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Note

A Fourth-Order Poisson Solver

1. Introduction

Consider the Poisson equation

$$\phi_{xx} + \phi_{yy} = \rho, \qquad 0 < x < a, \quad 0 < y < b. \tag{1}$$

When this equation is solved by finite differences, the most commonly used approximation is the five-point formula:

$$\phi_{i,j+1} + \phi_{i,j-1} + \phi_{i+1,j} + \phi_{i-1,j} - 4\phi_{i,j} = h^2 \rho_{i,j}. \tag{2}$$

This approximation has a truncation error of order h^2. An approximation of order h^4 can also be used to solve Eq. (1):

$$\begin{aligned} 4[\phi_{i,j+1} &+ \phi_{i,j-1} + \phi_{i+1,j} + \phi_{i-1,j}] \\ &+ \phi_{i+1,j+1} + \phi_{i+1,j-1} + \phi_{i-1,j+1} + \phi_{i-1,j-1} - 20\phi_{i,j} \\ &= 0.5h^2[\rho_{i+1,j} + \rho_{i-1,j} + \rho_{i,j+1} + \rho_{i,j-1} + 8\rho_{i,j}]. \end{aligned} \tag{3}$$

This nine-point formula, called a Mehrstellenverfahren by Collatz [3], has been known for almost 30 years (see also [5]). In recent years, several authors have derived high-order finite difference approximations for various partial differential equations, e.g., Hodie schemes [1, 7], O.C.I. methods [2] and SCHOS schemes [4, 8]. All of these approximations reduce to Eq. (3) for the case of the Poisson equation.

In this paper, we compare the accuracy and computational efficiency of the above difference approximations for a test problem. We also consider methods of approximating the values of $\partial\phi/\partial x$ and $\partial\phi/\partial y$ once the solution ϕ has been obtained. It is found that the standard central differences yield second-order-accurate values, irrespective of whether Eq. (2) or Eq. (3) is used to solve the Poisson equation. Some new difference approximations for computing the numerical values of these partial derivatives are introduced. These approximations are found to yield $O(h^4)$ accuracy, when used in conjunction with the nine-point formula (3).

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TABLE I

Average CPU Times for Direct Solver (sec)

	Nine-point		Five-point	
N	FACTOR	SOLVE	FACTOR	SOLVE
16	1.63	0.47	1.60	0.20
32	30.98	2.68	30.24	1.56

2. Computational Efficiency of Poisson Solvers

We examine the computational efficiency of the two Poisson solvers on the following problem:

$$\phi_{xx} + \phi_{yy} = \sin(\pi x k_1/8)\sin(\pi y k_2/8). \tag{4}$$

The exact solution is given by

$$\phi = -[(\pi/8)^2(k_1^2 + k_2^2)]^{-1}\sin(\pi x k_1/8)\sin(\pi y k_2/8). \tag{5}$$

This problem arises in the simulation of certain semi-bounded plasmas where both the electric potential ϕ and the electric fields grad ϕ are to be computed. This problem was considered by Knorr *et al.* [6] to test their fourth-order Poisson solver.

We solved Eq. (4) in the square $[0, 16] \times [0, 16]$ using a uniform mesh ($h = 16/N$) and approximated the Poisson equation at each interior mesh point by Eq. (2) or Eq. (3). The resulting algebraic systems were solved using a direct solver (LEQT1B) from I.M.S.L.; double precision arithmetic on IBM 4341. The average CPU times for factorizing the coefficient matrix (FACTOR) and solving the algebraic system (SOLVE) are given in Table I—the FACTOR times are almost identical with both difference approximations. The storage requirements of the band solver are almost identical for both formulas (Table II).

The maximum errors for ϕ are compared in Table III for a sample 32×32 mesh. As expected, Eq. (3) yields much better accuracy.

TABLE II

Storage Requirements of the Direct Solver (Number of Array Elements To Be Stored)

N	Nine-point	Five-point
16	11,475	10,800
32	95,139	92,256

TABLE III

Maximum Errors for ϕ ($N = 32$)

k_1, k_2	Five-point formula	Nine-point formula
1, 1	0.1044(−1)[a]	0.1336(−4)
2, 1	0.1425(−1)	0.5150(−4)
2, 2	0.1050(−1)	0.5304(−4)
3, 1	0.1734(−1)	0.2370(−3)
3, 2	0.1212(−1)	0.5621(−5)
3, 3	0.1060(−1)	0.1178(−3)

[a] $0.1044(-1) = 0.1044 \times 10^{-1}$.

3. Approximations of the First-Order Derivatives

Once the numerical solution of the Poisson equation has been obtained, one may compute the values of the first-order derivatives using the standard central differences:

$$(\partial\phi/\partial x)_{i,j} \cong (\phi_{i+1,j} - \phi_{i-1,j})/2h, \tag{6a}$$

$$(\partial\phi/\partial y)_{i,j} \cong (\phi_{i,j+1} - \phi_{i,j-1})/2h. \tag{6b}$$

Tables IV and V contain the maximum errors in the computed values of grad ϕ in the case of the five-point and the nine-point approximations. When the mesh is refined from 16×16 to 32×32, the errors decay by a factor of 4, thereby indicating $O(h^2)$ convergence in each case. This indicates that the $O(h^4)$ accuracy of the nine-point formula does not lead to comparably accurate values of grad ϕ.

We now examine a new finite difference approximation for grad ϕ, which can be used in conjunction with the nine-point formula:

$$\begin{aligned}(\partial\phi/\partial x)_{i,j} = {}& (\phi_{i+1,j} - \phi_{i-1,j})/3h + (\phi_{i+1,j+1} + \phi_{i+1,j-1} - \phi_{i-1,j+1} \\ & - \phi_{i-1,j-1})/12h - h(\rho_{i+1,j} - \rho_{i-1,j})/12;\end{aligned} \tag{7a}$$

$$\begin{aligned}(\partial\phi/\partial y)_{i,j} = {}& (\phi_{i,j+1} - \phi_{i,j-1})/3h + (\phi_{i+1,j+1} + \phi_{i-1,j+1} - \phi_{i+1,j-1} \\ & - \phi_{i-1,j-1})/12h - h(\rho_{i,j+1} - \rho_{i,j-1})/12.\end{aligned} \tag{7b}$$

The above approximations approximate grad ϕ with $O(h^4)$ accuracy. These approximations were obtained during development of high-order SCHOS approximations for general partial differential equations [4, 8]. Brief derivation of Eq. (7) is given in the Appendix.

TABLE IV

Maximum Errors for grad ϕ (Five-Point Formula) Central Differences

	$\partial\phi/\partial x$		$\partial\phi/\partial y$	
k_1, k_2	$N = 16$	$N = 32$	$N = 16$	$N = 32$
1, 1	0.1640(−1)	0.4093(−2)	0.1640(−1)	0.4093(−2)
2, 1	0.6049(−1)	0.1507(−1)	0.9226(−2)	0.2295(−2)
2, 2	0.3307(−1)	0.8202(−2)	0.3307(−1)	0.8202(−2)
3, 1	0.9778(−1)	0.2415(−1)	0.2128(−1)	0.5133(−2)
3, 2	0.8014(−1)	0.1993(−1)	0.3335(−2)	0.7154(−3)
3, 3	0.5026(−1)	0.1234(−1)	0.5026(−1)	0.1234(−1)

TABLE V

Maximum Errors for grad ϕ (Nine-Point Formula) Central Differences

	$\partial\phi/\partial x$		$\partial\phi/\partial y$	
k_1, k_2	$N = 16$	$N = 32$	$N = 16$	$N = 32$
1, 1	0.3255(−1)	0.8171(−2)	0.3255(−1)	0.8171(−2)
2, 1	0.1009(0)	0.2594(−1)	0.1266(−1)	0.3246(−2)
2, 2	0.6404(−1)	0.1628(−1)	0.6404(−1)	0.1628(−1)
3, 1	0.1611(0)	0.4316(−1)	0.4966(−2)	0.1541(−2)
3, 2	0.1266(0)	0.3339(−1)	0.3890(−1)	0.9988(−2)
3, 3	0.9317(−1)	0.2425(−1)	0.9317(−1)	0.2425(−1)

TABLE VI

Maximum Errors for grad ϕ (Nine-Point Formula) SCHOS Differences

	$\partial\phi/\partial x$		$\partial\phi/\partial y$	
k_1, k_2	$N = 16$	$N = 32$	$N = 16$	$N = 32$
1, 1	0.2546(−3)	0.1584(−4)	0.2546(−3)	0.1584(−4)
2, 1	0.6365(−2)	0.4070(−3)	0.2632(−2)	0.1712(−3)
2, 2	0.2092(−2)	0.1273(−3)	0.2092(−2)	0.1273(−3)
3, 1	0.2247(−1)	0.1474(−2)	0.7437(−2)	0.4981(−3)
3, 2	0.1763(−1)	0.1158(−2)	0.6344(−2)	0.4556(−3)
3, 3	0.7352(−2)	0.4545(−3)	0.7352(−2)	0.4345(−3)

When the above expressions were used to compute grad ϕ from the computed solutions of the nine-point approximation (3), the errors exhibited $O(h^4)$ convergence (see Table VI).

It is clear that the errors in Table VI are substantially smaller than those in Tables IV and V. These errors are comparable or better than those obtained by Knorr *et al.* [6]. The difference approximations presented here are simpler and more straightforward.

APPENDIX

The single-cell high-order schemes of [4, 8] are derived on a nine-point square cell with center (x_i, y_j) and sides of length $2h$. The other eight mesh points on the boundary of the square are $(x_i \pm h, y_j)$, $(x_i, y_j \pm h)$ and $(x_i \pm h, y_j \pm h)$. Taking the local origin at (x_i, y_j), the functions $\phi(x, y)$ and $\rho(x, y)$ are expressed locally by the power series

$$\phi(x, y) = \sum a_{tm}(x - x_i)^t (y - y_j)^m, \qquad \rho(x, y) = \sum c_{tm}(x - x_i)^t (y - y_j)^m,$$
$$x_i - h \leqslant x \leqslant x_i + h, \qquad y_j - h \leqslant y \leqslant y_j + h. \tag{A.1}$$

Substituting (A.1) into Eq. (1) and comparing powers of $(x - x_i)^t (y - y_j)^m$, we obtain the following constraints on the unknown coefficients a_{tm}:

$$\begin{aligned} c_{tm} &= (t + 1 - p)(t + 2 - p)\, a_{t-p+2,m-q} \\ &\quad + (m + 1 - q)(m + 2 - q)\, a_{t-p,m-q+2}, \qquad 0 \leqslant p \leqslant t, \quad 0 \leqslant q \leqslant m. \end{aligned} \tag{A.2}$$

The values of $\phi(x, y)$ at any point of the single cell can be expressed in terms of a_{tm} from (A.1), e.g.,

$$\begin{aligned} \phi_{i+1,j} &\equiv \phi(x_i + h, y_j) = a_{00} + a_{10}h + a_{20}h^2 + a_{30}h^3 + \cdots \\ \phi_{i+1,j+1} &\equiv \phi(x_i + h, y_j + h) = a_{00} + (a_{10} + a_{01})h + (a_{20} + a_{11} + a_{02})h^2 + \cdots. \end{aligned} \tag{A.3}$$

Equations (A.2) and (A.3) constitute a system of linear equations for the unknown coefficients a_{tm} in (A.1). The solution of this system yields a large class of finite difference schemes. The accuracy of a SCHOS scheme depends upon the number of equations used from (A.2) and (A.3).

If only one equation, viz., $c_{00} = 2a_{20} + 2a_{02}$, is used from (A.2), and five equations of the type (A.3) are used, a linear system of order 6×6 results. A particular choice leads to the following system:

$$\begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & -1 & 0 & 1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 2 & 0 & 2 \end{bmatrix} \begin{bmatrix} a_{00} \\ a_{10}h \\ a_{01}h \\ a_{20}h^2 \\ a_{11}h^2 \\ a_{02}h^2 \end{bmatrix} = \begin{bmatrix} \phi_{i+1,j} \\ \phi_{i,j+1} \\ \phi_{i-1,j} \\ \phi_{i,j-1} \\ \phi_{i+1,j+1} \\ c_{00}h^2 \end{bmatrix}. \tag{A.4}$$

The solution of this system gives a_{tm} in terms of c_{00}, h and ϕ_{ij}:

$$a_{00} = 0.25(\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} - h^2 c_{00}), \tag{A.5}$$

$$a_{10}h = 0.5(\phi_{i+1,j} - \phi_{i-1,j}), \qquad a_{01}h = 0.5(\phi_{i,j+1} - \phi_{i,j-1}). \tag{A.6}$$

From (A.1),

$$a_{00} = \phi(x_i, y_j), \qquad c_{00} = \rho(x_i, y_j), \qquad a_{10} = \partial\phi/\partial x(x_i, y_j)$$

and

$$a_{01} = \partial\phi/\partial y(x_i, y_j), \tag{A.7}$$

and Eqs. (A.5), (A.6) represent the five-point formula (2) and the central difference formulas (6), respectively.

For the fourth-order-accurate formulas, we need six constraints corresponding to c_{00}, c_{10}, c_{01}, c_{20}, c_{11}, c_{20} from (A.2) and nine equations of the type (A.3). This yields a 15×15 linear algebraic system similar to (A.4). On solution we obtain the following SCHOS approximations of fourth order:

$$\begin{aligned} a_{00} = {} & 0.2[\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}] \\ & + 0.05[\phi_{i+1,j+1} + \phi_{i+1,j-1} + \phi_{i-1,j+1} + \phi_{i-1,j-1}] \\ & - 0.3c_{00}h^2 - 0.05(c_{20} + c_{02})h^4; \end{aligned} \tag{A.8}$$

$$\begin{aligned} a_{10}h = {} & \tfrac{1}{3}[\phi_{i+1,j} - \phi_{i-1,j}] + \tfrac{5}{6}[\phi_{i+1,j+1} - \phi_{i-1,j+1} \\ & - \phi_{i-1,j-1} + \phi_{i+1,j-1}] - c_{10}h/6; \end{aligned} \tag{A.9}$$

$$\begin{aligned} a_{01}h = {} & \tfrac{1}{3}[\phi_{i,j+1} - \phi_{i,j-1}] + \tfrac{5}{6}[\phi_{i+1,j+1} + \phi_{i-1,j+1} \\ & - \phi_{i-1,j-1} - \phi_{i+1,j-1}] - c_{01}h/6. \end{aligned} \tag{A.10}$$

From (A.1),

$$\begin{aligned} c_{10} = \partial\rho/\partial x(x_i, y_j), & \qquad c_{01} = \partial\rho/\partial y(x_i, y_j), \\ c_{20} + c_{02} = \tfrac{1}{2}[\partial^2\rho/\partial x^2 & + \partial^2\rho/\partial y^2](x_i, y_j) \end{aligned} \tag{A.11}$$

and the SCHOS approximation for the Poisson equation (1) is obtained from (A.8) as

$$\begin{aligned}
&4[\phi_{i+1,j}+\phi_{i-1,j}+\phi_{i,j+1}+\phi_{i,j-1}] \\
&\qquad +\phi_{i+1,j+1}+\phi_{i-1,j+1}+\phi_{i-1,j-1}+\phi_{i+1,j-1}-20\phi_{ij} \\
&\quad = 6h^2\rho_{ij}+\tfrac{1}{2}h^4(\partial^2\rho/\partial x^2+\partial^2\rho/\partial y^2)_{ij}.
\end{aligned} \tag{A.12}$$

When the second term on the right-hand side of (A.12) is replaced by the difference approximation $\frac{1}{2}h^2[\rho_{i,j+1}+\rho_{i,j-1}+\rho_{i+1,j}+\rho_{i-1,j}-4\rho_{ij}]$, we obtain the Mehrstellen formula in Eq. (3). The difference approximations (7) for $\partial\phi/\partial x$ and $\partial\phi/\partial y$ are similarly obtained from (A.9), (A.10).

It is easy to show that these difference approximations have truncation error of order h^4.

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