The solution by fast Fourier transforms of Laplace's equation in a toroidal region with a rectangular cross-section

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ABSTRACT

The fast Fourier transform method is described for Laplace's equation in a toroidal region using the 9-point difference approximation to the Laplacian operator. Numerical results are given which indicate the efficiency and accuracy of the method. Accurate difference approximations are also derived for the determination of the electrostatic field in a toroidal region.

1. INTRODUCTION

The use of fast Fourier transforms for the numerical solution of Poisson's equation in a rectangular region was described by Hockney [1, 2] and Christiansen and Hockney [3] for the 5-point difference approximation, and by Pickering [4] for the 9-point approximation. Hughes [5] used the 5-point difference approximation and fast Fourier transforms for the solution of Poisson's equation in cylindrical coordinates. A 9-point difference approximation to Laplace's equation in cylindrical coordinates with rotational symmetry was used by the author for the determination of capacitance of a ring capacitor [6, 7, 8]. SOR iteration was used to solve the difference equations. In this paper, we describe the solution of these difference equations by fast Fourier transforms and compare the computer run-time to that of the SOR method. Difference approximations are derived for the determination of capacitance.

2. SOLUTION OF THE DIFFERENCE EQUATIONS USING SINE TRANSFORMS

Let

$$r = r_0 + ih,$$
 $i = 0, 1, ..., M$
 $z = jk,$ $j = 0, 1, ..., N$

with $N = 2^{IQ}$, and let $u(r_0 + ih, jk)$ be denoted by u (i, j). Assume that we have Dirichlet boundary conditions, i.e. u(i, 0), u(i, N), u(0, j) and u(M, j) are given for 0 < i < M, 0 < j < N. The 9-point difference approximation to $\Delta u = 0$ is [7] $a_1 u(i+1,j) + a_2 [u(i+1,j+1) + u(i+1,j-1)]$ $+ a_{3}[u(i, j+1) + u(i, j-1)] + a_{4}[u(i-1, j+1) + u(i-1, j-1)]$ and $t_{i} = -a_{2}u(i+1, N) - a_{3}u(i, N) - a_{4}u(i-1, N).$ + $a_5 u (i-1,j) - a_0 u (i,j) = 0$,

$$\label{eq:second} \begin{array}{l} 0 < i < M, \ 0 < j < N, \\ \mbox{with} \\ a_1 = (r+h/2)[(5k^2-h^2)/(6h^2k^2)] - 1/[12\,(r+h/2)], \\ a_2 = (r+h/2)[(h^2+k^2)/(12h^2k^2)], \\ a_3 = r\,[(5h^2-k^2)/(6h^2k^2)], \\ a_4 = (r-h/2)[(h^2+k^2)/(12h^2k^2)], \\ a_5 = (r-h/2)[(5k^2-h^2)/(6h^2k^2)] - 1/[12\,(r-h/2)] \\ and \\ a_0 = r[5(h^2+k^2)/(3h^2k^2)] - r/[6\,(r+h/2)(r-h/2)]. \\ \mbox{Let} \end{array}$$

$$u(i,j) = \sum_{k=1}^{N-1} \overline{u}(i,k) \sin(\pi k j/N)$$
 (2)

with

$$\overline{u}(i,k) = (2/N) \sum_{j=1}^{N-1} u(i,j) \sin (\pi k j/N)$$

Substituting (2) in (1) and using the orthogonality relations for the sine functions, we get

$$\begin{split} & [a_{1} + 2a_{2}\cos(\pi k/N)]\overline{u}(i+1,k) + [-a_{0} + 2a_{3}\cos(\pi k/N)]\overline{u}(i,k) \\ & + [a_{5} + 2a_{4}\cos(\pi k/N)]\overline{u}(i-1,k) \\ & = (2/N)\sin(\pi k/N)[s_{i} + (-1)^{k+1}t_{i}] \\ & \text{or} \\ & \beta_{i}\overline{u}(i+1,k) + \lambda_{i}\overline{u}(i,k) + \gamma_{i}\overline{u}(i-1,k) = \overline{q}(i,k) \\ & \text{where} \\ & s_{i} = -a_{2}u(i+1,0) - a_{3}u(i,0) - a_{4}u(i-1,0) \\ & \text{and} \end{split}$$

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(1)

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The system of equations (4) is solved by an adaption of Gauss elimination described by Richtmeyer and Morton [9].

The procedure is repeated for each harmonic and, finally u(i, j) is obtained by the inverse sine transform (2).

3. CAPACITANCE DETERMINATION

Nine-point approximations to u_r and u_z were derived in [7] and are given by :

$$\begin{split} \mathbf{u}_{r} &= \left[h/(12k^{2}) \right] \left[u(r+h,z+k) + u(r+h,z-k) \right. \\ &- u(r-h,z+k) - u(r-h,z-k) \right] \\ &+ \left\{ \left[1/(2h) \right] - \left[h/(6k^{2}) \right] \right\} \left[u(r+h,z) - u(r-h,z) \right] \\ &+ \left[(r+h/2)^{-1} u(r+h,z) + (r-h/2)^{-1} u(r-h,z) \right. \\ &- 2r(r+h/2)^{-1} (r-h/2)^{-1} u(r,z) \right] / 6 - (h^{2}/6) (\Delta u)_{r} \\ &+ 0 (h^{4}), \end{split}$$

and

$$\begin{split} \mathbf{u_{z}} &= (\mathbf{r} + \mathbf{h}/2)[\mathbf{k}/(12\,\mathbf{rh}^{2})][\mathbf{u}\,(\mathbf{r} + \mathbf{h}, \mathbf{z} + \mathbf{k}) - \mathbf{u}\,(\mathbf{r} + \mathbf{h}, \mathbf{z} - \mathbf{k})] \\ & \left\{ [1/(2k)] - [\mathbf{k}/(6h^{2})] \right\} [\mathbf{u}\,(\mathbf{r}, \mathbf{z} + \mathbf{k}) - \mathbf{u}\,(\mathbf{r}, \mathbf{z} - \mathbf{k})] \\ & + (\mathbf{r} - \mathbf{h}/2)[\mathbf{k}/(12\mathbf{rh}^{2})][\mathbf{u}\,(\mathbf{r} - \mathbf{h}, \mathbf{z} + \mathbf{k}) - \mathbf{u}\,(\mathbf{r} - \mathbf{h}, \mathbf{z} - \mathbf{k})] \\ & - (\mathbf{k}^{2}/6)\,(\Delta \mathbf{u})_{\mathbf{z}} + 0\,(\mathbf{h}^{4}). \end{split}$$

The capacitance determinations require the integration of the normal derivative of u(r, z) along a wall where u(r, z) = 0. The Laplacian of u(r, z) is given by

$$\Delta u = u_{rr} + (1/r) u_r + u_{zz} .$$
 (7)

Differentiation of the Laplacian gives

$$(\Delta u)_{rr} + (1/r) (\Delta u)_{r} - (\Delta u)_{zz}$$

= $u_{r}4 + (2/r)u_{r}3 - (1/r^{2})u_{r}2 + (1/r^{3})u_{r} - u_{z}4$.
(8)

Along the line $r = r_0$ with $u(r_0, z) = constant$, it follows from (7) and (8) that

$$u_{rr} = -(1/r)u_{r}$$

$$u_{r}^{4} = -(2/r)u_{r}^{3} - (2/r^{3})u_{r}$$
and
$$au(r, z) + bu(r + h, z) + cu(r + 2h, z)$$

$$= (a + b + c)u + \left[(b + 2c)h - (b + 4c)\frac{h^{2}}{2r} - (b + 16c)\frac{h^{4}}{12r^{3}} \right]$$

$$+ \left[(b + 8c)\frac{h^{3}}{6} - (b + 16c)\frac{h^{4}}{12r} \right] u_{r}^{3} + \dots$$

$$= u_{r} + 0(h^{4}) \qquad (9)$$

when $u \in C^6$,

$$b = 8 \left[1 - \frac{h}{r} \right] / D,$$

$$c = - \left[1 - \frac{h}{2r} \right] / D,$$

$$D = h \left[18 - 27(h/r) + 9(h + and + a - (b + c)) \right].$$

Along the line $z = z_0$ with

Along the line $z = z_0$ with $u(r, z_0) = \text{constant}$, it follows from (7) and (8) that if $u \in C^6$, $u_{zz} = u_z 4 = 0$ and

 $(r)^{2} + 2(h/r)^{3}]/3$

$$du(r,z) + eu(r,z+k) + fu(r,z+2k)$$

$$= (d + e + f)u + (e + 2f)ku_{z} + (e + 8f)(k^{3}/6)u_{z^{3}} + \dots$$

= $u_{z} + 0(k^{4})$ (10)

when
$$d = -7/(6k)$$
, $e = 4/(3k)$ and $f = -1/(6k)$.

The capacitance determination is similar to that described in [6, 7, 8] and is determined from the integral

$$C = -(4\pi)^{-1} \int_{\Gamma} (\partial u / \partial n) dS$$

where the contour of integration is either a section of the boundary of the region or a contour enclosing a section of the boundary. The normal derivative on the boundary of the region is determined from (9) or (10). Equation (5) or (6) is used to determine the normal derivative in the interior of the region. The integral is approximated by Simpson's quadrature rule.

4. NUMERICAL RESULTS

Fortran IV programs using the above numerical methods were compiled and run on an IBM model 3032. These programs are given in [10]. An abridged version of FOUR 67 [11] was used for the sine transforms.

Example 1

A boundary value problem was solved in the region $\{(r, z) | r_0 < r < r_0 + 1, 0 < z < 1\}$ with boundary values

u = 0 for $r = r_0$, z = 0 and z = 1

$$u = \sin(\pi z)$$
 for $r = r_1 = r_0 + 1$

The exact solution to this problem is

$$u_{r}^{(r, z)} = \frac{K_{0}(\pi r_{0})I_{0}(\pi r) - I_{0}(\pi r_{0})K_{0}(\pi r)}{K_{0}(\pi r_{0})I_{0}(\pi r_{1}) - I_{0}(\pi r_{0})K_{0}(\pi r_{1})} \sin(\pi z)$$

For $r_0 = 1/2$, table 1 gives numerical results obtained. A square mesh was used. Two capacitance determinations were made. The normal derivative is integrated over each of the sides $r = r_0$ and z = 0. The exact value of capacitance divided by the average circumference

TABLE 1.

Maximum error in finite difference determination of u(r, z), relative error in computed values of capacitance and CPU times for each determination for $r_0 = 1/2$.

	Maximum	Relative error		CPU times (secs.)	
h	error in $u(r, z)$	c ₁	c ₂	FFT	SOR
1/8	1.9 × 10 ⁻⁶	5.9×10^{-3}	5.9 × 10 ⁻⁴	0.007	0.046
1/16	1.3×10^{-7}	3.6×10^{-4}	3.7×10^{-5}	0.018	0.163
1/32	8.4×10^{-9}	2.3×10^{-5}	2.3 × 10 ⁻⁶	0.071	1.038
1/64	5.3×10^{-10}	1.4 × 10 ⁻⁶	1.5×10^{-7}	0.286	6.929
1/128	3.3×10^{-11}	9.1 × 10 ⁻⁸	9.2 × 10 ⁻⁹	1.220	
1/256	2.3×10^{-12}	5.7×10^{-9}	5.7×10^{-10}	5.254	



Fig. 1. Toroidal H-shaped region.

of the region is 0.012337 and 0.100123 in each of these two cases, respectively. The values C_1 and C_2 were obtained by approximating the derivatives by equations (9) and (10), respectively.

The CPU time includes only the time required for solution of the difference equations. The CPU time for solution by SOR includes input of the solution obtained with twice the current mesh size, interpolation, SOR iteration and output of the new solution. The optimum SOR relaxation factor was used and iteration was performed until the initial residue was reduced by 10^{-3} . Interpolation at a new point was performed by first taking the average of the four nearest points and, then, iterating over all new points using ten SOR iterations with a relaxation factor of 1.2.

Example 2

A boundary value problem was solved in the H-shaped region R, illustrated in figure 1, using a square mesh. The capacitance between the inner and outer walls of the region was approximated by integration of the charge distribution along the path which is at a distance h from the wall $r_0 + b$. This configuration represents a four-electrode capacitor and was studied by Makow and Campbell [6] and by Shields [12]. The boundary conditions are :

$$u(r, z) = 1 \text{ for } r = r_0$$

$$u(r, z) = 0$$
 elsewhere.

The procedure used to solve the problem is as follows :

Step 1

Approximate the solution in the gaps at z = 0 and z = c either by an analytic expression or by linear interpolation of a solution with twice the current mesh size. When an analytic approximation is used, u(r, z) is approximated by a logarithmic function in the gaps near the inner wall and by zero in the gaps near the outer wall.

Step 2

Solve the boundary value problem in the rectangular region $\{(r, z) | r_0 < r < r_0 + b, 0 < z < c\}$ by the fast Fourier transform method.

Step 3

Iterate the solution over mesh points contained in the regions

$$R_1 = R \cap \{ (r, z) \mid r_0 < r < r_0 + b, \ c - s < z < c + 4s \}$$

and

$$R_2 = R \cap \{(r, z) | r_0 < r < r_0 + b, -4s < z < s\}$$

using SOR iteration until the residual is sufficiently small. Since the region R and the boundary conditions are symmetric about the line z = c/2, it is sufficient to iterate in the region R_1 .

Step 4

Integrate the charge distribution over the contour Γ to obtain an estimate of capacitance. Equation (5) can be used to determine the normal derivative in this case. If this is the first time step 4 has been performed or if the present value of capacitance does not agree with the one calculated during the previous execution of step 4, repeat steps 2, 3 and 4.

Table 2 gives values of capacitance, C, calculated for $r_0 = 0.5$, b = 1, c = 1, s = 1/8 and s = 1/16. Four or

five repetitions of steps 2, 3, and 4 were required to obtain agreement to 8 digits of the computed values of capacitance.

TABLE 2

Values of $C/(\pi D)$ for $r_0 = 1/2$, b = c = 1.

D	is	the	average	diameter	of	the	region.
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h	s = 1/8	s = 1/16
1/16	0.0165257	
1/32	0.0166435	0.0159172
1/64	0.0166950	0.0159457
1/128	0.0167150	0.0159581

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