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Single Cell High Order Difference Methods for the Helmholtz Equation

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A procedure for deriving certain high order difference formulas for the Helmholtz equation is given. Families of formulas of order 2, 4, and 6 are derived. The distinction between "atomic" and "nonatomic" formulas is made, and a nonatomic formula of order 4 is given for a similar equation with variable coefficients. Numerical results using these formulas are given.

1. INTRODUCTION

In this paper we present the description of a simple technique for deriving finite difference formulas of high order for solving linear partial differential equations. The procedure is illustrated for the Helmholtz equation on a rectangle with Dirichlet boundary conditions. Our procedure has strong connections with the Mehrstellenverfahren of Collatz [1] and the HODIE method of Lynch and Rice [2]. Houstis and Papatheodorou [3] have studied the performance of fourth and sixth order HODIE formulas for the Helmholtz equation on a set of problems. Boisvert [4] derived two one-parameter families of fourth order HODIE formulas for the Helmholtz equation. Discretization which is optimal with respect to a certain norm of the truncation error was obtained by Boisvert for certain values of the parameter. Extensions yielding sixth order accuracy for the Helmholtz equation were also obtained.

Recently we have presented in [6–8] an alternative method for generating high order difference formulas for linear partial differential equations. When this procedure is applied to the Helmholtz equation, we not only obtain the discretizations given by the HODIE method but also several other fourth and sixth order schemes. Theoretically, it is possible to apply the procedure to obtain formulas of even higher order by using more than nine mesh points, however, such formulas have little practical interest. We therefore restrict ourselves to formulas that involve mesh points lying on a single cell or element. In this paper we present difference formulas of order two, four, and six for solving the Helmholtz equation and show how other formulas, including those derived by the HODIE method can be obtained from our formulas. Our procedure for generating formulas has been applied to a similar equation with variable coefficients. A numerical comparison of results obtained by using a variety of formulas on a set of problems is also given.

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2. Derivation of Difference Formulas

Consider the Helmholtz equation

$$u_{xx} + u_{yy} + \lambda u = f(x, y), \qquad x, y \text{ in } R \text{ and } \lambda \leqslant 0 \tag{2.1}$$

and

$$u = g(x, y) = \text{known for } (x, y) \text{ on the boundary } \partial R,$$

where R is a region such that a square mesh of size h can be used to subdivide the region. This assumption is made to simplify the presentation. A generalization of the procedure to arbitrary regions can be carried out on the same lines as presented here. Boundary conditions other than the Dirichlet type can also be incorporated in the procedure.

In order to obtain a difference formula for a mesh point it is convenient to consider a local coordinate system (x, y) with its origin at the mesh point. Next, the solution of the boundary value problem (2.1) in the neighbourhood of the mesh point is expanded in an infinite series whose terms are the solutions of the differential equation. An approximation to the solution is obtained by truncating the series. The unknown coefficients in the truncated series are expressed in terms of the nodal values of the solutions at those mesh points that are to be included in the difference formula. This procedure gives the required formula.

Rather than using the solutions of the differential equation, it is easier to expand the solution of (2.1) in a power series. A set of constraints on the coefficients is obtained by demanding that the differential equation be satisfied. In the present example, let

$$u = \sum\!\!\!\!\!\!- \; a_{i,j} x^i y^j \qquad \text{and} \qquad f(x, y) = \sum\!\!\!\!\!\!- \; c_{i,j} x^i y^j, \qquad i, j = 0, 1, 2, \ldots . \tag{2.2}$$

If u satisfies the differential equation, then we must have

$$c_{i,j} = (i+1)(i+2)\, a_{i+2,j} + (j+1)(j+2)\, a_{i,j+2} + \lambda a_{i,j}, \qquad i, j = 0, 1, 2, \ldots . \tag{2.3}$$

Furthermore, the interpolation of u on a set of mesh points (x_k, y_k) gives the following addition conditions:

$$u(x_k, y_k) = u_k = \sum a_{i,j} x_k^i y_k^j, \qquad k = 0, 1, 2, \ldots, M. \tag{2.4}$$

Before a difference formula over the stencil of mesh points (x_k, y_k) appearing in (2.4) is derived from Eqs. (2.3) and (2.4), it is necessary to introduce some approximations of u in the expansion (2.2). One way to do this is to set $a_{i,j} = 0$ for $i + j > n$ for some fixed n. Consequently, all the equations in (2.3) for which $i + j > n$ are eliminated and Eqs. (2.4) now involve finite sums. A difference formula exists if the systems of equations (2.3) and (2.4) are consistent. To obtain a formula, we form a

linear combination of the $c_{i,j}$ and express it in terms of $a_{i,j}$ using Eqs. (2.3). The coefficients of the linear combination of c_{ij} are chosen in such a way that it can be expressed in terms of the nodal values u_k, and all the $a_{i,j}$ are eliminated. This procedure can be described in terms of an $(n+1)(n+2)/2$-dimensional vector space S spanned by $a_{i,j}$. From Eq. (2.3) it is clear that $c_{i,j}$ also form a vector space S_1, which is a subspace of S. Similarly, from (2.4) it can be seen that u_k also form a vector space $S_2 \subset S$. Every nontrivial vector in $S_1 \cap S_2$, expressed in terms of $c_{i,j}$ and also in terms of u_k, provides a formula. A general formula may contain free parameters, the maximum number of such parameters depends upon the dimension of $S_1 \cap S_2$. Note that all $c_{i,j}$ are not linearly independent. For convenience, we choose the mesh points such that the u_k are linearly independent for the value of n chosen.

A difference formula obtained in this manner is exact at least for all polynomials of degree $\leqslant n$, that is, for polynomials in $\mathbb{P}_n$. In the case when the mesh is uniform, the truncation error is of order h^m, $m \geqslant n$. Such a formula is called "atomic" in the sequel. Another type of approximation leads to formulas which have truncation errors of order h^n, though, they many not be exact in $\mathbb{P}_n$. Such formulas are called "nonatomic."

When the mesh is uniform, it is possible to introduce another approximation. The Eqs. (2.3) are multiplied by h^{i+j+2} and all the terms of order h^m, $m > n$, are neglected in the set of Eqs. (2.3) and (2.4). As a consequence of this assumption all the terms containing $a_{i,j}$ for which $i+j > n$ are automatically eliminated. Now the same procedure described earlier is applied to derive a difference formula. During the process of elimination, any term of order h^m, $m > n$, is also neglected. Formulas obtained in this manner are not exact in $\mathbb{P}_n$, although, their truncation error is at least of order n. Hence, these formulas are nonatomic. From our numerical experiments it appears that the nonatomic formulas perform as well as the atomic ones, at least when the mesh is refined.

Some nonatomic formulas can be obtained directly from the atomic formulas by simply deleting the terms of order h^m, $m > n$. However, it is sometimes possible to obtain nonatomic formulas over a given stencil when no atomic formula exists. This indeed is the case for the Helmholtz equation with variable coefficients, for which a nonatomic formula of order 4 is derived for a 9-point stencil using a uniform mesh.

In practice, it is convenient to replace the linear combination of $c_{i,j}$ appearing in the formulas by an equivalent expression containing the values of the function f over a set of points (x_j^*, y_j^*) $j = 0, 1, \ldots, M^*$. The points (x_j^*, y_j^*) need not necessarily be the mesh points. In the case of atomic formulas, the replacement should be exact in $\mathbb{P}_n$. While in the nonatomic formulas, such a replacement should be exact to within the order h^n. Such a replacement results in HODIE type formulas. An atomic formula becomes nonatomic if the replacement is not exact in $\mathbb{P}_n$. Boisvert [5] has proposed a sixth order HODIE formula (2.15) for the Helmholtz equation which is not exact in $\mathbb{P}_6$.

In this paper we shall consider $n = 2$, 4, and 6 and give difference formulas for the Helmholtz equation (2.1) over a stencil of 5 and 9 points. The mesh is taken to be uniform. The general formulas contain some free parameters. All the HODIE-type

formulas for the Helmholtz equation over the 9-point stencil can be obtained by suitable choices of the parameters.

Over a 5-point stencil consisting of mesh points $(0, 0)$, $(\pm h, 0)$, and $(0, \pm h)$, an atomic formula of order 2 containing two parameters p and q $(p \neq 0)$ is given by

$$[p + \tfrac{1}{2}h^2 q]\, u_0 - [4p - \lambda h^2(p - 2q)]\, u_0 = p c_{0,0} h^2 + q(c_{2,0} + c_{0,2})\, h^4, \qquad \text{(A2)}$$

where $\diamond u_0 = u(h, 0) + u(-h, 0) + u(0, h) + u(0, -h)$. If the same stencil is chosen for the values of f, the right-hand side of (A2) can be replaced by

$$[\tfrac{1}{2}q\diamond f_0 + (p - 2q) f_0]\, h^2. \qquad (2.5)$$

The principal error term of formula (A2) is

$$[(12 - h^2)q - 2p](a_{4,0} + a_{0,4})\, h^4 + 4q a_{2,2} h^4 \qquad (2.6)$$

which shows that formula (A2) is not exact for polynomials of degree 4 but is exact in $\mathbb{P}_3$. The truncation error of (A2) is of order h^2. No choices of p and q can anihilate expression (2.6). Thus, there does not exist a fourth order formula over the 5-point stencil considered here.

One of the simplest choices of p and q is $p = 1$ and $q = 0$, which gives the standard 5-point formula

$$\diamond u_0 - (4 - \lambda h^2)\, u_0 = c_{0,0} h^2 = f_0 h^2. \qquad (2.7)$$

Other choices of p and q can also be made.

Using the same procedure and a 9-point stencil formed by the addition of the four mesh points $(\pm h, \pm h)$ and defining $\square u_0$ by

$$\square u_0 = u(h, h) + u(-h, h) + u(-h, -k) + u(h, -h),$$

we can write a general fourth order atomic formula as

$$\begin{aligned} &[4p + \tfrac{1}{2}\lambda h^2(q - r)]\, \diamond u_0 + [p + \tfrac{1}{4}\lambda h^2 r]\, \square u_0 \\ &\quad - \left[20p - \lambda h^2(6p - 2q + r) + \frac{\lambda^2}{2} h^4 (p - q)\right] u_0 \qquad \text{(A4)} \\ &= [6p - \tfrac{1}{2}\lambda h^2(p - q)]\, c_{0,0} h^2 + p[c_{2,0} + c_{0,2}]\, h^4 + q[c_{4,0} + c_{0,4}]\, h^6 + r c_{2,2} h^6 \end{aligned}$$

The parameters p, q, and r are arbitrary except that $p \neq 0$. The right-hand side of (A4) can be replaced in terms of the values of f over a set of 13 points as

$$\begin{aligned} &[r + (8 + \tfrac{1}{2}\lambda h^2)q - (4 + \tfrac{1}{2}\lambda h^2)p]\, f_0 h^2 + \tfrac{8}{3}(p - q)\, h^2 \diamond f_0 \\ &\quad - \tfrac{1}{6}\,[p - 4q + 3r]\, h^2 \diamond f_0 + \frac{r}{4} h^2 \square f_0 \qquad (2.8) \end{aligned}$$

or as

$$[r + (3 + \tfrac{1}{2}\lambda h^2)q + (1 - \tfrac{1}{2}\lambda h^2)p]f_0 h^2 + \tfrac{4}{3}(p - q)\, h^2 \underline{\square} f_0 + \tfrac{1}{2}(q - r)\, h^2 \diamond f_0 + \tfrac{1}{12}(3r - p + q)\, h^2 \square f_0, \tag{2.9}$$

where

$$\underline{\diamond} f_0 = f\left(\frac{h}{2}, 0\right) + f\left(-\frac{h}{2}, 0\right) + f\left(0, \frac{h}{2}\right) + f\left(0, -\frac{h}{2}\right)$$

and

$$\underline{\square} f_0 = f\left(\frac{h}{2}, \frac{h}{2}\right) + f\left(-\frac{h}{2}, \frac{h}{2}\right) + f\left(-\frac{h}{2}, -\frac{h}{2}\right) + f\left(\frac{h}{2}, -\frac{h}{2}\right).$$

All the atomic formulas of order 4 over the 9-point stencil given by Boisvert [5] can be obtained from (A4) and (2.8) or (2.9). For example, the choice of $p = q = 1$ and $r = 0$ gives the formula proposed by Boisvert [5, p. 70]. One simple special case of (A4) is obtained by setting $p = 1$, $q = r = 0$. We also replace $c_{i,j}$ in terms of the values of f at the same 5 points. This replacement is exact only upto h^4 and hence this formula is no longer atomic. Such a formula is given by

$$4 \diamond u_0 + \square u_0 - (20 - 6\lambda h^2 + \tfrac{1}{2}\lambda^2 h^4)\, u_0 = (4 - \lambda h^2/2) f_0 h^2 + (h^2/2) \diamond f_0. \tag{2.10}$$

The principal error term of (A4) is given by

$$(30q - 12p - \lambda h^2 q)(a_{6,0} + a_{0,6})\, h^6 + (2q + 12r - 4p - \lambda h^2 r)(a_{4,2} + a_{2,4})\, h^6. \tag{2.11}$$

It is possible to anihilate the expression in (2.11) by choosing

$$p = 1 - \frac{7}{66}\lambda h^2 + \frac{\lambda^2 h^4}{360}, \qquad q = \frac{2}{5} - \frac{\lambda h^2}{30}, \qquad \text{and} \qquad r = \frac{4}{15} - \frac{\lambda h^2}{90} \tag{2.12}$$

and obtain a sixth order formula. The resulting formula is a special case of a more general sixth order formula containing three parameters p, q, and r and given by

$$\left[4 + \left(\frac{1}{15} + 4p\right)\lambda h^2 + \frac{1}{2}(q - r)\lambda^2 h^4\right] \diamond u_0 + \left[1 + \left(\frac{1}{15} + p\right)\lambda h^2 + \frac{r}{4}\lambda^2 h^4\right] \square u_0 - \left[20 + \lambda h^2\left(20p - \frac{82}{15}\right) + \lambda^2 h^4\left(2q - 6p - r + \frac{3}{10}\right) - \frac{1}{2}(p - q)\lambda^3 h^6\right] u_0$$
$$= \left[6 + \left(6p - \frac{3}{10}\right)\lambda h^2 + \frac{1}{2}(q - p)\lambda^2 h^4\right] c_{0,0} h^2 + [1 + p\lambda h^2](c_{2,0} + c_{0,2})\, h^4$$

$$+\left[\frac{2}{5}+q\lambda h^2\right](c_{4,0}+c_{0,4})\,h^6+\left[\frac{4}{15}+r\lambda h^2\right]c_{2,2}h^6$$

$$+\left[12p-30q+\frac{2}{5}+q\lambda h^2\right](c_{6,0}+c_{0,6})\,h^8$$

$$+\left[\frac{4}{15}+4p-2q-12r+r\lambda h^2\right](c_{4,2}+c_{2,4})\,h^8. \tag{A6}$$

A study of the principal error term of (A6) shows that it is not possible to get an eight order formula on the 9-point stencil used in (A6). Some special cases of (A6) are

(1) $$p=q=\tfrac{1}{120}, \qquad r=\tfrac{1}{72} \tag{2.13}$$

which is the formula given by Houstis and Papatheodorou [3]. With these choices of p, q, and r the right-hand side of (A6) can be expressed in terms of f_0, $\diamond f_0$, $\square f_0$, and $\underline{\square} f_0$ so that the resulting formulas is still atomic.

(2) $$p=-\tfrac{1}{240}(13+\lambda h^2/8), \qquad q=-\tfrac{1}{60}(1+\lambda h^2/32), \qquad r=\tfrac{1}{720} \tag{2.14}$$

gives a formula in which the right-hand side can be expressed in terms of the values f_0, $\diamond f_0$, $\underline{\diamond} f_0$, and $\underline{\square} f_0$ and the formula remains atomic.

(3) $$p=q=r=0 \tag{2.15}$$

gives a formula which appears to be simpler than the other formulas. However, the right-hand side cannot be replaced in terms of f_0, $\diamond f_0$, $\underline{\diamond} f_0$, and $\underline{\square} f_0$. Additional points are required if the formula is to remain atomic. However, if this requirement is relaxed, we obtain the formula given by Boisvert [5, p. 119–120] which is not exact in $\mathbb{P}_6$, which has the truncation error of order h^6. We have solved several problems using this and other formulas and have found that the nonatomic formulas perform as well as the atomic formulas. Similar observations have been made by Boisvert, although this distinction is not made clear.

(4) $$p=-\frac{7}{60}+\frac{\lambda h^2}{360}, \qquad q=-\frac{1}{30}, \qquad r=-\frac{1}{90}. \tag{2.16}$$

This choice eliminates the coefficients, $c_{6,0}$, $c_{0,6}$, $c_{4,2}$, and $c_{4,2}$ and gives formula (2.12) obtained from formula (A4) earlier. Again an atomic formula is not obtainable in terms of f_0, $\diamond f_0$, and $\square f_0$.

3. Formulas for Variable Coefficients

Following the procedure, described in Section 2, we now give formulas of order 2 and 4 for the equation

$$a(x, y)\, u_{xx} + b(x, y)\, u_{yy} + w(x, y)u = f(x, y). \tag{3.1}$$

Using the expansions

$$a(x, y) = \sum \alpha_{i,j} x^i y^j, \qquad b(x, y) = \sum \beta_{i,j} x^i y^j, \qquad w(x, y) = \sum \omega_{i,j} x^i y^j$$

along with the expansions of u and f given in (2.2). The standard 5-point formula of order 2 and a nonatomic formula of order 4 over the 9-point stencil are given here using the notation

$$u_1 = u(h, 0), \qquad u_2 = u(0, h), \qquad u_3 = u(-h, 0), \qquad u_4 = u(0, -h),$$
$$u_5 = u(h, h), \qquad u_6 = u(-h, h), \qquad u_7 = u(-h, -h), \qquad u_8 = u(h, -h).$$

Formula of order 2:

$$\alpha_{0,0}(u_1 + u_3) + \beta_{0,0}(u_2 + u_4) - u_0(2\alpha_{0,0} + 2\beta_{0,0} - \omega_{0,0}h^2) = c_{0,0}h^2 = f_0 h^2. \tag{3.2}$$

This formula is exact in $\mathbb{P}_3$ and has a truncation error of order 2. A nonatomic formula of order 4 in which

$$\bar{\alpha}_{1,0} = \alpha_{1,0}/\alpha_{0,0} \qquad \text{and} \qquad \bar{\beta}_{0,1} = \beta_{0,1}/\beta_{0,0}$$

is given by

$$\begin{aligned}
&(u_1 + u_3)[5\alpha_{0,0} - \beta_{0,0} - h^2(\bar{\alpha}_{1,0}\alpha_{1,0} + \bar{\beta}_{0,1}\alpha_{0,1}) + h^2(\alpha_{2,0} + \alpha_{0,2} + \omega_{0,0}/2)] \\
&\quad + (u_2 + u_4)[5\beta_{0,0} - \alpha_{0,0} - h^2(\bar{\beta}_{0,1}\beta_{0,1} + \bar{\alpha}_{1,0}\beta_{1,0}) + h^2(\beta_{2,0} + \beta_{0,2} + \omega_{0,0}/2)] \\
&\quad - h(u_1 - u_3)[\beta_{1,0} - \beta_{0,0}\bar{\alpha}_{1,0} + h^2(\bar{\alpha}_{1,0}\omega_{0,0} - \omega_{1,0})/2] \\
&\quad - h(u_2 - u_4)[\alpha_{0,1} - \alpha_{0,0}\bar{\beta}_{0,1} + h^2(\bar{\beta}_{0,1}\omega_{0,0} - \omega_{0,1})/2] \\
&\quad + (\alpha_{0,0} + \beta_{0,0})\,\square u_0/2 + h(\alpha_{0,1} - \alpha_{0,0}\bar{\beta}_{0,1})(u_5 + u_6 - u_7 - u_8)/2 \\
&\quad + h(\beta_{1,0} - \beta_{0,0}\bar{\alpha}_{1,0})(u_5 - u_6 - u_7 + u_8)/2 \\
&\quad - u_0[10(\alpha_{0,0} + \beta_{0,0}) - 2h^2\{\bar{\alpha}_{1,0}(\alpha_{1,0} + \beta_{1,0}) + \bar{\beta}_{0,1}(\alpha_{0,1} + \beta_{0,1})\} \\
&\quad + 2h^2(\alpha_{2,0} + \alpha_{0,2} + \beta_{2,0} + \beta_{0,2} - 2\omega_{0,0}) + h^4(\omega_{1,0}\bar{\alpha}_{1,0} + \omega_{0,1}\bar{\beta}_{0,1}) \\
&\quad - h^4(\omega_{2,0} + \omega_{0,2})] \\
&= 6h^2 c_{0,0} - h^4(\bar{\alpha}_{1,0}c_{1,0} + \bar{\beta}_{0,1}c_{0,1}) + h^4(c_{2,0} + c_{0,2}).
\end{aligned} \tag{3.3}$$

The truncation error of formula (3.2) is of order h^4. When $\alpha_{i,j}$, $\beta_{i,j}$, $\omega_{i,j}$, and $f_{i,j}$ are replaced by the values of the functions a, b, w, and f, respectively, due care must be taken to preserve the order. This does require the use of additional points such as $(h/2, 0)$, $(-h/2, 0)$, etc. Numerical results obtained by using both formulas (3.2) and (3.3) are given in the next section.

4. Numerical Results

We have solved many different boundary value problems given by (2.1) over a unit square for various values of $g(x, y)$ and λ. Table I we compare the numerical results obtained for three problems using various atomic and nonatomic methods.

Method 1 uses the second order atomic formula (2.7). Methods 2 and 4 use the atomic fourth and sixth order formulas (2.9 with $p = q = 1$ and $r = 0$) and (2.13), respectively. While Methods 3 and 5 use the nonatomic fourth and sixth order formulas (2.10) and (2.16), respectively. The convergence rates were estimated by

$$\ln(e_{h_1}/e_{h_2})/\ln(h_1/h_2),$$

where e_{h_1} and e_{h_2} are the maximum errors for $h_1 = \frac{1}{8}$ and $h_2 = \frac{1}{16}$. The matrix equations were solved using successive over relaxation (SOR) in single precision on a DEC 2060.

TABLE I

Maximum errors, (N) = 10^N

Problem	Method	h = 1/4	h = 1/8	h = 1/16	Convergence Rate
1	1	0.7351(-1)	0.3229(-1)	0.9081(-2)	1.83
	2	0.2991(-1)	0.2888(-2)	0.1833(-3)	3.98
	3	0.1038(-1)	0.1612(-2)	0.1171(-3)	3.78
	4	0.1277(-3)	0.7093(-5)	0.3502(-6)*	4.34
	5	0.1047(-2)	0.4428(-4)	0.8661(-6)	5.68
2	1	0.1272	0.1078	0.4001(-1)	1.43
	2	0.1837	0.3671(-1)	0.3186(-2)	3.53
	3	0.6983(-1)	0.1944(-1)	0.1813(-2)	3.42
	4	0.3172(-2)	0.3582(-3)	0.9239(-5)	5.28
	5	0.4039(-2)	0.2969(-3)	0.7179(-5)	5.37
3	1	0.1414(2)	0.1602(1)	0.3092(0)	2.37
	2	0.1318(2)	0.2627(0)	0.1865(-1)	3.82
	3	0.1332(2)	0.3050(0)	0.1864(-1)	4.03
	4	0.8336(1)	0.8447(-1)	0.8142(-3)	6.70
	5	0.8445(1)	0.7947(-1)	0.7082(-3)	6.81

* affected by roundoff error.

Problems 1–3 were chosen from Houstis and Papatheodorou [3]. They are:

Problem 1:

$$u = (\cosh 10x + \cosh 10y)/\cosh 10, \qquad \lambda = -100.$$

Problem 2:

$$u = \frac{\cosh 10x}{\cosh 10} + \frac{\cosh 20y}{\cosh 20}, \qquad \lambda = -100.$$

Problem 3:

$$u = \cos 20y + \sin 20(x - y), \qquad \lambda = -30.$$

To demonstrate the effectiveness of formula (3.3) for solving Eq. (3.1), we compare in Table II the numerical results obtained using the second order method (3.2) and our fourth order method (3.3). The problems chosen were:

Problem 4:

$$u = x^2y^2(x^2 + y^2), \qquad a = x^2, \qquad b = y^2, \qquad w = -14.$$

Problem 5:

$$u = \frac{\cosh 10x}{\cosh 10} + \frac{\cosh 4y}{\cosh 4}, \quad a = \frac{\cosh 4y}{\cosh 4}, \quad b = \frac{\cosh 10x}{\cosh 10}, \quad w = -100\frac{\cosh 4y}{\cosh 4}.$$

Problem 6:

$$u = x^2y^2 \exp(x + y), \qquad a = 1/(x^2 + 4x + 2), \qquad b = 1(y^2 + 4y + 2),$$
$$w = -1/(10 + x^2 + y^2).$$

TABLE II

Maximum errors for $au_{xx} + bu_{yy} + wu = f$

Problem	Method	h = 1/4	h = 1/8	h = 1/16	Convergence Rate
4	1	0.2063(-2)	0.5401(-3)	0.1362(-3)	1.98
	2	0.1756(-2)	0.1156(-3)	0.8217(-5)	3.81
5	1	0.4141(-1)	0.2096(-1)	0.5734(-2)	1.87
	2	0.2542(-1)	0.2038(-2)	0.1257(-3)	4.01
6	1	0.1378(-1)	0.3968(-2)	0.1052(-2)	1.91
	2	0.4408(-2)	0.3123(-3)	0.1445(-4)	4.43

5. Concluding Remarks

The convergence rates estimated from the numerical results for a variety of problems demonstrate that the order of the method is as expected. One would normally expect that the atomic formulas would be more accurate than the nonatomic ones. This indeed is the case for solutions which are polynomials of a certain degree. For example, the sixth order atomic formulas are exact for polynomials of degree up to 7, however, the nonatomic formulas are not. But, as the size of the mesh is decreased, the reduction of the error is at a rate predicted by the order of the method. It may be mentioned here that the higher order methods do require that the solution satisfies certain smoothness requirements. If the solution does not satisfy these smoothness conditions, a higher order method may not perform any better than a lower order method.

We tested a large number of second, fourth, and sixth order methods by choosing the free parameters from a study of the truncation error, so as to optimize certain properties. However, we were not able to find a best all round method. One can construct problems for which one of the methods of a particular order performs better than all of the other methods. However, it is always possible to construct a problem where this situation is reversed.

The method described here has been applied to generate nonatomic fourth order difference formulas in the case of more general elliptic equations with variable coefficients, and to some three-dimensional problems. These formulas have given excellent numerical results over a wide range of problems.

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