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Abstract. Let $u_{j,k,\ell} = u(jh,kh,\ell h)$ denote values of a function on a cubic lattice. Let $\sum_{r^2} u_{j,k,\ell}$ denote the sum of values of u at lattice points a distance r from $(jh,kh,\ell h)$. Let

$$L_h u_{j,k,\ell} = \{-128u_{j,k,\ell} + 14 \sum_{r^2=h^2} u_{j,k,\ell} + 3 \sum_{r^2=2h^2} u_{j,k,\ell} + \sum_{r^2=3h^2} u_{j,k,\ell}\}/(30h^2)$$

$$F_h f_{j,k,\ell} = \{ 280f_{j,k,\ell} + 8 \sum_{r^2=h^2} f_{j,k,\ell} +48 \sum_{r^2=3h^2/4} u_{j,k,\ell} + \sum_{r^2=3h^2} f_{j,k,\ell}\}/720$$

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

where I denotes the identity, $\nabla^2 = X^2 + Y^2 + Z^2$ denotes the Laplacian, and $X = \partial/\partial x$, $Y = \partial/\partial y$, $Z = \partial/\partial z$.

We show that if u has continuous eighth derivatives and $f = \nabla^2 u$, then $L_h u_{j,k,\ell} = M_h \nabla^2 u_{j,k,\ell} + O(h^6) = M_h f_{j,k,\ell} + O(h^6) = F_h f_{j,k,\ell} + O(h^6)$. Solutions of $L_h U_{j,k,\ell} = M_h f_{j,k,\ell}$ or

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$L_h U_{j,k,\ell} = F_h f_{j,k,\ell}$, subject to Dirichlet boundary conditions yield $O(h^6)$ estimates of u at lattice points. If the region is a cartesian product of three intervals, then tensor product or Fast Fourier Transform techniques can be used to solve the discrete problem. Experimental results are given which confirm the $O(h^6)$ behavior of the discretization error.

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

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1. $O(h^6)$ discretization to solutions of the Poisson equation in terms of f and its derivatives. Consider the Poisson equation:

$$\nabla^2 u \equiv \partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \partial^2 u/\partial z^2 = f$$

With $X = \partial/\partial x$, $Y = \partial/\partial y$, $Z = \partial/\partial z$, the Laplacian can be written as

$$\nabla^2 = X^2 + Y^2 + Z^2$$

Taylor's series representations of an anlytic function can be written as

$$u(x+h,y,z) = u(x,y,z) + h\,Xu(x,y,z) + (h^2/2)\,X^2u(x,y,z) + \ldots$$

$$= e^{hX}u(x,y,z)$$

$$u(x+h,y+h,z) = e^{h(X+Y)}u(x,y,z)$$

$$u(x+h,y+h,z+h) = e^{h(X+Y+Z)}u(x,y,z)$$

and so on. Divided central differences can then be represented conveniently, for example

$$\delta_x^2\, u(x,y,z) = [u(x-h,y,z) - 2u(x,y,z) + u(x+h,y,z)]/h^2$$

$$= [X^2 + (h^2/12)\,X^4 + (h^4/360)\,X^6\,]\,u(x,y,z) + O(h^6)$$

* This report records a derivation of a specific difference approximation. It is not intended for publication and is, therefore, not in polished form. The derivation is elementary and once the approximation is available, it can easily be verified directly.

and, similarly,

$$\delta_y^2 = Y^2 + (h^2/12)\ Y^4 + (h^4/360)\ Y^6 + O(h^6)$$

$$\delta_z^2 = Z^2 + (h^2/12)\ Z^4 + (h^4/360)\ Z^6 + O(h^6)$$

$$\delta_x^2\delta_y^2 = X^2Y^2 + (h^2/12)[X^4Y^2 + X^2Y^4] + O(h^4)$$

$$\delta_x^2\delta_y^2\delta_z^2 = X^2Y^2Z^2 + O(h^2)$$

and so on.

We use the operators A_h,B_h, and C_h defined by

$$A_h \equiv \delta_x^2 + \delta_y^2 + \delta_z^2 = (X^2 + Y^2 + Z^2) + (h^2/12)[X^4 + Y^4 + Z^4] + \ldots$$

$$= \nabla^2 + (h^2/12)[\nabla^4 - 2(X^2Y^2+\ldots)]$$

$$+ (h^4/360)[\nabla^6 - 3(X^4Y^2+X^2Y^4+Y^4Z^2+Y^2Z^4+Z^4X^2+Z^2Y^4) - 6\ X^2Y^2Z^2]$$

$$+ O(h^6)$$

$$= \nabla^2 + (h^2/12)[\nabla^4 - 2(X^2Y^2+\ldots)]$$

$$+ (h^4/360)[\nabla^6 - 3(X^2Y^2+\ldots)\nabla^2 - 3\ X^2Y^2Z^2] + O(h^6)$$

$$B_h = \delta_x^2\delta_y^2 + \delta_y^2\delta_z^2 + \delta_z^2\delta_x^2 = (X^2Y^2+\ldots)$$
$$+(h^2/12)[(X^2Y^2+\ldots)\nabla^2 - 3X^2Y^2Z^2] + O(h^4)$$

$$C_h = \delta_x^2\delta_y^2\delta_z^2 = X^2Y^2Z^2 + O(h^2)$$

where here and below we use the abbreviation

$$(X^2Y^2+\ldots) = (X^2Y^2 + Y^2Z^2 + Z^2X^2)$$

We define operators M_h and L_h in terms of A_h, B_h, C_h as

(1-1a) $$M_h = I + (h^2/12)\nabla^2 + (h^4/360)[\nabla^4 + 2(X^2Y^2 + \ldots)]$$

(1-1b) $$L_h = A_h + (h^2/6)\, B_h + (h^4/30)\, C_h = M_h\nabla^2 + O(h^6)$$

where I denotes the identity operator.

To express the operator L_h in terms of coefficients of a stencil, let $\sum_{r^2} u_{j,k,\ell}$ denote the sum of values of u at lattice points a distance r from $(jh, kh, \ell h)$. Then we have

$$A_h u_{j,k,\ell} = [-6u_{j,k,\ell} + \sum_{r^2=h^2} u_{j,k,\ell}]/h^2$$

$$D_h u_{j,k,\ell} = [-12u_{j,k,\ell} + \sum_{r^2=2h^2} u_{j,k,\ell}]/h^2$$

$$= [4\, A_h + h^2\, B_h]\, u_{j,k,\ell}$$

$$= \{4\nabla^2 + (h^2/12)[4\nabla^4 + 4(X^2Y^2 + \ldots)] + \ldots\}\, u_{j,k,}$$

$$E_h u_{j,k,\ell} = [-8u_{j,k,\ell} + \sum_{r^2=3h^2} u_{j,k,\ell}]/h^2 = [4A_h + 2h^2B_h + h^4C_h]u_{j,k,\ell}$$

$$= \{4\nabla^2 + (h^2/12)[4\nabla^4 + 16(X^2Y^2 + \ldots)] + \ldots\}\, u_{j,k,\ell}$$

$$L_h u_{j,k,\ell} = [24\, A_h + 8\, B_h + C_h]\, u_{j,k,\ell}$$

(1-2) $$= [-128\, u_{j,k,\ell} + 14 \sum_{r^2=h^2} u_{j,k,\ell} + 3 \sum_{r^2=2h^2} u_{j,k,\ell} + \sum_{r^2=3h^2} u_{j,k,\ell}]/(30h^2)$$

THEOREM 1: Let R denote a connected domain made up of the union of cubes, each of which has volume h_0^3, with disjoint interiors and edges parallel to coordinate axes. Let ∂R denote the boundary of R

Let one of the vertices of a cube be the origin. For an integer $N \geq 2$, let $h = h_0/N$ and let $(jh,kh,\ell h)$, with j,k,ℓ integers, denote points of a cubic lattice with contains the vertices of the cubes as a sublattice. Let R_h denote the set of lattice points in R and ∂R_h the set of lattice points in ∂R. Let u denote a function with continuous eighth derivatives and let f and g denote functions

$$f = \nabla^2 u,\ (x,y,z) \in R, \quad \text{and} \quad g = u,\ (x,y,z) \in \partial R$$

Let $U^{(h)}$ denote the solution of

$$\text{(1-3a)} \qquad L_h\, U^{(h)}_{j,k,\ell} = M_h\, f_{j,k,\ell}, \quad (jh,kh,\ell h) \in R_h$$

$$\text{(1-3b)} \qquad U^{(h)}_{j,k,\ell} = g_{j,k,\ell}, \quad (jh,kh,\ell h) \in \partial R_h$$

There exists a constant K which depends on u but not on h or $(jh,kh,\ell h)$ such that

$$\text{(1-4)} \qquad |u_{j,k,\ell} - U^{(h)}_{j,k,\ell}| \leq K\, h^6, \quad (jh,kh,\ h) \in R_h$$

Furthermore, no other coefficients in (1-1b) or (1-2) can give a higher order of accuracy.

Proof: The error, $e = u - U^{(h)}$ satisfies (1-3a) with right side replaced with $O(h^6)$ and zero boundary conditions (1-3b). For functions which are zero at the boundary, the operator L_h is of monotone type ($L_h v \leq 0$ implies $v \geq 0$), and L_h applied to $(Kh^6/6)[x^2 + y^2 + z^2 - r^2]$ yields Kh^6. Hence, for sufficiently large r and K, this function bounds the error. Hence (1-4) follows.

The last statement of the Theorem follows from the polynomial displayed in the proof of Theorem 11 in Birkhoff and Gulati [1974]. This polynomial is an eighth degree harmonic polynomial in two independent variable which is $O(h^8)$ on the nine points $(0,0)$, $(\pm h,0)$, $(0,\pm h)$, $(\pm h,\pm h)$. Application of L_h to this polynomial gives, therefore, $O(h^6)$, whereas the right side of (1-3a) is zero.

The coefficients in (1-2) are given by Mikeladze [1937]. He also displays the terms through $O(h^2)$ in the M_h. He did not realize, apparently, that (1-3a) yields $O(h^6)$ accuracy, for he only proved $O(h^4)$.

2. $O(h^6)$ <u>discretization error for solutions in terms of values of</u> f. Rather than evaluate derivatives of f to obtain values of the right side of (1-3a), we construct $O(h^6)$ difference approximation to the operator M_h.

One cannot obtain an $O(h^6)$ approximation by using only the 27 lattice points used for the operator L_h. This is because one obtains ∇^2 and ∇^4 only from A_h; they do not appear in B_h or C_h. In A_h, these have coefficients 1 and $h^2/12$, respectively, with ratio $12/h^2$, whereas the coefficients of these in M_h are $h^2/12$ and $h^4/360$ with ratio $30/h^2$.

There are a number of disadvantages of using values of f at other lattice points in addition to the 27 used in the operator L_h. These include the following: A linear combination of $A_h, B_h, C_h, A_{2h}, B_{2h}, C_{2h}$ which gives an $O(h^6)$ approximation to the derivative terms in M_h leads to negative coefficients of some of the values of f; there is a close relationship between the solution of (1-3) in terms of values of f and quadrature and it is customary in quadrature formulas to use positive coefficients to reduce round-off error. [The connection is: elements of the inverse of the matrix associocated with the system of difference equations has elements which approximate the Green's function of the Poisson equation problem, the product of the inverse and the vector of right-side-values of the difference equation gives components which approximate the integral of the Green's function and the right side of the Poisson equation.] For lattice points adjacent to the boundary values of f must be evaluated outside the region. The coefficient in the error term is larger than if values of f are taken in and on the cube of volume $8h^3$ centered at an interior lattice point.

Thus, we use additional values of f in a cube of volume $8h^3$. There are a number of choices. We choose to use the operators A_h, D_h, E_h defined in Section 2 and also $E_{h/2}$:

$$E_{h/2} = 4\nabla^2 + (h^2/12)[\nabla^4 + 4(X^2Y^2 + \dots)] + O(h^4)$$

$$E_{h/2}\, f_{j,k,\ell} = 4[-8\, f_{j,k,\ell} + \textstyle\sum_{r^2=3h^2/4} f_{j,k,\ell}]/h^2$$

This requires evaluation of f at the eight half-lattice points: $(jh \pm h/2, kh \pm h/2, \ell h \pm h/2)$. Thus, f is evaluated at points of a body-centered cubic lattice and there is on the average two evaluations of f for each lattice point.

One obtains $O(h^6)$ approximation to M_h by using F_h defined by

$$F_h = I + (h^2/90)A_h + (h^2/60)E_{h/2} + (h^2/720)E_h$$

so that

$$\begin{aligned} F_h f_{j,k,\ell} &= [280 f_{j,k,\ell} + 8 \textstyle\sum_{r^2=h^2} f_{j,k,\ell} + 48 \sum_{r^2=3h^2/4} f_{j,k,\ell} \\ &\qquad + \textstyle\sum_{r^2=3h^2} f_{j,k,\ell}]/720 \\ &= M_h f_{j,k,} + O(h^6) \end{aligned}$$

By changing the coefficients, one can include a term proportional to D_h in the approximation, but this increases the amount of calculation required to evaluate F_h applied to f.

Except for reference to specific equations, the proof of Theorem 1 is the same as the proof of the following.

THEOREM 2: The results stated in Theorem 1 hold when (1-3a) is replaced with

(2-1) $$L_h U^{(h)}_{j,k,\ell} = F_h f_{j,k,\ell}, \quad (jh,kh,\ell h) \in R_h$$

For the case that $\partial u/\partial z \equiv 0$, the difference equation reduces to a two variable equation. The stencil for L_h is

(2-2) $$1/(6h^2)\begin{bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{bmatrix}$$

and the stencil at half-lattice points for F_h is

$$(1/360)\begin{bmatrix} 1 & 0 & 4 & 0 & 1 \\ 0 & 48 & 0 & 48 & 0 \\ 4 & 0 & 148 & 0 & 4 \\ 0 & 48 & 0 & 48 & 0 \\ 1 & 0 & 4 & 0 & 1 \end{bmatrix}$$

Milne, p. 136 [1953] and others give expressions for the stencil in (2-2) in terms of derivatives. Milne is the only source we know of which displays the term proportional to h^6. Using the result in Milne, we have

$$L_h u = \nabla^2 u + (h^2/12)\nabla^4 u + (h^4/360)[\nabla^6 u + 2X^2Y^2\nabla^2 u] + (h^6/8!)[12\nabla^8 u + 64X^2Y^2\nabla^4 u + 80X^4Y^4 u] + O(h^8)$$

from which it is clear that the stencil in (2-2) cannot yield $O(h^8)$ approximation to solutions of the Poisson equation in two variable, but can obtain $O(h^6)$ approximation.

If $\partial u/\partial y \equiv 0$, $\partial u/\partial z \equiv 0$, then (2-1) reduces to

$$[U_{j-1} - 2U_j + U_{j+1})/h^2 = [f_{j-1} + 16f_{j-1/2} + 26f_j + 16f_{j+1/2} + f_{j+1}]/60 \quad (2\text{-}3)$$

In contrast to multi-dimensional problems involving elliptic second order partial differential equations in n independent variables, an approximation with finite difference operators made up of the cartesian product of n set of three points of a lattice along the coordinate directions, such as L_h, there is no limit to the order of accuracy of approximation of second order ordinary differential operators. See Lynch and Rice [1976,1977].

Rosser [1976] has given an $O(h^6)$ scheme for the Poisson equation on a two dimensional region with f evaluated only at mesh points in the region; some of their coefficients are negative.

4. Evaluation by tensor product methods. If the domain R is the cartesian product of three intervals of lengths $N_x h$, $N_y h$, $N_z h$ with N_x, N_y, N_z integers, then tensor product methods--which are equivalent to separation of variables--yield very efficient computational schemes for solving either (1-3a) or (2-1) subject to Dirichlet conditions in (2-3b) as well as a variety of other standard boundary conditions. The use of tensor products for solving difference equations is discussed by a number of authors, see for example, Lynch, Rice and Thomas [1964a,1964b,1965]. Application to the difference approximation to the Poisson equation in three variables on a mesh with $N_x = N_y = N_z = N$ requires order N^4 operations. Since the discretization error is decreasing as N^{-6}, asymptotically, the error is halved with a 59% increase in work. Use of Fast Fourier Transforms reduces the work from order N^4 to order $N^3 \log_2 N$; for $N = 2,4,8,16$, this gives a savings of factors of order 2, 2, 2.6, 4, respectively. For such techniques, see Hockney 1970.

Figure 1 shows experimental results for the Poisson equation subject to zero boundary conditions on the unit cube. The function f was chosen so that the solution is

$$u(x,y,z) = x(x-1)y(y-1)z(z-1)\exp(x+y+z)$$

The maximum error is plotted versus N and so is the solution time as well as K/N^6 and CN^4 for some constants K and C. The calculation was done on Purdue University's CDC 6500 computer which uses floating point numbers accurate to about 1 part in 10^{15}. For information which can be used to convert these times to other computers, we note that the solution time required for the solution of

50 linear algebraic equations with Gauss elimination, Crout reduction and one step of iterative refinement of the solution takes about 1.75 seconds.

Values used to plot the graphs in Figure 1 are given in Table 1.

Table 1

Values of N, number of unknowns, maximum error, and solution time for solving

$$u_{xx} + u_{yy} + u_{zz} = f, \quad u = 0 \text{ on unit cube}$$

with u taken as $x(x-1)y(y-1)z(z-1)\exp(x+y+z)$ and tensor product methods.

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

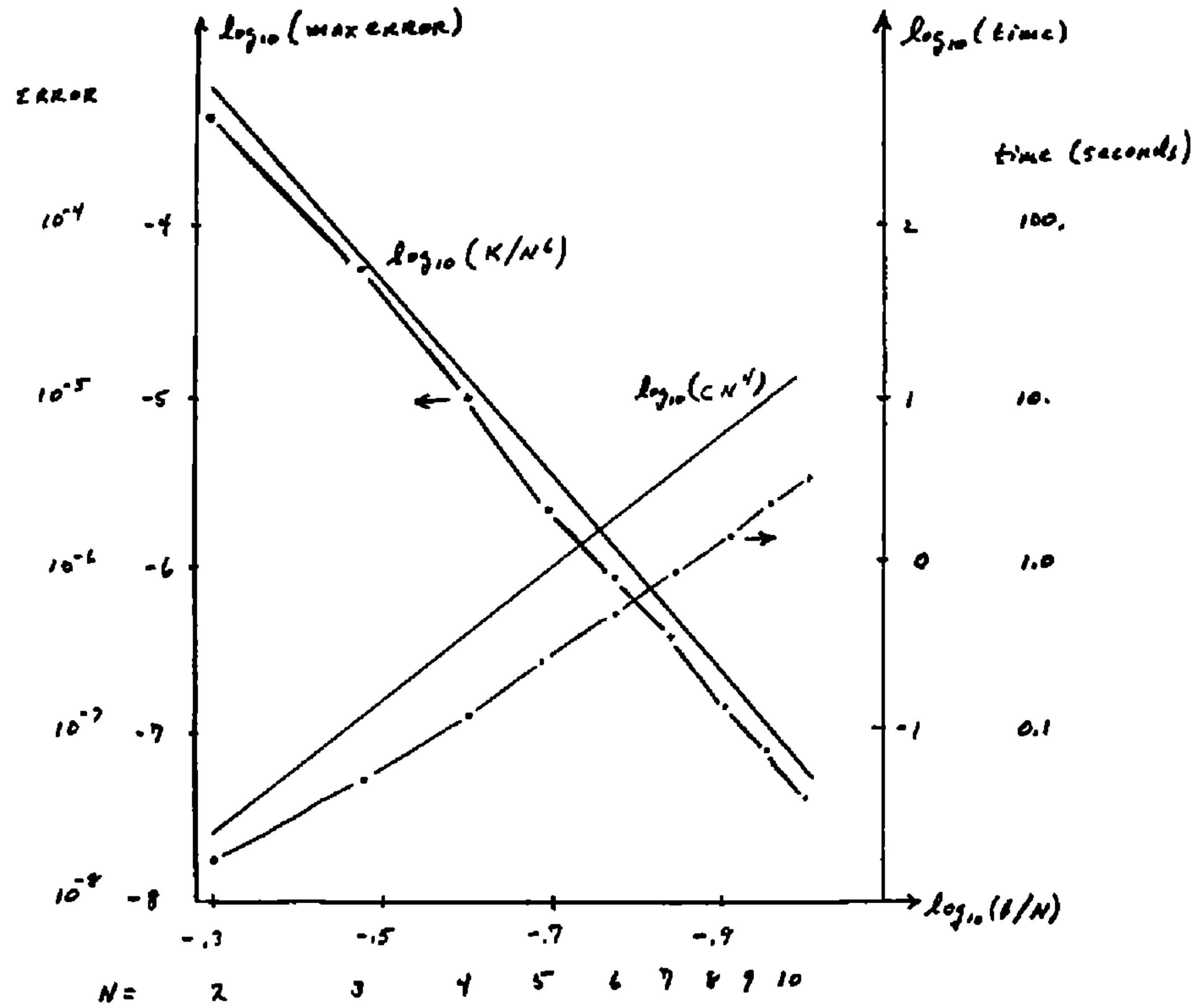

Figure 1. Experimental results for $u_{xx} + u_{yy} + u_{zz} = f$ and $u = 0$ on the surface of a unit cube. f chosen so that $u(x,y,z) = x(x-1)\,y(y-1)\,z(z-1)\exp(x+y+z)$. $\Delta x = \Delta y = \Delta z = 1/N$

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