random walk to get within some smaller ε, say $\varepsilon/10$, of the boundary. We then score the *difference* in the estimates of the coefficients between applying the ε or $\varepsilon/10$ rule for termination to the *same* random walk. Thus we can estimate how different our answer would have been if the random walks had terminated within $\varepsilon/10$ of the boundary rather than within ε. (For the example $\varepsilon = 10^{-12}$ and the difference in a_0 between using $\varepsilon/10$ and ε was $-2.1\text{E} - 12$, significantly less than the statistical error of $1.9\text{E} - 11$).

Application to Other Coordinate System

There is nothing special about the polar coordinate expansion coefficients. The expansion coefficients can be generated for any coordinate system in which Eq. (1) is separable because the expansion coefficients always involve an integral that may be estimated by Monte Carlo. In the next section, for example, we show how to estimate the expansion coefficients in Cartesian coordinates.

DIRICHLET PROBLEM IN CARTESIAN COORDINATES

If the variables are separated into x, y coordinates, the solution to

$$\begin{array}{ccc} & 0, b \quad f_3(x) \quad a, b & \\ f_2(y) & \boxed{u_{xx} + u_{yy} - \alpha^2 u = 0} & f_4(y) \\ & 0, 0 \quad f_1(x) \quad a, 0 & \end{array}$$

with the indicated boundary conditions f_i is $u(x, y) = u_1(x, y) + u_2(x, y) + u_3(x, y) + u_4(x, y)$, where (see Appendix)

$$u_1(x, y) = \sum_{n=1}^{\infty} \frac{2}{\sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2} b\}} \frac{1}{a} \int_0^a f_1(x') \sin \frac{n\pi x'}{a} dx' \times \sin(n\pi x/a) \sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2}(b - y)\}, \tag{15}$$

$$u_2(x, y) = \sum_{n=1}^{\infty} \frac{2}{\sinh\{(\alpha^2 + (n\pi/b)^2)^{1/2} a\}} \frac{1}{b} \int_0^b f_2(y') \sin \frac{n\pi y'}{b} dy' \times \sin(n\pi y/b) \sinh\{(\alpha^2 + (n\pi/b)^2)^{1/2}(a - x)\}, \tag{16}$$

$$u_3(x, y) = \sum_{n=1}^{\infty} \frac{2}{\sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2} b\}} \frac{1}{a} \int_0^a f_3(x') \sin \frac{n\pi x'}{a} dx' \times \sin(n\pi x/a) \sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2} y\}, \tag{17}$$

$$u_4(x, y) = \sum_{n=1}^{\infty} \frac{2}{\sinh\{(\alpha^2 + (n\pi/b)^2)^{1/2} a\}} \frac{1}{b} \int_0^b f_4(y') \sin \frac{n\pi y'}{b} dy' \times \sin(n\pi y/b) \sinh\{(\alpha^2 + (n\pi/b)^2)^{1/2} x\}. \tag{18}$$

Thus, we need to estimate

$$\begin{aligned} c_{n1} &= \frac{1}{a} \int_0^a f_1(x) \sin \frac{n\pi x}{a} dx, \qquad c_{n2} = \frac{1}{b} \int_0^b f_2(y) \sin \frac{n\pi y}{b} dy \\ c_{n3} &= \frac{1}{a} \int_0^a f_3(x) \sin \frac{n\pi x}{a} dx, \qquad c_{n4} = \frac{1}{b} \int_0^b f_4(y) \sin \frac{n\pi y}{b} dy. \end{aligned} \tag{19}$$

These are easily estimated in the following manner:

$$\hat{c}_{n1} = \frac{1}{M_1} \sum_{m=1}^{M_1} f_1(x_m) \sin \frac{n\pi x_m}{a}, \qquad x_m \text{ uniform on } (0, a). \tag{20}$$

Again, we do not know $f_1(x_m)$, so we use the single point theory to get a one particle estimate and we write

$$\hat{\hat{c}}_{n1} = \frac{1}{M_1} \sum_{m=1}^{M_1} \hat{f}_1(x_m) \sin \frac{n\pi x_m}{a}. \tag{21}$$

For convenience let $\hat{d}_{n1}$ be the entire expansion coefficient, that is

$$\hat{d}_{n1} = \hat{\hat{c}}_{n1}(2/\sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2}\, b\}). \tag{22}$$

As with the circular method (Eq. (10)), if we go outside the rectangle, the higher order terms have factors like

$$R_n = \sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2}(b-y)\}/\sinh\{(\alpha^2 + (n\pi/a)^2)^{1/2}\, b\} \tag{23}$$

that tend to infinity with n.

Convergence of the Estimates for the c_{ni}

The convergence properties for the c_{ni} estimates are essentially the same as for the a_n and b_n estimates. For example, with a change of variables ($\theta_0 = (2\pi/a)\, x$),

$$\frac{1}{a}\int_0^a f_1(x) \sin \frac{n\pi x}{a}\, dx = \frac{1}{2\pi}\int_0^{2\pi} h_1(\theta_0) \sin \frac{n\theta_0}{2}\, d\theta_0, \qquad h_1(\theta_0) = f_1(x). \tag{24}$$

To prove that the estimate for c_{n1} converges (for α real), one need only replace u of [1, Eq. (24)] with $h_1 \sin(n\theta_0/2)$.

Comments

As mentioned earlier, the technique may be applied in any separable coordinate system. Thus, the technique can easily be generalized to N dimensions; in general, Monte Carlo methods become more competitive with deterministic methods as the dimension and complexity increase. Although this technique is undoubtedly currently *much* slower than standard deterministic techniques, it should be remembered that special sampling techniques can theoretically produce zero-variance solutions. In Monte Carlo particle transport problems, for example, it is not uncommon to see factors of 10^6 to 10^8 improvement over an analog Monte Carlo sampling. Furthermore, automatic learning procedures have been developed [6] to *automatically* produce low–variance samplings for the particle transport field.

APPENDIX: Separation of Variables Solution in Cartesian Coordinates

Consider the equation

$$u_{xx} + u_{yy} - \alpha^2 u = 0. \tag{25}$$

Now separate variables

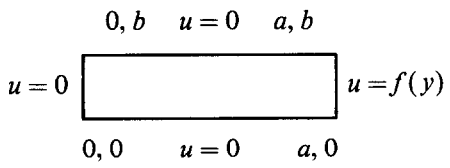
$$u(x, y) = \chi(x)\, Y(y) \tag{26}$$

and substitute into

$$\chi'' Y + \chi Y'' - \alpha^2 \chi Y = 0 \qquad \text{or} \qquad (-\chi''/\chi) + \alpha^2 = (Y''/Y) = -\beta^2, \tag{27}$$

with separation constant β^2.

Suppose we wish to solve the problem



The solution to the Y equation is

$$Y = c \cos \beta y + d \sin \beta y. \tag{28}$$

Imposing the boundary conditions $Y(0) = Y(b) = 0$ results in the set of solutions (with $\beta_n = n\pi/b$)

$$Y_n = d_n \sin \beta_n y. \tag{29}$$

The solution to the χ equation is (with $\gamma_n^2 = \alpha^2 + \beta_n^2$)

$$\chi = e_n \cosh \gamma_n x + f_n \sinh \gamma_n x. \tag{30}$$

Imposing the boundary condition $\chi(0) = 0$ implies $e_n = 0$. We thus have

$$u(x, y) = \sum_{n=1}^{\infty} g_n \sin(\beta_n y) \sin h(\gamma_n x). \tag{31}$$

Now we may determine the g_n by applying $u(a, y) = f(y)$ in Eq. (31), multiplying by $\sin \beta_m y$, and integrating over $0 \leqslant y \leqslant b$ to obtain

$$g_n = \frac{2}{\sinh \gamma_n a} \frac{1}{b} \int_0^b f(y) \sin \beta_n y \, dy. \tag{32}$$

Thus

$$u(x,y) = \sum_{n=1}^{\infty} \frac{2}{\sinh\{(\alpha^2 + (n\pi/b)^2)^{1/2}\, a\}} \frac{1}{b} \int_0^b f(y') \sin\frac{n\pi y'}{b}\, dy'$$

$$\times \sin(n\pi y/b) \sinh\{(\alpha^2 + (n\pi/b)^2)^{1/2}\, x\}.$$

This is essentially $u_4(x,y)$ of Eq. (18). The other $u_i(x,y)$ may be obtained by inspection.

REFERENCES

1. T. E. BOOTH, *J. Comput. Phys.* **39** (1981), 396.
2. A. HAJI-SHEIKH, "Application of Monte Carlo Methods to Thermal Conduction Problems," Ph.D. thesis, University Microfilms, Inc., University of Michigan, Ann Arbor, 1965.
3. P. R. GARABEDIAN, "Partial Differential Equations," Wiley, New York, 1964.
4. S. SELBY, Ed., "CRC Standard Mathematical Tables," 22nd ed., CRC Press, Cleveland, 1975.
5. G. N. WATSON, "A Treatise of Bessel Functions," 2nd ed., p. 20–21.
6. T. E. BOOTH, *Trans. Amer. Nucl. Soc.* **41** (1982), 308.