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Abstract. A finite difference approximation is given which gives $O(h^6)$ accurate approximations to smooth solutions of the Poisson equation in three independent variables. Experimental results are given which confirm this behavior of the error.

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$O(h^6)$ DISCRETIZATION ERROR FINITE DIFFERENCE APPROXIMATION TO SOLUTIONS OF THE POISSON EQUATION IN THREE VARIABLES

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1. Finite difference approximation. We consider approximation of smooth solutions of the Poisson equation

$$u_{xx} + u_{yy} + u_{zz} = f$$

at mesh points of a cubic lattice with mesh spacing h. It is sufficient to regard one of the mesh points as the origin.

Let $\sum_{r^2} U$ denote the sum of values of U at lattice points a distance r from the origin. Let $X = \partial/\partial x$, $Y = \partial/\partial y$, $Z = \partial/\partial z$, so that the Laplacian is given by $\nabla^2 = X^2 + Y^2 + Z^2$.

Let the difference operators L_h and I_h and the differential operator M_h be defined by

$$L_hU = [-128\ U + 14 \sum_{r^2=h^2} U + 3 \sum_{r^2=2h^2} U + \sum_{r^2=3h^2} U\ ]/(30h^2)$$

$$I_hf = [\ 280\ f + \ 8 \sum_{r^2=h^2} f + 48 \sum_{r^2=3h^2/3} f + \sum_{r^2=3h^2} f\ ]/720$$

$$M_hf = f + (h^2/12)\nabla^2 f + (h^4/360)[\nabla^4 f + 2(X^2Y^2 + Y^2Z^2 + Z^2X^2)f]$$

The following relations are easy to verify for u with

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continuous eighth derivatives and $f = \nabla^2 u$:

$$L_h u = M_h \nabla^2 u + O(h^6) = M_h f + O(h^6)$$

$$I_h f = M_h f \quad + O(h^6)$$

Alternatively, these can be easily derived by use of Taylor's Theorem; use of operators such as $\exp(hX) = I + hX + (h^2/2)X^2 + \ldots$ $\exp(h[X+Y]) = I + h(X+Y) + \ldots$, and so on, together with symmetry and simple identities among symmetric polynomials simplifies the derivation. A complete derivation is given by Lynch [1977].

It follows that if the function U defined at mesh points satisfies the system of differnce equations $L_h U = I_h f$, one equation for each interior mesh point, then the error $e = U - u$ satisfies $L_h e = I_h f - L_h u = O(h^6)$. If the function U takes on the values of u at boundary mesh points, then e is zero on the boundary. The operator L_h on the space of functions which are zero at boundary mesh points is of monotone type ($L_h v \geqq 0$ implies $v \leqq 0$), hence the function $Kh^6(r^2 - x^2 - y^2 - z^2)$ bounds the magnitude of the error provided K and r are sufficiently large. Consequently, one obtains $O(h^6)$ discretization error.

The difference operator L_h was given by Mikeladze [1937] and he proved $O(h^4)$ discretization for the approximation $L_h U = M_h f$. Apparently he was not aware that this gives $O(h^6)$ accuracy.

The value $I_h f$ gives $O(h^2)$ approximation to f and I_h can, therefore, be regarded as a perturbation, or expansion, of the identity. The approximation $L_h U = I_h f$ is an example of a High Order Difference approximation with Identity Expansion, called a HODIE approximation by Lynch and Rice [1975,1977]. Lynch and Rice [1977] display the coefficients of L_h and I_h, but they do not present the experimental results described in the next section.

Note that f is evaluated only in the mesh cube of side $2h$ centered at the origin; this cube also contains the 27 stencil points of the operator L_h. The function f is evaluated close to the central stencil point and f does not have to be evaluated outside the region on which it is defined. Also note that the coefficients of f in the operator I_h are all positive. Rosser [1975] has proposed an $O(h^6)$ approximation for the Poisson equation in two variables whose generalization to three dimensions does not have the two features mentioned above, namely, his scheme requires evaluation of f outside the cube of side 2h (but not outside the region of definition of f) and some of the coefficients of f are negative (see Lynch [1977]). Consider the matrix formulation of the system of difference equations, suppose it is $AU = b$ with solution $U = A^{-1}b$. The components of A^{-1} are estimates of values of the Green's Function of the differential equation problem. A component of $A^{-1}b$ is an estimate of a value of u and is thus an estimate of the integral of the product of the Green's Function and f. This can be regarded as a type of quadrature formula. Components of b are $I_h f$ (plus, in certain cases, values of the boundary values). If the coefficients of $I_h f$ were negative, then one would have a quadrature formula with negative weights; it is well-known that such formulas are to be avoided because of the build-up of round-off error.

There is no 27-point difference operator, such as L_h but with different coefficients, which can give higher than $O(h^6)$ accuracy for the Poisson equation in three variables. This follows from the eighth degree polynomial in two variables

$$p_8(x,y) = (x^8-28x^6y^2+70x^4y^4-28x^2y^6+y^8) - h^4(x^4-6x^2y^2+y^4) + 20h^8$$

This polynomial is harmonic, it is equal to $20h^8$ at the origin, and it is equal to zero at the other 26 stencil points. Application of any difference operator which approximates the Laplacian gives, therefore, $20h^6$ for p_8 and any linear combination of values of f and its derivatives on the right side of the difference equations is zero. The polynomial p_8 was used by Birkhoff and Gulati [1974] in the proof of the similar result for approximation of the Poisson equation in two variables with nine-point stencils.

In the special case that f and the boundary conditions do not depend on z, then the $O(h^6)$ difference approximation reduces to a nine-point scheme on the plane. In stencil form, the operators L_h and I_h are given by

$$6h^2 L_h U = \begin{bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{bmatrix} U \qquad 360 I_h f = \begin{bmatrix} 1 & & 4 & & 1 \\ & 48 & & 48 & \\ 4 & & 148 & & 4 \\ & 48 & & 48 & \\ 1 & & 4 & & 1 \end{bmatrix} f$$

The HODIE approximation $L_h U = I_h f$ gives $O(h^6)$ accuracy for the two-dimensional generalization of the Poisson equation to $-div(p\ grad[u]) + q\ u = f$, see Lynch and Rice [1977]; we expect that $O(h^6)$ approximation for the three-dimensional problem is also possible.

2. Experimental results. Solution of a finite difference approximation (or any other kind of approximation) of an elliptic partial differential equation in three independent variables can be quite costly with current computers and computer costs. A problem with domain a cube and N subintervals in each coordinate direction has N^3 unknowns. The coefficient-matrix, with the usual ordering of unknowns, is a banded N^3-by-N^3 matrix with band-width N^2; Gauss elimination requires order $N^7/3$ arithmetic operations but there are more efficient elimination methods.

The Poisson equation on a cube is separable and tensor product methods can be used; see, for example, Lynch, Rice, and Thomas [1964a, 1964b]. This reduces the number of operations to order N^4. Even more savings is realized with Fast Fourier Transform techniques which require order $N^3 \log_2 N$ operations, see Hockney [1970]. The tensor product method is very easy to program an applicable to all values of N and since we were interested in N between 2 and 10 for which Fast Fourier Transforms are only about 2 to 3 times faster, we chose to use tensor product methods for our experiments.

Results are given in Table 1 and are displayed graphically in Figure 1. The right side of the Poisson equation was chosen so that its solution was $x(x-1)y(y-1)z(z-1)\exp(x+y+z)$. The experiments were performed on Purdue University's CDC 6500 computer which uses a floating point number with about 15 decimal digits of significance. For comparison, the solution of 50 linear algebraic equations with Gauss elimination by Crout reduction and one iterative refinement takes about 1.75 seconds.

Table 1

Experimental results from tensor product solutions of $O(h^6)$ finite difference approximation for the Poisson equation in three variables on a unit cube. Solution chosen as $x(x-1)y(y-1)z(z-1)\exp(x+y+z)$. $\Delta x = \Delta y = \Delta z = 1/N$. 4.36(-4) denotes 4.36×10^{-4}.

N	$(N-1)^3$	maximum error	time (seconds)
2	1	4.36(-4)	0.018
3	8	5.54(-5)	0.053
4	27	9.92(-6)	0.126
5	64	2.34(-6)	0.272
6	125	8.28(-7)	0.526
7	216	3.37(-7)	0.947
8	343	1.49(-7)	1.582
9	521	7.24(-8)	2.499
10	729	3.94(-8)	3.756

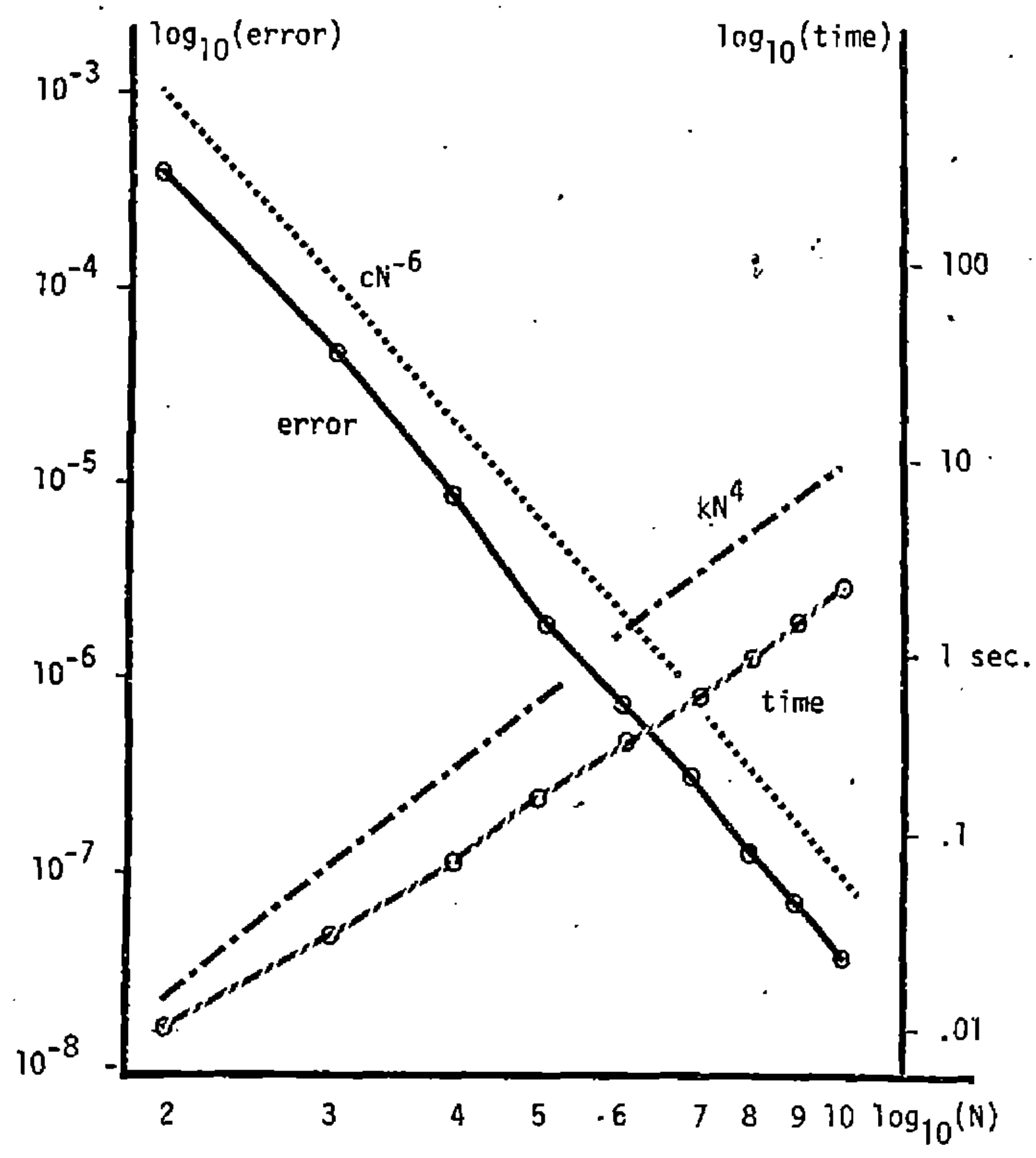

Figure 1. Experimental results for $u_{xx}+u_{yy}+u_{zz}=f$ on unit cube and zero Dirichlet boundary conditions with f chosen so $u = x(x-1)y(y-1)z(z-1)\exp(x+y+z)$. Graphs of logarithms of $|\max \text{error}|$, execution time, cN^{-6}, and kN^4 versus logarithm of N are shown for equal spaced mesh: $\Delta x = \Delta y = \Delta z = 1/N$.

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