A Multidimensional Compact Higher-Order Scheme for 3-D Poisson's Equation

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A multidimensional compact finite-difference scheme is applied to the solution of a threedimensional Poisson's equation. Excellent precision is obtained by means of a moderate discretization net. The presence of Neumann boundary conditions calls for special attention because these normal conditions affect the global precision. The numerical results for a test case involving five Neumann conditions and one Dirichlet condition on the six faces of a unit cube show good agreement with the analytical solution.

1. INTRODUCTION

We are interested in solving Poisson's equation

$$p_{xx} + p_{yy} + p_{zz} = q \tag{1}$$

in a three-dimensional parallelepiped R where the function p is known on a portion ∂R_1 of the boundary (Dirichlet conditions) and its normal derivative on the remaining portion ∂R_2 (Neumann conditions) $[\partial R_1 \cup \partial R_2 = \partial R$ is the total boundary of the domain R]. The computational solution of such an equation must approach the exact solution within a given precision, in minimum computer time, and with a limited computer memory. For a fixed order of precision, the use of high-order finite-difference methods improves the latter two efficiency criteria.

The precision of a finite-difference method rests essentially on the accuracy of the basic function derivatives. Consider the discretized form of the Poisson's equation at a point P. The second derivative in a direction may be classically evaluated at P as a linear combination of the basic function values in the proximity of P. The precision is improved when the linear combination includes more terms. The hermitian compact method used here is based on another principle: the equation must be satisfied simultaneously at many points and the derivative known at these different points. The discrete relation between the basic function and its derivative may therefore include the value of the derivative at more than one point and the result is a gain in precision. We take optimal advantage of this fact in the three spatial directions, while considering only three consecutive points in each direction.

One-dimensional higher-order finite-difference expressions between a function and its derivatives are well known (Collatz [1]). The application of these hermitian compact relations in solving partial differential equations in fluid dynamics is more recent (Orszag and Israëli [2]). Many test problems have been given (Hirsh [3]; Adam [4]) that show the advantage of this procedure. These latter papers show a gain in precision over the classical second-order methods.

The numerical solution of the three-dimensional Poisson's equation has already been studied. Wilhelmson and Ericksen [5] analyse the extension of many twodimensional second-order direct methods based on cyclic reduction and the Fourier transform. Shaanan and Ferziger [6] reduce the three-dimensional equation to two dimensions by a Fourier transform along the third direction, and then apply finite differences by compact relations in the two remaining dimensions. An interesting feature of our method is the excellent precision obtained by using three-dimensional compact relations between the known values q of the right-hand side of Eq. (1) and the unknown values of function p. A special treatment of the Neumann boundary conditions has also been investigated and has improved the previous handling of this condition, as it was proposed in [6]. This study is in fact a particular case of a more general problem in incompressible fluid dynamics and enables us to solve a pressure equation characterized by Neumann conditions on five of the six faces of a parallelepipedic domain.

2. BASIC ONE-DIMENSIONAL COMPACT RELATIONS

The one-dimensional compact relations are derived by setting to zero certain expressions of the form

$$E \equiv \sum_{r=-k}^{r=+k} (a_r p_{l+r} + b_r p'_{l+r} + c_r p''_{l+r}),$$

where p_{i+r} , p'_{i+r} , and p''_{i+r} are respectively the variable and its first and second derivatives at the discretization points near point P_i . As a first basic choice, the value of k is 1 in order to give the expression a tridiagonal structure. According to the desired relation, some parameters a_r , b_r , or c_r (r = -1, 0, 1) may be set to zero as a second option. Thereafter the remaining parameters are optimized to cancel E as well as possible. This is accomplished by expanding p_{i+r} , p'_{i+r} , p''_{i+r} , as Taylor series centered around P_i and by setting the coefficients of powers of the spatial step h equal to zero to as high a power of h as possible (Collatz [1]).

At an interior point P_i , the following relation is obtained when the b_r are set to zero:

$$p_{i-1} - 2p_i + p_{i+1} = \frac{h^2}{12} \left(p_{i-1}'' + 10p_i'' + p_{i+1}'' \right) + \theta \left[-\frac{h^6}{240} p_i^{(6)} \right].$$
(2)

For points P_0 and P_m on boundaries with a Neumann condition, the tridiagonal structure of the system is maintained with the following two-point relations $(a_{-1}, b_{-1}, c_{-1}, b_1 = 0 \text{ or } a_1, b_1, c_1, b_{-1} = 0)$:

$$p_{1} - p_{0} = \frac{h^{2}}{6} \left(p_{1}'' + 2p_{0}'' \right) + hp_{0}' + \theta \left[-\frac{h^{4}}{24} p_{0}^{(4)} \right],$$
$$p_{m-1} - p_{m} = \frac{h^{2}}{6} \left(p_{m-1}'' + 2p_{m}'' \right) - hp_{m}' + \theta \left[-\frac{h^{4}}{24} p_{m}^{(4)} \right].$$

The decrease in precision of these boundary relations justifies a mesh refinement near to the boundaries with Neumann conditions. Suppose that the spatial step between the boundary node and the nearest node in the normal direction is half the spatial step h inside the domain.

In case of Dirichlet and Neumann conditions, the sequence of mesh points is therefore: P_0 , P_1 ,..., P_l , $P_{l+1/2}$. (On a unit length, h = 2/(2l+1).) For two Neumann conditions, the mesh points are P_0 , $P_{1/2}$, $P_{3/2}$,..., $P_{m-1/2}$, P_m . (h = 1/m.)

The expressions at the boundary node P_0 and the first interior node $P_{1/2}$ become

$$p_{1/2} - p_0 = \frac{h^2}{24} \left(p_{1/2}'' + 2p_0'' \right) + \frac{h}{2} p_0' + \theta \left[-\frac{h^4}{384} p_0^{(4)} \right],$$
(3a)

$$2p_0 - 3p_{1/2} + p_{3/2} = \frac{h^2}{48} \left(-2p_0'' + 33p_{1/2}'' + 5p_{3/2}'' \right) + \theta \left[-\frac{h^5}{96} p_{1/2}^{(5)} \right], \qquad (4a)$$

and, correspondingly, at P_m and $P_{m-1/2}$,

$$p_{m-1/2} - p_m = \frac{h^2}{24} \left(p_{m-1/2}'' + 2p_m'' \right) - \frac{h}{2} p_m' + \theta \left[-\frac{h^4}{384} p_m^{(4)} \right], \tag{3b}$$

$$2p_{m} - 3p_{m-1/2} + p_{m-3/2} = \frac{h^{2}}{48} \left(-2p_{m}'' + 33p_{m-1/2}'' + 5p_{m-3/2}''\right) + \theta \left[+ \frac{h^{5}}{96} p_{m-1/2}^{(5)} \right].$$
(4b)

The boundary mesh refinement provides a division by 16 of the truncation error in the relations centered at P_0 and P_m . It represents a gain of one order of magnitude and brings the precision at the boundary nearer to that inside the domain.

The use of a higher-order boundary condition instead of the mesh refinement technique does not prove interesting. There exists no sixth-order relationship of the form

$$ap_0 + bp_1 + cp_2 = dp_0'' + ep_1'' + fp_2'' + gp_0' + \theta[h^6 p_0^{(6)}],$$

where g does not vanish.

The restriction $g \neq 0$ reduces the order to h^5 . By cancelling the coefficient of $p_2''(f=0)$, one finds

$$p_2 - p_0 = \frac{2}{3} h^2 (p_0'' + 2p_1'') + 2hp_0' + \theta \left[\frac{2h^5}{45} p_0^{(5)}\right].$$

This equation makes use of information at the second interior point which might be "far" from the boundary, while p_1 does not appear.

3. PRINCIPLE OF THE MULTIDIMENSIONAL COMPACT METHOD

Let us consider as an example the two-dimensional operator

$$M(p) = p_{xx} + p_{yy}$$

and the associated Poisson's equation

$$M(p) = q.$$

Consider a set of 3×3 discretization nodes centered at point (i_0, j_0) . On rows $j_0 - 1, j_0, j_0 + 1$, relations of type (2) may be written between p_{xx} and p. On columns $i_0 - 1, i_0, i_0 + 1$, relations of type (2) may also be expressed between p_{yy} and p. By addition of these six relations with a multiplicator 10 for row j_0 and column i_0 , one obtains in each node of the nine-point set the expression $p_{xx} + p_{yy}$, i.e., the operator M(p). The resulting compact relation is depicted in Fig. 1; on the left-hand side, a

$$M(p) \neq P_{xx} + P_{yy}$$

$$\begin{pmatrix} c^{4} & c^{3} & c^{4} \\ * & * & * \\ & & \\ c^{2} & c^{1} & c^{2} \\ * & * & * \\ c^{4} & c^{3} & c^{4} \\ * & * & * \end{pmatrix} \qquad p = \begin{pmatrix} 1 & 10 & 1 \\ * & * & * \\ 10 & 100 & 10 \\ * & * & * \\ 1 & 10 & 1 \\ * & * & * \end{pmatrix} M(p)$$

 $X = 1/h_{\chi}^2$, $Y = 1/h_{\chi}^2$

c1 = -240 (X + Y) c2 = 120X - 24Y FIG. 1. General two-dimensional compact relation. linear combination of the $M(p) \equiv q$ known values at the nine nodes appears, and on the right-hand side a linear combination of the unknown values of p at the same nine points appears.

An analogous operation may be carried out on an 27-node set for the threedimensional operator

$$N(p) = p_{xx} + p_{yy} + p_{zz}$$

and the associated Poisson's equation

$$N(p) = q$$

Figure 2 presents the compact relation obtained with relations of type (2) in the three spatial directions.

Let us retain the general form of the one-dimensional compact discrete expressions (2)-(4):

$$a_i^{-}[S(p)]_{i-1} + a_i^{0}[S(p)]_i + a_i^{+}[S(p)]_{i+1} = b_i^{-}p_{i-1} + b_i^{0}p_i + b_i^{+}p_{i+1} + c_i^{0},$$

N(P) # P_{XX} + P_{yy} + P_{zz}

$X = 1/h_X^2$, $Y = 1/h_y^2$, $Z = 1/h_z^2$

c1 = -2400 (X + Y + Z)c5 = -24Z + 120 (X + Y)c2 = 1200X - 240 (Y + Z)c6 = -24X + 120 (Y + Z)c3 = 1200Y - 240 (X + Z)c7 = -24Y + 120 (X + Z)c4 = 1200Z - 240 (X + Y)c8 = 12 (X + Y + Z)

FIG. 2. General three-dimensional compact relation.

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where index *i* is relative to the chosen direction and S(p) is the second derivative of *p* in this direction. By linear combination of such expressions written in the three spatial directions, we obtain a set of multidimensional compact relations as in Fig. 2.

An interesting feature of the compact relations between the unknown p and the multidimensional operator M(p) or N(p) is that the operator values are known everywhere in the domain and on its boundary $[M(p) \equiv q]$, and that we do not have to separately evaluate the second derivatives p_{xx} , p_{yy} , and p_{zz} whose boundary values are not known precisely.

Let us finally note that these multidimensional compact relations are of the highest order of precision on the set of fixed nodes.

4. SOLUTION OF THE NUMERICAL SYSTEM

At each point of the discretization net of the parallelepiped where Poisson's equation (1) is to be solved, one can write an implicit compact relation between the unknown values of p and the right-hand side values of q. When assembled, these relations form a tridiagonal system exhibiting tridiagonal blocks of tridiagonal blocks.

First of all, let us observe the system organization due to the structure of the onedimensional relations (2)-(4). Figure 1 shows a bidimensional combination between relations of type (2). One observes a symmetry in both directions x and y, resulting from that of relation (2). On the other hand, Fig. 3 presents a combination between relation (2) in the x-direction and relation (4) in the y-direction. The symmetry still exists along x, but disappears along y.

The global system includes the multidimensional compact relations centered at each node. The boundary conditions influence the block structure and determine the appearance of symmetry in these blocks. The numerical algorithm for solving the global system depends on this structure.

If two Dirichlet boundary conditions appear in one direction, only relations of type (2) are used in that direction and the presence of symmetric tridiagonal blocks is observed in the global system matrix. Otherwise, relations of type (3) and (4) are used with Neumann boundary condition and an asymmetry results in the tridiagonal blocks.

When Neumann boundary conditions occur in at most one direction, a direct method may be considered to solve the global system. This is based on the diagonalization of symmetric tridiagonal blocks for which the eigenvalues and eigenvectors can be easily evaluated. The method is described for a two-dimensional problem by Shaanan and Ferziger [6]. If the index relative to the only direction where the Neumann boundary conditions occur, varies faster than the other two indices, the matrix of the system has a symmetric block tridiagonal structure exhibiting symmetric tridiagonal blocks of tridiagonal blocks.

The diagonalization procedure works in two steps. In the first one, the global system of $L \times M \times N$ equations is reduced to N symmetric block tridiagonal systems



of tridiagonal blocks of $L \times M$ equations. The second step reduces each of the N systems to M tridiagonal systems of L equations. These two successive diagonalizations apply the algorithm described in [6].

Here we consider the solution of Poisson's equation with Neumann conditions imposed on five on the six faces of a parallelepiped. The previous direct method cannot be used so it was decided to resort to a successive overrelaxation method (SOR). As the structure of the system is tridiagonal, a single line SOR method improves the rate of convergence: when the relaxation factor is 1 (Gauss-Seidel), the convergence rate is twice that of the corresponding SOR method by points (Ames [7]). Let us note that an iterative method may prove competitive in practice with a direct method. It depends on the number of iterations needed to achieve the required accuracy.

5. PRECISION AND TESTS

A one-dimensional precision analysis of the discrete relationships was first worked out. Consider the one-dimensional problem corresponding to the Poisson's equation: knowing the second derivative values p'' at the nodes of a one-dimensional discretization net, we have to compute the function p at the same nodes.

The basic relations (2)-(4) present a truncation error in terms of higher powers of

the spatial step and higher-order derivatives. The set of relations relative to each node may therefore be expressed by a numerical system of the form

$$A\mathbf{x} = \mathbf{y} + \mathbf{\hat{y}},$$

where $\hat{\mathbf{y}}$ is the truncation error vector. Nevertheless, we solve in fact the system

$$A\mathbf{x}' = \mathbf{y}.$$

The solution of this last system is different from the exact solution x. Defining

$$\mathbf{x}' = \mathbf{x} + \mathbf{\hat{x}},$$

the following error system is obtained:

$$A\hat{\mathbf{x}} = -\hat{\mathbf{y}}.$$

From the evaluation of the truncation errors $\hat{\mathbf{y}}$, it is possible to know the error distribution on the solution. The nature of boundary condition (Dirichlet or Neumann) and the presence or the absence of a mesh refinement near the boundary have an influence on both A and $\hat{\mathbf{y}}$. On the other hand, the mesh size value does not appear in the coefficients of the A matrix, but affects only $\hat{\mathbf{y}}$.

With Dirichlet conditions on both boundaries, one uses a relation of type (2) at every node. The matrix A of the system can be inverted and the *r*th component of the error vector $\hat{\mathbf{x}}$ takes the general form

$$\hat{x}_r = (-A^{-1}\hat{\mathbf{y}})_r = \frac{1}{n+1} \left[(n+1-r) \sum_{i=1}^{r-1} i \hat{y}_i + r \sum_{i=r}^n (n+1-i) \hat{y}_i \right],$$

where \hat{y}_i is the *i*th component of \hat{y} and *n* the order of the system. As the matrix -A is of monotone kind [8], one deduces that $\hat{x}_1 \leq \hat{x} \leq \hat{x}_2$ if there exists \hat{x}_1 and \hat{x}_2 with $-A\hat{x}_1 \leq \hat{y} \leq -A\hat{x}_2$. Therefore, if \hat{y}_u is an upper bound of \hat{y} , then the solution \hat{x}_u of the system $-A\hat{x} = \hat{y}_u$ is also an upper bound of the error \hat{x} , component by component. The truncation error in the tridiagonal relation (2) written at a node is proportional to the sixth power of the spatial step *h* and to the sixth derivative $p^{(6)}$ of *p* evaluated at this point. One may consider a vector \hat{y}_u with identical components, each of them equal to $C = (h^6/240) \max_i p_i^{(6)}$. The components of \hat{x}_u are then

$$(\hat{\mathbf{x}}_u)_r = \frac{C}{2}r(n+1-r).$$

The error distribution on the solution \mathbf{x} of the basic system is therefore quadratic along the discretization net. The maximum error occurs at the center of the net and is proportional to the square of the number of steps and to the sixth power of h. It follows that by halving the spatial step h, the maximum error is divided by 16 and the global precision is thus $\theta(h^4)$. A local refinement of the mesh size near a boundary with Dirichlet condition has no favourable effect because the local error at the refinement node goes down from $\theta(h^6)$ to $\theta(h^5)$.

The presence of a Neumann condition at one boundary reduces the global precision. A local error $\theta(h^4)$ in the boundary node relation overcomes the errors $\theta(h^6)$ at the other nodes. The general component of the error vector $\hat{\mathbf{x}}$ is now

$$\hat{x}_r = \sum_{i=1}^{r-1} i \hat{y}_i + r \sum_{i=r}^n \hat{y}_i.$$

The matrix -A is again of monotone kind and for an upper bound \hat{y}_u whose components \hat{y}_i are of the type

$$ah^6$$
, $i = 1,..., n - 1$,
 ch^4 , $i = n$,

the components of $\hat{\mathbf{x}}_{u}$ become

$$(\hat{\mathbf{x}}_u)_r = ah^6[r(r-1)/2 + r(n-r)] + ch^4r.$$

In practice, the second term exceeds the first one, and the distribution of the global error is essentially linear with a maximum value at the Neumann boundary. This value is proportional to the number of discretization nodes and to the fourth power of h. By halving the mesh size, the maximum error is divided by 8 and the global precision is $\theta(h^3)$.

Now, the treatment of a boundary with Neumann condition by a local refinement has a favorable effect. At the boundary node, the local error is evaluated with the step h/2 instead of h so it is smaller by a factor 16. The basic system generates an error vector $\hat{\mathbf{x}}$ whose components are

$$\hat{x}_{r} = \begin{cases} \sum_{i=1}^{r-1} i \cdot \hat{y}_{i} + r \sum_{i=r}^{n-1} \hat{y}_{i} + 2r\hat{y}_{n}, & 1 \leq r \leq n-1 \\ \sum_{i=1}^{n-1} i \cdot \hat{y}_{i} + (2n-1)\hat{y}_{n}, & r = n. \end{cases}$$

The matrix -A is always of monotone kind and an upper bound \hat{y}_u with components \hat{y}_i of the form

$$ah^{6}, \quad i = 1,..., n-2$$

 $bh^{5}, \quad i = n-1,$
 $c(h/2)^{4}, \quad i = n,$

TABLE 1

Two-Dimensional Tests

Test func	tion $p: [0, 1] \times [0, 1] \rightarrow [0, 1]: (x, y)$	$(y) \rightsquigarrow p = \sin(\pi/2)x$	$\cos 2\pi y$
		Mesh size	Maximum error
Second order	Dirichlet on all boundaries	1/32	-3.08 (-3)
Compact method	Dirichlet on all boundaries	1/32	-5.91 (6)
Compact method	Dirichlet on all boundaries	1/16	-9.51 (-5)
Compact method	Dirichlet on all boundaries	1/8	-1.55 (-3)
Second order	Dirichlet along X	1/32	-2.26 (-3)
	Neumann along Y		
Compact method	Dirichlet along X	1/32	-6.58 (-5)
	Neumann along Y		
Compact method	Dirichlet along X	1/16	-4.48 (-4)
	Neumann along Y		
Compact method	Dirichlet along X	1/8	-2.02 (-3)
	Neumann along Y		
Shaanan and Ferziger	Dir.–Neum. along X	1/32	6.03 (-1)
	NeumNeum. along Y		
Compact method	Dir.–Neum. along X	2/63, 1/32	-2.21 (-4)
	NeumNeum. along Y		

gives the following components for $\hat{\mathbf{x}}_{\mu}$:

$$(\hat{\mathbf{x}}_{u})_{r} = \begin{cases} h^{4}r \left[\frac{a}{2} h^{2}(2n-3-r) + bh + \frac{c}{8} \right], & 1 \leq r \leq n-1 \\ h^{4} \left[\frac{a}{2} h^{2}(n-2)(n-1) + bh(n-1) + \frac{c}{16} (2n-1) \right], & r = n. \end{cases}$$

The last term is again predominant. The global error varies linearly and its maximum appears at the Neumann boundary. However this maximum value is of the order of $ch^4n/8$ in lieu of ch^4n without refinement. The global effect of a local refinement (division by 2) of the spatial step near the Neumann boundary is therefore the reduction of the maximum error by a factor 8. This is an important increase of the precision at a low cost.

The comparison of the solution of a two-dimensional Poisson's equation by the present compact method and a classical second-order method shows the difference of precision (Table 1). In our test case, the compact method achieves the same level of precision as a second-order method, but with four times less points in each direction. The algorithm of Sweet [9] is used for the second-order method.

Shaanan and Ferziger treats the 2-D test function of Table 1 with Dirichlet-Neumann conditions in the x-direction and Neumann-Neumann conditions in the y-direction. A first-order treatment of the Neumann conditions is proposed by using an artificial row of exterior points outside the integration domain. The result

ſ	4	
μ	4	
ρ	9	
2	5	

TABLE 2 Three-Dimensional Tests

	Taat Burnation				Errors	
	$p: [0, 1] \times [0, 1] \times [0, 1] \to [0, 1]$	h_x, h_y, h_z	$\omega_{ m optimum}$	ε max.	$(\sum \varepsilon /n)^a$	$(\sum \varepsilon^2/n)^a$
Ξ	64x(1-x) y(1-y) z(1-z)	$\frac{1}{10}, \frac{1}{10}, \frac{2}{15}$	1.7	-1.74(-14)	I	ļ
(2)	$64x(1-x) y(1-y) z^3(1-z^3)$	$\frac{1}{10}, \frac{1}{10}, \frac{2}{15}$	1.7	1.12(3)	7.46(—4)	7.95(4)
(3)	$64x^3(1-x^3)y(1-y)z(1-z)$	$\frac{1}{10}, \frac{1}{10}, \frac{2}{15}$	1.7	2.15(3)	9.85(—4)	1.07(-3)
(4)	$64x^3(1-x^3)y^3(1-y^3)z^3(1-z^3)$	$\frac{1}{10}, \frac{1}{10}, \frac{2}{13}$	1.7	1.82(-3)	8.63(4)	9.31(4)
(5)	$64x^3(1-x^3)y^3(1-y^3)z^3(1-z^3)$	$\frac{1}{20}, \frac{1}{20}, \frac{2}{31}$	1.55	2.41(4)	8.87(5)	9.85(-5)
9	$\sin(\pi/2)x \sin(\pi/2)y (e^z - 1)/(e - 1)$	$\frac{1}{10}, \frac{1}{10}, \frac{2}{15}$	1.7	-1.41(-5)	7.78(6)	8.28(6)

^a n is the number of calculation points.

obtained by this procedure is poor. The error value given in [6] corresponds to the imposition of Dirichlet conditions on all the boundaries.

Different tests are then performed on the multidimensional compact method by solving a three-dimensional Poisson's equation in a unit cube with Neumann conditions on five of the six faces and a Dirichlet condition on the sixth side (z = 1). This set of boundary conditions is particularly unfavourable and represents a severe test of precision. A reduction by two of the spatial step was set up near the Neumann boundaries. Table 2 shows the results. The first test with a product of polynomial functions in x, y, and z of order less than or equal to 3 yields the exact solution. The second test involves a higher-order polynomial in the z-direction, where a Neumann and a Dirichlet boundary conditions are applied, while in test 3, the higher-order polynomial is used in the x-direction with two Neumann conditions. A decrease of the accuracy is noted when there is one Neumann condition more, especially as $h_r = 2/15$ is greater than $h_r = 1/10$ (comparison test 2-test 3). If the mesh size is divided by 2, the error is divided by 7.55, 9.73 or 9.45, according to the error definition (comparison test 4-test 5). Finally the use of higher-order polynomial functions constitutes a severe precision test because of the high values of the higherorder derivatives, which have a direct influence on the error, (comparison test 4-test 6).

6. CONCLUSION

Summarily, the previous tests show:

(i) a global precision of order h^3 with Neumann boundary conditions, the error being proportional to the number of nodes in the normal direction to the boundary and to the local error $\theta(h^4)$;

(ii) a global precision of order h^4 with Dirichlet boundary conditions, the error being proportional to the square of the number of nodes in a direction and to the local error $\theta(h^6)$.

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