Finite difference techniques for ring capacitors

J. B. CAMPBELL

Computation Centre, National Research Council, Ottawa, Canada

SUMMARY

This paper describes finite difference techniques used to calculate the capacitance of a ring capacitor. The determination of capacitance involves the solution of a Dirichlet boundary value problem and the calculation of the gradient of the solution obtained. Circular cylindrical coordinates are used. Nine point difference approximations are used for the Laplacian and the first derivatives of a function. If this function satisfies Laplace's equation and is sufficiently differentiable, the discretization error of each approximation is $O(h^4)$ where h is the maximum mesh size.

1. Introduction

A nine point finite difference approximation to the Laplacian in rectangular coordinates in 2 dimensions is given by [1]

$$L_h u = a[u(x+h, y+k) + u(x+h, y-k) + u(x-h, y+k) + u(x-h, y-k)]$$
$$+ b[u(x+h, y) + u(x-h, y)] + c[u(x, y+k) + u(x, y-k)] - du(x, y) \qquad (1)$$

with

$$a = (h^2 + k^2)/(12h^2 k^2),$$
$$b = (5k^2 - h^2)/(6h^2 k^2),$$
$$c = (5h^2 - k^2)/(6h^2 k^2),$$

and

$$d = 5(h^2 + k^2)/(3h^2 k^2).$$

If $u(x, y)$ satisfies Laplace's equation and $u(x, y) \in C^6$ in a neighborhood of the point (x, y), then

$$L_h u = \Delta u + O[\max(h^4, k^4)]. \qquad (2)$$

If $h = k$ and if $u(x, y) \in C^8$ in a neighborhood of the point (x, y), we have $L_h u = \Delta u + O(h^6)$.

In this paper, I give a nine point difference approximation to the Laplacian in cylindrical coordinates valid for axially symmetric functions and apply it to the calculation of the capacitance of ring capacitors described in [2]. The derivatives of the potential function are used to calculate the capacitance and are also approximated by nine point differences.

2. Difference approximations for regular points

In circular cylindrical coordinates (r, ϕ, z), the Laplacian of an axially symmetric function $u(r, z)$ is given by

$$\Delta u = \partial^2 u/(\partial r)^2 + \partial^2 u/(\partial z)^2 + (1/r)\partial u/\partial r. \qquad (3)$$

The derivation of difference approximations is similar to that given in [3, p. 337]. It is given in detail in [8]. A rectangular mesh is used with mesh lengths h and k in the r and z directions, respectively. A condition which is usually imposed on a difference equation such as eqn. (1) is that the coefficients a, b and c be positive, i.e., the matrix is of "positive type". This restricts

the values h and k. In the remainder of this paper I will assume that $k = O(h)$ and hence $O[\max(h^4, k^4)] = O(h^4)$.

The operators Δ_r and Δ_z are defined as

$$\Delta_r u = h^{-2}[(r+h/2)u(r+h, z)+(r-h/2)u(r-h, z)-2ru(r, z)],$$

and

$$\Delta_z u = k^{-2}[u(r, z+k)+u(r, z-k)-2u(r, z)].$$

If $u(r, z) \in C^6$ then, by Taylor series expansion in powers of h and k, it follows that

$$\Delta_r u + r\Delta_z u + [(h^2+k^2)/12]\Delta_r\Delta_z u = r\Delta u + (h^2/12)[r(\Delta u)_r]_r$$
$$+ (k^2/12)r(\Delta u)_{zz} + (h^2/12)(u_r/r)_r + O(h^4). \quad (4)$$

Substitution in (4) of the difference approximation

$$(u_r/r)_r = h^{-2}[(r+h/2)^{-1}u(r+h, z)+(r-h/2)^{-1}u(r-h, z)$$
$$-2r(r+h/2)^{-1}(r-h/2)^{-1}u(r, z)]+O(h^2),$$

gives an approximation L_h to the operator $r\Delta u$ which is defined by the following equation:

$$L_h u = -a_0 u(r, z)+a_1 u(r+h, z)+a_2[u(r+h, z+k)+u(r+h, z-k)]$$
$$+ a_3[u(r, z+k)+u(r, z-k)]+a_4[u(r-h, z+k)+u(r-h, z-k)]$$
$$+ a_5 u(r-h, z) \quad (5)$$

with

$$a_1 = (r+h/2)[(5k^2-h^2)/(6h^2 k^2)]-1/[12(r+h/2)],$$
$$a_2 = (r+h/2)[(h^2+k^2)/(12h^2 k^2)],$$
$$a_3 = r[(5h^2-k^2)/(6h^2 k^2)], \quad (6)$$
$$a_4 = (r-h/2)[(h^2+k^2)/(12h^2 k^2)],$$
$$a_5 = (r-h/2)[(5k^2-h^2)/(6h^2 k^2)]-1/[12(r-h/2)],$$

and

$$a_0 = r[5(h^2+k^2)/(3h^2 k^2)]-r/[6(r+h/2)(r-h/2)].$$

If $u(r, z) \in C^6$ in a neighborhood of the point (r, z), then

$$L_h u = r\Delta u + (h^2/12)[r(\Delta u)_r]_r + (k^2/12)r(\Delta u)_{zz} + O(h^4).$$

In a similar manner, the following approximations for u_r and u_z are obtained:

$$u_r = [h/(12k^2)][u(r+h, z+k)+u(r+h, z-k)-u(r-h, z+k)-u(r-h, z-k)]$$
$$+ \{[1/(2h)]-[h/(6k^2)]\}[u(r+h, z)-u(r-h, z)]$$
$$+ [(r+h/2)^{-1}u(r+h, z)+(r-h/2)^{-1}u(r-h, z)$$
$$-2r(r+h/2)^{-1}(r-h/2)^{-1}u(r, z)]/6-(h^2/6)(\Delta u)_r+O(h^4), \quad (7)$$

and

$$u_z = (r+h/2)[k/(12rh^2)][u(r+h, z+k)-u(r+h, z-k)]$$
$$+ \{[1/(2k)]-[k/(6h^2)]\}[u(r, z+k)-u(r, z-k)]$$
$$+ (r-h/2)[k/(12rh^2)][u(r-h, z+k)-u(r-h, z-k)]$$
$$- (k^2/6)(\Delta u)_z+O(h^4). \quad (8)$$

3. Difference approximations for irregular points

For points close to the boundary of the bounded region R where we are attempting to solve the differential equation, it may not be possible to use an approximation of the form (5).

Following [3, p. 338], each derivative of the differential equation can be approximated by a four point unbalanced difference, i.e., for $0 < \lambda \leq 1$, $0 < \mu \leq 1$ and $u \in C^4$,

$$u_{rr} = h^{-2} \left[\frac{\lambda-1}{\lambda+2} u(r+2h, z) + \frac{2(2-\lambda)}{\lambda+1} u(r+h, z) \right.$$

$$\left. + \frac{6}{\lambda(\lambda+1)(\lambda+2)} u(r-\lambda h, z) - \frac{3-\lambda}{\lambda} u(r, z) \right] + O(h^2),$$

$$u_{zz} = k^{-2} \left[\frac{\mu-1}{\mu+2} u(r, z+2k) + \frac{2(2-\mu)}{\mu+1} u(r, z+k) \right.$$

$$\left. + \frac{6}{\mu(\mu+1)(\mu+2)} u(r, z-\mu k) - \frac{3-\mu}{\mu} u(r, z) \right] + O(k^2),$$

$$u_r = h^{-1} \left[\frac{\lambda}{\lambda+1} u(r+h, z) - \frac{1}{\lambda(\lambda+1)} u(r-\lambda h, z) - \frac{\lambda-1}{\lambda} u(r, z) \right] + O(h^2). \tag{9}$$

A more accurate approximation can sometimes be obtained in the form:

$$\begin{aligned}
L_h u &\equiv -a_0 u(r, z) + a_1 u(r+d_1 h, z) + a_2 u(r+d_2 h, z+d_2 k) + a_3 u(r, z+d_3 k) \\
&\quad + a_4 u(r-d_4 h, z+d_4 k) + a_5 u(r-d_5 h, z) + a_6 u(r-d_6 h, z-d_6 k) \\
&\quad + a_7 u(r, z-d_7 k) + a_8 u(r+d_8 h, z-d_8 k) \\
&= \Delta u + c_1 (\Delta u)_r + c_2 (\Delta u)_z + c_3 (\Delta u)_{rr} + c_4 (\Delta u)_{rz} + c_5 (\Delta u)_{zz} + O(h^3),
\end{aligned}$$
$$0 < d_i \leqq 1, \quad i = 1, 2, \ldots, 8. \tag{10}$$

In order that the discretization error in the solution of the difference equation be $O(h^4)$ when the difference approximation (5) is used at interior points of R, it is sufficient [3] that $u(r, z) \in C^6$ in D, the coefficients a_i of (6) are positive and the approximation L_h used at points close to the boundary has strict diagonal dominance and satisfies

$$L_h u/a_0 = \Delta u/a_0 + O(h^4).$$

Let C^* denote the set of mesh points on the boundary of R and let P_i denote the mesh point corresponding to a_i in (10). The requirement of strict diagonal dominance is equivalent to the existence of a positive number $\delta < 1$, independent of h and k, such that

$$\sum_{\substack{i=1 \\ P_i \notin C^*}}^{8} |a_i| < \delta |a_0|. \tag{11}$$

Equating coefficients of derivatives of u of orders up to and including order 4 in (10), we get a system of 15 equations in 14 unknowns $a_0, a_1, \ldots, a_8, c_1, c_2 \ldots, c_5$ which is overdetermined. For $h=k$ the coefficients of $u_{r^3 z}$ and u_{rz^3} are the same. If $u \in C^5$ and u satisfies (3) and if a_i, $i=0, 1, \ldots, 8$, c_i, $i=1, 2, \ldots, 5$ is a solution of (10) except for the coefficients of u_{rz^3} and with $a_i/a_0 \geqq 0$ for all i, then

$$L_h u/a_0 = hk(k^2-h^2)(d_2^4 a_2 - d_4^4 a_4 + d_6^4 a_6 - d_8^4 a_8)u_{rz^3}/(6a_0) + O(h^5)$$
and
$$|L_h u/a_0| \leqq hk|k^2-h^2| \, |u_{rz^3}|/6 + O(h^5) = O(h^4).$$

If $h=k$, then $L_h u/a_0 = O(h^5)$.

If we equate coefficients of derivatives of u of orders up to and including order 3 in (10), we get a system of 10 equations in 14 unknowns. If we solve the system for $a_0, a_1, \ldots, a_8, c_1$ and c_2 with $a_i = 0$ for some i and $c_3 = c_4 = c_5 = 0$, and if $a_i/a_0 \geqq 0$ for all i, then $L_h u/a_0 = O(h^4)$.

The method being used to derive a difference equation for irregular points is:

(i) Determine values of $a_0, a_1, \ldots, a_8, c_1, c_2, \ldots, c_5$ such that coefficients of derivatives of u of orders up to and including order 4 in (10) are equal except for the coefficients of u_{rz^3}. If $a_i/a_0 \geqq 0$ for all i and Eq. (11) is satisfied with $\delta = 24/25$, then these values define a difference equation. If $a_i/a_0 < 0$ for some i or Eq. (11) is not satisfied, then:

(ii) Determine values of $a_0, a_1, \ldots, a_8, c_1, c_2, \ldots, c_5$ such that coefficients of derivatives of u of orders up to and including order 3 in (10) are equal, $a_i = 0$ for some $i = i_0$ and $c_3 = c_4 = c_5 = 0$. The index i_0 is chosen by checking the signs of the values a_i/a_0 of the solution obtained in (i). If j is the first index for which $a_i/a_0 < 0$, then set $i_0 = j+1$ if $a_{j+2}/a_0 < 0$ and set $i_0 = j$ if $a_{j+2}/a_0 \geqq 0$. If $a_i/a_0 \geqq 0$ for all i and Eq. (11) is satisfied with $\delta = 24/25$, then these values define a difference equation. If $a_i/a_0 < 0$ for some i or Eq. (11) is not satisfied, then:

(iii) Use (9) to derive a difference equation.

4. Solution of the difference equations

Iterative methods used to solve the difference equations are discussed in [1] and [5]. When reducing the equation $L_h u = 0$ to matrix form it is assumed that the natural ordering of the mesh points is used. In matrix form the difference equation $L_h u = 0$ reduces to

$$Au = b$$

where A is a square non-singular matrix. In a rectangular region with no irregular points the equation $L_h u = 0$ produces a symmetric matrix A.
Let

$$A = B + D,$$
$$B = L + U,$$

where

$$l_{ij} = 0 \quad \text{for} \quad j \geqq i,$$
$$u_{ij} = 0 \quad \text{for} \quad j \leqq i,$$

and

$$d_{ii} \neq 0, \quad d_{ij} = 0 \quad \text{for} \quad i \neq j.$$

The successive iterates $u^{(n)}$ of the successive overrelaxation method (SOR) are defined as

$$u^{(n+1)} = \mathscr{L}_\omega u^{(n)} + (I - \omega L)^{-1} \omega c$$

with

$$\mathscr{L}_\omega = (I - \omega L)^{-1} [\omega U + (1 - \omega) I]$$

and

$$c = D^{-1} b.$$

The successive iterates $u^{(n)}$ of symmetric successive overrelaxation (SSOR) are given by

$$u^{(n+1)} = \mathscr{T}_\omega u^{(n)} + \omega(2 - \omega)(I - \omega U)^{-1}(I - \omega L)^{-1} c$$

with

$$\mathscr{T}_\omega = \mathscr{U}_\omega \mathscr{L}_\omega$$

where

$$\mathscr{U}_\omega = (I - \omega U)^{-1} [\omega L + (1 - \omega) I].$$

If A is symmetric with positive diagonal elements and ω is real, the eigenvalues of $\mathscr{T}_\omega$ are real and non-negative. The successive iterates $v^{(n)}$ for the SSOR method with semi-iteration (SSOR-SI) are given by [5, p. 471]

$$v^{(n+1)} = \rho_{n+1}(1 - \bar\lambda/2)^{-1}[(\mathscr{T}_\omega - \bar\lambda I/2)v^{(n)} + k] + (1 - \rho_{n+1})v^{(n-1)},$$

where

$$\rho_1 = 1, \quad \rho_2 = 2z^2/(2z^2 - 1),$$
$$\rho_{n+1} = [1 - \rho_n/(4z^2)]^{-1}, \quad n = 2, 3, \ldots,$$
$$z = (2/\bar\lambda) - 1,$$

the eigenvalues λ of $\mathscr{T}_\omega$ are contained in the interval

$$0 \leqq \lambda \leqq \bar\lambda = S(\mathscr{T}_\omega)$$

and
$$k = \omega(2-\omega)(I-\omega U)^{-1}(I-\omega L)^{-1}c .$$

If A is a positive definite matrix and if $\mu = S(D^{-1}B)$ then, according to [5, p. 464], if

$$\omega_1 = 2/\{1+[2(1-\mu)]^{\frac{1}{2}}\} \tag{12}$$

then
$$\bar{\lambda}_1 = S(\mathcal{T}_{\omega_1}) \leqq \{1-[(1-\mu)/2]^{\frac{1}{2}}\}/\{1+[(1-\mu)/2]^{\frac{1}{2}}\} . \tag{13}$$

As the radial coordinate becomes infinite, the difference approximation (5) approaches the difference approximation (1). It has been found that the optimum iteration parameters for each of the methods SOR and SSOR do not significantly depend on the radius but only on the boundary of the region, *e.g.*, in Figure 1 the optimum iteration parameters are, for practical purposes, independent of a. For a square region $0 < x < 1, 0 < y < 1$, with a square mesh the optimal relaxation factor for SOR for the difference equation (1) is given by [1]

$$\omega = 2 - 2.116(\pi h) + 2.24(\pi h)^2 + O(h^3) , \tag{14}$$

and for this relaxation factor, the spectral radius of the matrix $\mathcal{L}_\omega$ is given by
$$S(\mathcal{L}_\omega) = 1 - 1.791(\pi h) + 1.60(\pi h)^2 + O(h^3) . \tag{15}$$

The spectral radius μ of the Jacobi matrix $D^{-1}B$ for the same region is given by [1]

$$\mu = 0.2[\cos^2(\pi h) + 4\cos(\pi h)] . \tag{16}$$

This can be used with (12) and (13) to obtain a reasonably efficient estimate for the parameters needed for the SSOR-SI method.

TABLE 1

Solution of the difference equations in a square region. The number of iterations given is for $a \to \infty$.

h	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$
No. of SOR iterations	54	92	183
No. of SSOR-SI iterations with $\omega_0, \bar{\lambda}_0$	21	30	43
No. of SSOR-SI iterations with $\omega_1, \bar{\lambda}_1$	26	37	52
Error in test problem. $a = 10^{16}$	2.07×10^{-7}	3.28×10^{-9}	5.13×10^{-11}
Error in test problem. $a = \frac{1}{2}$	1.93×10^{-6}	1.31×10^{-7}	8.39×10^{-9}

Table 1 gives a comparison of SOR and SSOR-SI for the solution of the Dirichlet problem on the unit square with a square mesh $(h = k)$. The optimum relaxation factor ω for SOR was obtained from (14). The optimum SSOR-SI parameters, ω_0 and $\bar{\lambda}_0$, were obtained by numerical experiments. ω_0 minimizes $S(\mathcal{T}_\omega)$ for the difference equation (1) and $\bar{\lambda}_0 = S(\mathcal{T}_{\omega_0})$. The SSOR-SI parameters, ω_1 and $\bar{\lambda}_1$, were obtained from (12), (13) and (16). The table gives the number of iterations required to reduce the maximum residual of the difference equation to 10^{-14} when the value of the solution on the boundary of the unit square is zero and the initial approximation at each mesh point in the interior of the unit square is unity. Each SSOR-SI iteration requires approximately three times as many arithmetic operations as does an SOR iteration. A test boundary value problem was solved and the maximum discretization error was computed. The test problem was solved in the region $a < r < a+1, 0 < z < 1$ with boundary values $u = 0$ for $r = a, z = 0$ and $z = 1$ and $u = \sin(\pi z)$ for $r = a+1$. For $a = \frac{1}{2}$ the discretization error should be proportional to h^4 and for $a - > \infty$, the discretization error should be proportional to h^6.
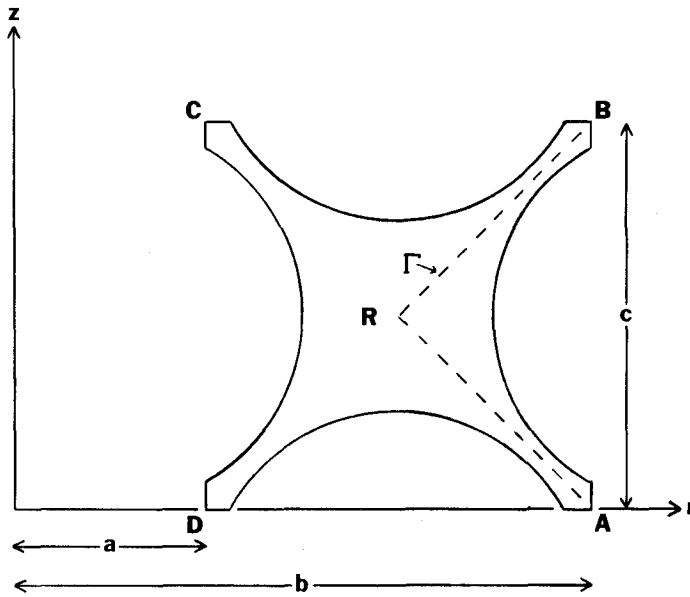
Figure 1. Axisymmetric region R bounded by four axisymmetric shells AB, BC, CD, and DA.

For an irregular region, the main difficulty in applying SOR or SSOR-SI is the determination of the optimum iteration parameters. The matrix obtained from the difference equations for an irregular region is not symmetric. The techniques used to determine the optimum parameters for SOR and SSOR-SI usually assume a symmetric matrix.

Let the region R shown in Figure 1 be the axisymmetric region with boundary the axisymmetric shells AB, BC, CD and DA. The test problem

$$u(r, z) = \frac{I_0(\pi r/c)/I_0(\pi a/c) - K_0(\pi r/c)/K_0(\pi a/c)}{I_0(\pi b/c)/I_0(\pi a/c) - K_0(\pi b/c)/K_0(\pi a/c)} \sin(\pi z/c)$$

with $b = a + 1$ and $c = 1$ was solved by finite differences in the region R using a square mesh. SOR iteration was used with the iteration parameter $\omega = 2/[1 + (1 - \mu^2)^{\frac{1}{2}}]$. An approximation to μ, the spectral radius of the Jacobi matrix, was determined by iteration [6, Chapter V]. The maximum discretization error was computed as before. A comparison was made of the solutions obtained using two different approximations for irregular points, i.e., Method 1 uses Eqs. (9) for irregular points, and Method 2 uses a nine-point difference equation defined by Eq. (10), when possible, for irregular points and, if not possible, Eqs. (9) are used. Computed results

TABLE 2

Maximum discretization error for an irregular region

h	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$
No. of difference equations	52	204	800
Error with Method 1. $a = 10^{16}$	1.2×10^{-4}	4.2×10^{-6}	2.7×10^{-7}
Error with Method 2. $a = 10^{16}$	3.9×10^{-7}	1.3×10^{-7}	1.0×10^{-8}
Error with Method 1. $a = \frac{1}{2}$	1.2×10^{-4}	4.9×10^{-6}	3.1×10^{-7}
Error with Method 2. $a = \frac{1}{2}$	1.6×10^{-5}	8.5×10^{-8}	7.2×10^{-9}

are given in Table 2. The number of difference equations given in Table 2 is the number in the region $0 < z \leqq \frac{1}{2} \cap R$.

5. Calculation of capacitance

Referring to Fig. 1, the capacitance between AB and CD is defined as the charge on AB when CD is at unit potential and AB, BC and DA are at zero potential. Thus, if u is the solution to the resulting boundary value problem, then C, the capacitance between AB and CD, is given by

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

$$= -1/(4\pi) \int_{\Gamma} (\partial u)/(\partial n) dS \tag{15}$$

where Γ is the contour shown in Figure 1. The derivative in the integrand is the outward normal derivative.

A uniform mesh is used in the region R. The differential equation is approximated at each mesh point by a difference equation described in sections 2 and 3. The difference approximations of u_r and u_z, given by (7) and (8), are used to approximate the normal derivative in (15). The integration is done by Simpson's rule. If the discretization error in the solution of the difference equation is $O(h^4)$, we can expect the discretization error in the computed values of u_r and u_z to be at least $O(h^3)$. It follows from the results given in [4] that if $u(r, z) \in C^6$ in R then, for an interior point of R, the discretization error in the computed values of u_r and u_z is $O(h^4)$. Furthermore, a uniform $O(h^4)$ discretization error in u_r and u_z is not expected unless the approximation to the differential equation at irregular points is $O(h^3)$. Because of the narrowness of the gaps between the electrodes in the region R of Fig. 1, one would expect that the singularities at the corners of the region would have no significant effect on the solution of the difference equation in a neighborhood of the surface Γ. Based on this assumption, if we integrate the charge over the surface Γ to obtain the capacitance, we would expect that if C_h is the computed value of capacitance obtained, then

$$C_h = C + O(h^4) .$$

The capacitance was computed between opposite faces of the capacitor shown in Figure 1, i.e., between AB and CD, with $b = a + 1$ and $c = 1$. An infinite radius a was used. The true value of capacitance per unit length is known in this case [7] and is equal to $\ln 2/(4\pi^2)$. Table 3 gives the relative error in the value of capacitance per unit length calculated by finite differences. The charge was integrated over the path Γ to obtain the computed value of capacitance. Method 1 and Method 2 are the same two methods used for irregular points in the computed results for Table 2.

TABLE 3

Relative error in the computed value of capacitance. $Error = (C - C_h)/C.$

h	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$
Error with Method 1	-2.3×10^{-3}	-5.3×10^{-5}	4.0×10^{-6}
Error with Method 2	-3.6×10^{-4} .	2.9×10^{-6}	6.4×10^{-8}

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