1977

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Report Number:
77-223

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CSD-TR 223

February 21, 1977
(Revised September 30, 1977)

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Abstract. A new an flexible finite difference method is described which gives approximate solutions of linear elliptic partial differential equations, $Lu = G$, subject to general linear boundary conditions. The method gives high-order accuracy. The values of the unknown approximating function U are dertermined at mesh points by solving a system of finite difference equations $L_h U = I_h G$. $L_h U$ is a linear combination of values of U at points of a standard stencil (nine-point for two-dimensional problems, 27-point for three-dimensional) and $I_h G$ is a linear combination of values of the given function G at mesh points as well as at other points. A local calculation is carried out to determine the coefficients of the operators L_h and I_h so that the approximation is exact on a specific linear space of functions. Having the coefficients of each difference equation one solves the resulting system by standard techniques to obtain U at all interior mesh points. Special cases generalize well-known $O(h^6)$ approximation of smooth solutions of the Poisson equation to $O(h^6)$ approximation for the variable coefficient equation $-\mathrm{div}(p\ \mathrm{grad}[u]) + p\ u = G$. The method can be applied to other than elliptic problems.

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1. The HODIE finite difference approximation. We first consider finite difference approximation for the real linear elliptic Dirichlet boundary value problem:

$$L[u] = Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G, \quad AC > B^2 \qquad [1]$$

The coefficients $A,\ldots,F,G$ are assumed given smooth functions on a connected region R with piecewise smooth boundary ∂R. For a given function g, $u = g$ on the boundary.

We first consider the case of a square mesh with mesh length h and approximation away from the boundary. We approximate u by values of U, defined at mesh points in the interior of R, as the solution of the linear difference equation

$$L_hU \equiv (1/h^2) \sum_{i=0}^{8} \alpha_i U_i = \sum_{j=1}^{J} \beta_j G_j \equiv I_h G. \qquad [2]$$

In [2], the sum of the $\alpha_i U_i$ is taken over nine mesh points in the interior of R called stencil points which are shown as small circles in Figure 1. We use S_h to denote the square of side $2h$ with corners labeled 5,6,7,8 and we call the point labeled 0 the central stencil point.

One key idea of the method we discuss is the use of the right side of [1] at several points in S_h. In [2], $I_h G$ is a linear combination of values G_j of G at J auxiliary points. They include non-stencil points, such as those indicated by the x's in Figure 1, as well as stencil points. The use of these auxiliary points gives the high accuracy of the scheme. The Mehrstellenverfahren ("Hermitian" method) of Collatz (1) uses linear combinations of G and its derivatives, but only at stencil points.

A second key idea of the method we discuss consists in choosing the coefficients α_i, β_j to make the approximation exact on some given finite dimensional linear space S, such as the space $\mathbb{P}_K$ of polynomials of degree at most K. That is, for any basis $s_0,\ldots,s_K$ of S, the coefficients satisfy

$$(1/h^2) \sum_{i=0}^{8} \alpha_i (s_k)_i = \sum_{j=1}^{J} \beta_j (Ls_k)_j, \quad k=0,\ldots,K. \qquad [3]$$

In this respect, this method is different from the Mehrstellenverfahren in which coefficients are obtained by equating terms of Taylor's series expansions.

A third key idea is the use of nine stencil points which leads to a block tridiagonal matrix equation for the values of U. Such equations are ameanable to standard, efficient computational schemes.

A fourth key idea is the ease of approximation of general linear boundary conditions given on curved boundaries (see Section 5). The block tridiagonal structure mentioned above is preserved and evaluation of $A,\ldots,F,G$ outside the closed region $\bar{R}$ is not needed.

If the coefficients of [2] are normalized by making the sum of the β_j's equal to unity, then $I_h G = G_0 + O(h)$. Thus the operator I_h is a perturbation of the identity operator. We call the scheme described above <u>High Order Difference approximation with Identity Expansion</u> and use the acronym HODIE. A complete analysis of the HODIE method as applied to ordinary differential equations is given by Lynch and Rice (2).

2. <u>Examples.</u> As a simple example, we consider a new $O(h^6)$ approximation to the Poisson equation: $\nabla^2 u = u_{xx} + u_{yy} = G$. Using the space $S = \mathbb{P}_7$, one obtains the well-known 9-point approximation for the Laplacian (4) for L_h. Using auxiliary points consisting of the stencil points and the centers of the four mesh squares indicated by the x's in Figure 1, we obtain

$$\frac{1}{6h^2}\begin{array}{|c|c|c|}\hline 1 & 4 & 1 \\ \hline 4 & -20 & 4 \\ \hline 1 & 4 & 1 \\ \hline \end{array}\ U = \frac{1}{360}\begin{array}{|c|c|c|c|c|}\hline 1 & & 4 & & 1 \\ \hline & 48 & & 48 & \\ \hline 4 & & 148 & & 4 \\ \hline & 48 & & 48 & \\ \hline 1 & & 4 & & 1 \\ \hline \end{array}\ G \qquad [4]$$

The value of the right side requires, on the average, two evaluations of G for each interior mesh point. For a different approximation, see Rosser (5).

If U and G are replaced by u and $\nabla^2 u$, where u is in $C^8(\overline{R})$, the space of functions with continous eighth derivatives on $\overline{R}$, then [4] fails to be an equality by terms of order $O(h^6)$. Thus, the <u>truncation error</u> is $O(h^6)$ for $u \in C^8(\overline{R})$. Moreover, the difference operator L_h is of monotone type: for v zero on the boundary, $L_h v \geqq 0$ implies that $v \leqq 0$. It follows that the <u>discretization error</u>, defined as the maximum of $|U - u|$ at mesh points, is also $O(h^6)$ if $u \in C^8(\overline{R})$ and if $\overline{R}$ is the union of squares S_h.

With S a space of polynomial, $O(h^6)$ approximation is <u>optimal</u> for the nine point stencil of Figure 1. This follows from Theorem 11 of Birkhoff and Gulati (6) who display an eighth degree harmonic polynomial which is nonzero at the central stencil point and zero at the other eight stencil points.

However, the HODIE method gives $O(h^6)$ approximation not only to sufficiently smooth solutions of the Poisson equation, but also to the more general differential equation

$$-\mathrm{div}(p\ \mathrm{grad}[u]) + F\, u = G. \tag{[5]}$$

This equation is important in applications such as nuclear reactor design and petroleum reservoir analysis. For this, we have used 20 auxiliary points: the nine stencil points, the points at the centers of the four unit squares which make up S_h, and seven of the eight midpoints of their outer edges. We used a basis for $\mathbb{P}_6$ and solved [3] to obtain the coefficients α_i, β_j for each set of nine stencil points in R.

We report on results from one of our test cases:

$$-(\exp(xy)u_x)_x - (\exp(xy)u_y)_y + 2(x^2+y^2)\exp(xy)u = G, \tag{[6]}$$

for R the unit square. In order to measure the discretization error as a function of mesh length h, we <u>chose</u> analytic solutions, u, and from them determined G and the boundary function g. Specifically, we considered

$$\begin{aligned}
&\text{(I)} \quad u(x,y) = \exp(xy) \text{ with } G(x,y) = 0,\\
&\text{(II)} \quad u(x,y) = \exp(-xy) \text{ with } G(x,y) = 2(x^2+y^2),\\
&\text{(III)} \quad u(x,y) = (3-x^2-y^2)^{1/3}.
\end{aligned} \tag{[7]}$$

Table 1 lists values of the discretization error for various values of h and also these errors divided by h^p for p = 6 or p = 7 which shows the error is $O(h^7)$ for Case (I) and $O(h^6)$ for the other two cases.

TABLE 1

[a]: Discretization error, [b]: (discretization error)/h^7, and [c]: (discretization error)/h^6 for equation [6] and the solutions given in [7]. 4.92-6 denotes 4.92×10^{-6}.

	(I)		(II)		(III)	
h	[a]	[b]	[a]	[c]	[a]	[c]
1/4	4.92-6	.0805	2.29-4	.000940	5.67-5	.232
1/6	3.30-7	.0923	8.03-9	.000374	6.80-6	.317
1/8	4.63-8	.0970	1.25-9	.000326	1.38-6	.362
1/10	9.83-9	.0983	3.39-10	.000339	3.78-7	.378

3. Computational techniques and complexity. Appropriate choice of basis elements simplifies the evaluation of the α_i, β_j. For $S = \mathbb{P}_M$, we use a basis which makes the system [3] reducible. We choose basis elements $s_0, \ldots, s_8$ which span the space of biquadratic polynomials. For the other basis elements, we use polynomials vanishing at all stencil points.

We first solve the system

$$\beta_1 = 1 \qquad [7a]$$

$$\sum_{j=2}^{J} \beta_j (Ls_k)_j = -(Ls_k)_1, \quad k = 9, 10, \ldots, K, \qquad [7b]$$

to obtain the β_j's. Typically we used $K = J+9$ so that there are as many equations as unknowns. But in some cases, such as those mentioned in Section 2, the symmetry of the operator L allows [7b] to be solved for some K greater than $J+9$.

After the β_j's are evaluated, we solve the system

$$(1/h^2) \sum_{i=0}^{8} \alpha_i (s_k)_i = \sum_{j=1}^{J} \beta_j (Ls_k)_j, \quad k = 0, \ldots, 8, \qquad [8]$$

to obtain the stencil coefficients α_i.

Having the coefficients of L_h, I_h for all S_h, we evaluate $I_h G$ and then solve the system of difference equations [2] to obtain the estimates U of u.

For sufficiently smooth u, the discretization error as a function of h depends on the number J of auxiliary points and the number, say h^{-2}, of interior mesh points. Since J is fixed, the amount of work in determining the α_i, β_j increases as the number of difference equations,

h^{-2}. But, the work involved in solving the system of difference equations to obtain U increases at a faster rate. For example if band-elimination is used, this work increases as h^{-4}. Consequently, the major part of the work occurs in the solution of the difference equations and the work involved in determining the coefficients α_i, β_j which give high accuracy is minor. For a more detailed analysis, see Lynch and Rice*.

4. Outline of theoretical results. For a given space Q of functions in the domain of L, the truncation operator T_h is defined by $T_h q = -L_h q + I_h L q$, $q \varepsilon Q$, and the truncation error as the max norm of $T_h q$. If the solution u is in Q, so that $Lu = G$, then one obtains an equation for the error $e = U - u$ in terms of the truncation operator:

$$L_h e = L_h U - L_h u = I_h G - L_h u = T_h u. \qquad [9]$$

In some cases, such as when L_h is of monotone type, one can show that an $O(h^p)$ bound on the truncation error gives and $O(h^p)$ bound on the discretization error defined as the max norm of e.

We begin by considering [1] with constant coefficients and use lower case letter to denote constants:

$$Lu = au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = G \qquad [10]$$

Consider approximation with $S = \mathbb{P}_M$. For $p \varepsilon \mathbb{P}_M$, $Lp \varepsilon \mathbb{P}_M$ and if $f \neq 0$, then the mapping is onto $\mathbb{P}_M$ provided f is not an eigenvalue of the operator $Lu - fu$. One sees that [7b] with $K = J+9$ has one and only one solution except when f is an eigenvalue of the linear system. Since s_k, $k = 0,\ldots,8$, in [8] form a basis for the biquadratic polynomials, there is a unique set of u_i which satisfy [8]. Hence with few exceptions, there exist a unique set of α_i,β_j which satisfy [7] and [8] provided $f \neq 0$.

If $f = 0$ and $d \neq 0$ or $e \neq 0$, then one also gets unique α_i,β_j which satisfy [7] and [8] with only a few exceptions. If the coefficients $A,\ldots,F$ in [1] are differentiable, then terms in the equations [7] and [8] for the variable coefficient case differ by $O(h)$ from the terms for some constant coefficient operator L. Hence for $K = J+9$ and any sufficiently small h, there are unique α_i, β_j which satisfy [7] and [8] provided one of D, E, or F is nonzero -- and again with only a few exceptions.

If, however, in [10] the constants d, e, and f are each zero, then L maps $\mathbb{P}_M$ into $\mathbb{P}_{M-2}$. Furthermore, there is a subspace $\mathbb{N}_M$ of $\mathbb{P}_M$ which has dimension $(M+1)(M+2)/2$ which is also a subspace of the null space of L. For $L = \nabla^2$, this is the space of harmonic polynomials of degree M. For s_k in $\mathbb{N}_M$, [3] reduces to

$$(1/h^2) \sum_{i=0}^{8} \alpha_i (s_k)_i = 0$$

and if this (for all s_k in $\mathbb{N}_M$) implies that $\alpha_i = 0,\ldots,8$, then the sum in [2] which involves the approximation U vanishes. In this case one obtains no estimate U of u, i.e., there is no nontrivial HODIE approximation which is exact on $\mathbb{P}_M$. By determining the minimum degree M for which the HODIE approximation must have all coefficients α_i, β_j equal to zero, one obtains the following

THEOREM. <u>Consider</u> [10] <u>with constant coefficients and the HODIE approximation which is exact on</u> $\mathbb{P}_M$:

(a) <u>If</u> $Lu = u_{xx} + u_{yy}$, <u>then one can obtain a HODIE approximation with</u> $S = \mathbb{P}_7$ <u>but not with</u> $S = \mathbb{P}_8$; <u>for</u> $S = \mathbb{P}_7$, <u>the truncation error is</u> $O(h^6)$ <u>with respect to</u> $C^8(\overline{R})$.

(b) _If_ $Lu = u_{xx} + cu_{yy}$ _or_ $Lu = u_{xx} + 2bu_{xy} + u_{yy}$ _with_ $b \neq 0$, $0 \neq c \neq 1$, _then one can obtain a nontrivial HODIE approximation with_ $S = \mathbb{P}_5$ _but not with_ $S = \mathbb{P}_6$; _for_ $S = \mathbb{P}_5$, _the truncation error is_ $O(h^4)$ _with respect to_ $C^6(\overline{R})$.

(c) _If_ $Lu = u_{xx} + 2bu_{xy} + cu_{yy}$, $b \neq 0$, $0 \neq c \neq 1$, _then one can obtain a nontrivial HODIE approximation with_ $S = \mathbb{P}_3$ _but not with_ $S = \mathbb{P}_4$; _for_ $S = \mathbb{P}_3$, _the truncation error is_ $O(h^2)$ _with respect to_ $C^4(\overline{R})$ _and one such scheme is the divided central difference approximation to_ L _and a single auxiliary point at the central stencil point_.

If L is the Laplacian and if a rectangular mesh is used with spacing Δx, Δy, $\Delta x \neq \Delta y$, then the change of scale $x \to x$, $y \to (\Delta x/\Delta y)y$, transforms the mesh to a square mesh and the operator transforms as $\nabla^2 u \to u_{xx} + (\Delta y/\Delta x)^2 u_{yy}$. Case (b) then applies and one gets only $O(h^4)$ truncation error. Similarly, there is a rectangular mesh for which one obtains a HODIE $O(h^6)$ approximation to $Lu = u_{xx} + cu_{yy}$. After a change of scale and a rotation, one can obtain a HODIE $O(h^6)$ approximation to $Lu = u_{xx} + 2bu_{xy} + cu_{yy}$.

5. Extensions and generalizations. The HODIE method is not limited to second order operators, to elliptic operators, to operators in two independent variables as in [1a], or to a nine-point stencil in two dimensions. For example, there is a three dimensional $O(h^6)$ analogue of [4] which uses 27 stencil points and 23 auxiliary points, see Lynch‡.

Although we have only done computer experiments with S a space of polynomials, other spaces can be used. For example, near a corner where a derivative of u has a singularity, an appropriate space can be used provided the nature of the singularity is known. Dershem ( ) has obtained $O(h^2)$ approximation to solutions of ordinary differential equations which behave as x^ν, $0 < \nu < 1$ by using a single auxiliary point.

The limit of $O(h^6)$ for approximation to the Laplacian with S a space of polynomials is due to the fact that harmonic polynomials of arbitrarily high degree exist. When lower order derivatives also appear, however, there is, in principle, no reason for this limitation. We have experimented with a number of operators and the numerical computations have been stable; the results in Table 1 for Case (I) illustrates one example in which $O(h^7)$ discretization error is obtained.

Finally, the difference equation [2] can be modified to take into account general linear boundary conditions

$$L_B u = Pu + Qu_x + Tu_y = g, \quad (x,y) \in \partial R, \quad P^2 + Q^2 + T^2 \neq 0 \qquad [11]$$

on curved portions of the boundary. We assume that h is sufficiently small so that the portion of the boundary which cuts through a square S_h is smooth as indicated in Figure 2. The difference equation is

$$(1/h^2) \sum_{i=0}^{I} \alpha_i U_i = \sum_{j=0}^{J} \beta_j G_j + \sum_{m=1}^{M} \gamma_m g_m \qquad [12]$$

As above, U_i denotes the value of U at a stencil point, but here the stencil points are the mesh points in the intersection $S_h \cap R$; G_j denotes values of G at auxiliary points in the same intersection. The values g_m are taken at M boundary auxiliary points; these are points on the boundary which cuts through S_h and are indicated by small squares in Figure 2. The equations which give the coefficients are

$$(1/h^2) \sum_{i=0}^{I} \alpha_i (s_k)_i = \sum_{j=1}^{J} \beta_j (Ls_k)_j + \sum_{m=1}^{M} \gamma_m (L_B s_k)_m, \quad k = 0,\ldots,K.$$

After the coefficients are evaluated, the value of the right side of [12] is known since G and g are given. Note that the structure of the coefficient matrix which arises from the left side of the difference equation [12] has the same structure as the nine-point approximation to L because the only unknowns are U at interior mesh points.

Acknowledgment: We thank the National Science Foundation for partial support under NSF grant MCS 76-10225.

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Footnotes.

[line 7 of page 8]:

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[line 5 of page 12]:

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Figure captions [2 figures]

Figure 1. The nine stencil points for approximation away from the boundary are indicated by small circles. Four non-stencil auxiliary points are indicated by small x's.

Figure 2. An example of points used in S_h when the boundary cuts through S_h. Five stencil points are indicated by small circles. Four non-stencil auxiliary points are indicated by small x's. Six boundary auxiliary points are indicated by small squares.

Figure 1

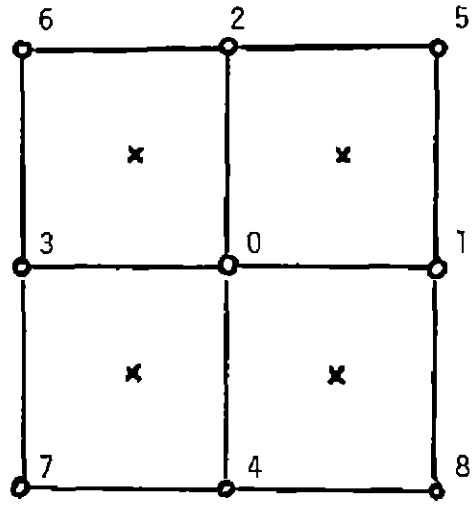

Figure 2