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Note

Poisson's Equation, Hexagonal Grids and FFT Methods: Periodic Boundary Conditions

1. Introduction

In a recent article Pickering [1] described a fourth-order method for solving the discrete Poisson equation on a regular hexagonal grid using FFT techniques. The model problem considered in that article assumed Dirichlet boundary conditions and the results obtained were compared with those obtained on a rectangular grid and also with the results derived from other algorithms, notably Christiansen and Hockney [2] and Houstis and Papatheodorou [3]. The configuration of the grid used in [1], in which each hexagon is divided into equilateral triangles of side h, is shown in Fig. 1 and the approximation to Poisson's equation

$$\nabla^2\phi(x, y) = q(x, y), \tag{1}$$

was written in the form

$$\begin{aligned} &-6\phi_{i,j} + \phi_{i,j-2} + \phi_{i,j+2} + \phi_{i+1,j+1} + \phi_{i-1,j+1} + \phi_{i+1,j-1} + \phi_{i-1,j-1} \\ &\quad = Q_{i,j} + O(h^6) \qquad (i = 1, 2, ..., n; j = 1, 2, ..., J+1), \end{aligned} \tag{2}$$

where

$$Q_{i,j} = 3h^2 q_{i,j}/2 + 3h^4\, \nabla^2 q_{i,j}/32,$$

n is odd, and J is even.

The purpose of this note is to demonstrate how the techniques developed in [1] can be extended to deal with the cases where the boundary conditions are periodic in the j direction and where the boundary conditions are periodic in both the i and j directions. The relevant equations are given in Sections 2 and 3. The first of these cases was briefly outlined in [1], whereas the second has not previously been considered. Numerical illustrations are given in Section 4 for both types of boundary conditions.

2. Periodic Conditions in the j Direction

Here we consider solving Poisson's equation over the grid shown in Fig. 1 using the finite-difference relation (2) with periodic conditions in the j direction and Dirichlet conditions in the i direction.

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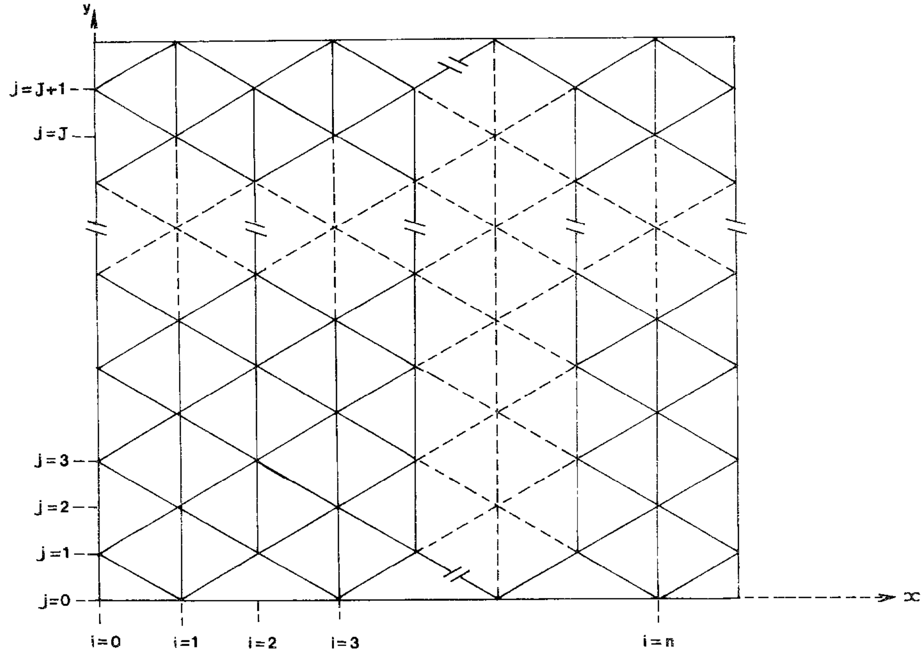

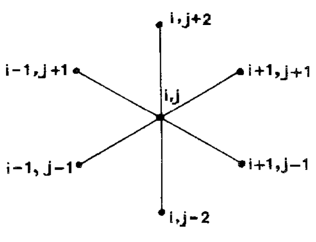

FIG. 1. The solution domain and finite difference molecule

For j even we define

$$\begin{aligned} \boldsymbol{\phi}_j &= (\phi_{1,j}, \phi_{3,j}, ..., \phi_{n,j})^{\mathrm{T}} \\ \mathbf{r}_j &= (Q_{1,j}, Q_{3,j}, ..., Q_{n,j})^{\mathrm{T}} \end{aligned} \tag{3}$$

and for j odd,

$$\begin{aligned} \boldsymbol{\psi}_j &= (\phi_{2,j}, \phi_{4,j}, ..., \phi_{n-1,j})^{\mathrm{T}} \\ \mathbf{s}_j &= (Q_{2,j}, Q_{4,j}, ..., Q_{n-1,j})^{\mathrm{T}}. \end{aligned} \tag{4}$$

The vectors (3) have $m=(n+1)/2$ components and the vectors (4) have $m-1$ components. Hence for j even, relation (2) may be written as

$$-6\boldsymbol{\phi}_j+\boldsymbol{\phi}_{j-2}+\boldsymbol{\phi}_{j+2}+B(\boldsymbol{\psi}_{j-1}+\boldsymbol{\psi}_{j+1})=\mathbf{r}_j^*, \tag{5}$$

and for j odd,

$$-6\boldsymbol{\psi}_j+\boldsymbol{\psi}_{j-2}+\boldsymbol{\psi}_{j+2}+B^{\mathrm{T}}(\boldsymbol{\phi}_{j-1}+\boldsymbol{\phi}_{j+1})=\mathbf{s}_j, \tag{6}$$

where

$$B=\begin{bmatrix}1 & 0 & \cdot & \cdot & \cdot & 0\\ 1 & 1 & 0 & \cdot & \cdot & 0\\ 0 & 1 & 1 & 0 & \cdot & 0\\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot\\ 0 & \cdot & \cdot & 0 & 1 & 1\\ 0 & \cdot & \cdot & \cdot & 0 & 1\end{bmatrix}_{mx(m-1)} \tag{7}$$

and

$$\mathbf{r}_0^*=\mathbf{r}_0-(\phi_{0,J+1}+\phi_{0,1},0,\ldots,0,\phi_{n+1,J+1}+\phi_{n+1,1})^{\mathrm{T}} \tag{8}$$

$$\mathbf{r}_j^*=\mathbf{r}_j-(\phi_{0,j-1}+\phi_{0,j+1},0,\ldots,0,\phi_{n+1,j-1}+\phi_{n+1,j+1})^{\mathrm{T}} \tag{9}$$

$(j=2,4,\ldots,J)$.

The grid point values of ϕ in (8) and (9) are known boundary values and the periodicity of ϕ in the j direction has been used in (8). Thus, following the development in [1], the vectors $\boldsymbol{\psi}_j$ may be eliminated and, for a domain which is periodic in the j direction, we obtain the equations

$$\begin{aligned}
&U\boldsymbol{\phi}_0+V\boldsymbol{\phi}_2-\boldsymbol{\phi}_4 && -\boldsymbol{\phi}_{J-2}+V\boldsymbol{\phi}_J=\mathbf{R}_0^*\\
&V\boldsymbol{\phi}_0+U\boldsymbol{\phi}_2+V\boldsymbol{\phi}_4-\boldsymbol{\phi}_6 && -\boldsymbol{\phi}_J=\mathbf{R}_2^*\\
&-\boldsymbol{\phi}_{j-4}+V\boldsymbol{\phi}_{j-2}+U\boldsymbol{\phi}_j+V\boldsymbol{\phi}_{j+2}-\boldsymbol{\phi}_{j+4} && =\mathbf{R}_j^*\\
& && (j=4,6,\ldots,J-4)\\
&-\boldsymbol{\phi}_0 && -\boldsymbol{\phi}_{J-6}+V\boldsymbol{\phi}_{J-4}+U\boldsymbol{\phi}_{J-2}+V\boldsymbol{\phi}_J=\mathbf{R}_{J-2}^*\\
&V\boldsymbol{\phi}_0-\boldsymbol{\phi}_2 && -\boldsymbol{\phi}_{J-4}+V\boldsymbol{\phi}_{J-2}+U\boldsymbol{\phi}_J=\mathbf{R}_J^*,
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{R}_0^*&=6\mathbf{r}_0^*-(\mathbf{r}_2^*+\mathbf{r}_J^*)+B(\mathbf{s}_1+\mathbf{s}_{J+1}),\\
\mathbf{R}_j^*&=6\mathbf{r}_j^*-(\mathbf{r}_{j-2}^*+\mathbf{r}_{j+2}^*)+B(\mathbf{s}_{j-1}+\mathbf{s}_{j+1}),\\
&\qquad (j=2,4,\ldots,J-2)
\end{aligned} \tag{11}$$

$$\begin{aligned} \mathbf{R}_J^* &= 6\mathbf{r}_J^* - (\mathbf{r}_0^* + \mathbf{r}_{J-2}^*) + B(\mathbf{s}_{J-1} + \mathbf{s}_{J+1}), \\ U &= 2(H - 15I), \qquad V = H + 16I, \end{aligned} \tag{12}$$

and

$$H = BB^{\mathrm{T}} - 4I = \begin{bmatrix} -3 & 1 & 0 & \cdot & \cdot & \cdot & 0 \\ 1 & -2 & 1 & \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & -2 & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 0 & 1 & -2 & 1 \\ 0 & \cdot & \cdot & \cdot & 0 & 1 & -3 \end{bmatrix}, \tag{13}$$

where I is the unit matrix of order m.

By expanding $\boldsymbol{\phi}_j$ and $\mathbf{R}_j^*$ in terms of the eigenvectors of H [1], systems of cyclic pentadiagonal equations are obtained for the appropriate Fourier harmonics. These, equations may be solved using an algorithm given by Benson and Evans [4] and the $\boldsymbol{\phi}_j$'s synthesized in the usual manner. The solution for j odd may be recovered by solving

$$\begin{aligned} -6\boldsymbol{\psi}_1 + \boldsymbol{\psi}_3 \qquad\qquad + \boldsymbol{\psi}_{J+1} &= \mathbf{s}_1 - B^{\mathrm{T}}(\boldsymbol{\phi}_0 + \boldsymbol{\phi}_2) \\ \boldsymbol{\psi}_{j-2} - 6\boldsymbol{\psi}_j + \boldsymbol{\psi}_{j+2} \qquad &= \mathbf{s}_j - B^{\mathrm{T}}(\boldsymbol{\phi}_{j-1} + \boldsymbol{\phi}_{j+1}) \\ &\quad (j = 3, 5, ..., J-1) \\ \boldsymbol{\psi}_1 \qquad + \boldsymbol{\psi}_{J-3} - 6\boldsymbol{\psi}_{J+1} &= \mathbf{s}_{J+1} - B^{\mathrm{T}}(\boldsymbol{\phi}_0 + \boldsymbol{\phi}_J). \end{aligned} \tag{14}$$

These equations immediately decouple into $m-1$ cyclic tridiagonal systems for the components $\psi_j^{(k)}$ and each system may be solved, for example, using an algorithm given by Ahlberg *et al.* [5].

3. Periodic Conditions in Both i and j Directions

For this case, when j is even, we define the vectors $\boldsymbol{\phi}_j$ and $\mathbf{r}_j$ by relations (3) and, when j is odd, we let $\boldsymbol{\psi}_j$ and $\mathbf{s}_j$ be the m component vectors

$$\boldsymbol{\psi}_j = (\phi_{0,j}, \phi_{2,j}, ..., \phi_{n-1,j})^{\mathrm{T}}$$

and (15)

$$\mathbf{s}_j = (Q_{0,j}, Q_{2,j}, ..., Q_{n-1,j})^{\mathrm{T}}.$$

Thus, taking account of the periodicity in the i-direction, the equations corresponding to (5) and (6) may be written as

$$-6\boldsymbol{\phi}_j + \boldsymbol{\phi}_{j-2} + \boldsymbol{\phi}_{j+2} + (P+I)(\boldsymbol{\psi}_{j-1} + \boldsymbol{\psi}_{j+1}) = \mathbf{r}_j \tag{16}$$

$$-6\boldsymbol{\psi}_j + \boldsymbol{\psi}_{j-2} + \boldsymbol{\psi}_{j+2} + (P^T+I)(\boldsymbol{\phi}_{j-1} + \boldsymbol{\phi}_{j+1}) = \mathbf{s}_j, \tag{17}$$

where P is the $m \times m$ permutation matrix given by

$$P = \begin{bmatrix} 0 & 1 & 0 & \cdot & \cdot & 0 \\ 0 & 0 & 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & 0 & 1 \\ 1 & 0 & 0 & \cdot & 0 & 0 \end{bmatrix}. \tag{18}$$

It follows that the totality of equations for j even, assuming that the domain is also periodic in the j direction, may be written in the form (10) with

$$U = 2(M - 15I), \qquad V = M + 16I, \tag{19}$$

where

$$M = (P+I)(P^{\mathrm{T}}+I) - 4I = \begin{bmatrix} -2 & 1 & 0 & 0 & \cdot & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdot & \cdot & 0 \\ 0 & 1 & -2 & 1 & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 0 & 1 & -2 & 1 \\ 1 & 0 & \cdot & \cdot & 0 & 1 & -2 \end{bmatrix}. \tag{20}$$

The appropriate eigenvector expansions thus require the use of the standard real periodic Fourier transform. Furthermore, for doubly periodic conditions, the solution of Poisson's equation involves an arbitrary additive constant and this is reflected in the fact that the system of equations (10) is singular. It is easily verified that the relevant singular system for the Fourier harmonics corresponds to the case of a zero eigenvalue of the matrix M. The right-hand sides of (10) are here given by (11) with the matrix B replaced by $P+I$ and the vector $\mathbf{r}_j^*$ replaced by $\mathbf{r}_j$, $j = 0, 2, ..., J$. The equations for j odd are of the same form as (14) with the matrix B^{T} replaced by $P^{\mathrm{T}} + I$.

4. Model Problems and Computational Results

The solution domain was chosen as $0 \leqslant x \leqslant 1$, $0 \leqslant y \leqslant 1/\sqrt{3}$ with grid sizes defined by

$$n = 2^{\gamma} - 1, \tag{21}$$

where $\gamma \geqslant 4$, $m = (n+1)/2$, $J = n - 1$, and $h = 1/m\sqrt{3}$.

For the problem with periodic conditions in the j direction we chose

$$q(x, y) = e^{x}(\sin^2 \sqrt{3}\pi y + 6\pi^2 \cos 2\sqrt{3}\pi y), \tag{22}$$

for which

$$\phi(x, y) = e^{x} \sin^2 \sqrt{3}\pi y, \tag{23}$$

and the appropriate Dirichlet conditions on $i = 0$, $n+1$ were computed from (23).

For the doubly periodic problem we chose

$$q(x, y) = -16\pi^2 \sin 2\pi x \cos 2\sqrt{3}\pi y, \tag{24}$$

for which

$$\phi(x, y) = \sin 2\pi x \cos 2\sqrt{3}\pi y, \tag{25}$$

so that

$$\iint q \, dx \, dy = 0, \tag{26}$$

where (26) denotes integration over the solution domain.

For the purposes of comparison with (25), the arbitrary constant in the final solution was chosen so that the mean of the computed solution values was equal to the mean of grid-point values of (25). In general the mean solution value may be known from physical considerations or may be truly arbitrary. The relevant

TABLE I

Values of Maximum Modulus Error and RMS Error for the Two Problems Considered

		Periodic j direction		Doubly periodic	
γ	m	Max mod error	RMS error	Max mod error	RMS error
4	8	7.08, −4	3.97, −4	1.02, −3	5.50, −4
5	16	4.41, −5	2.39, −5	6.55, −5	3.34, −5
6	32	2.75, −6	1.48, −6	4.12, −6	2.07, −6
7	64	1.72, −7	9.18, −8	2.57, −7	1.29, −7

TABLE II

Execution Times for the Three Types of Boundary Conditions

γ	m	Periodic j-direction	Doubly periodic	Dirichlet
4	8	0.081	0.046	0.057
5	16	0.27	0.18	0.25
6	32	0.88	0.65	0.75
7	64	3.63	2.51	2.77

singular system of Eqs. (10) was solved by choosing one Fourier harmonic arbitrarily and several different values of the arbitrary harmonic were used in test runs with negligible observed effect on the computed errors in the final solution. The overall computational procedure for both problems follows the same lines as that described in [1]. The programs were written in Fortran 77 and run on a Prime 9950 machine with approximately 13 decimal digit precision.

Table I shows values of maximum modulus error and RMS error for various values of γ. For both problems the maximum modulus error and RMS error decrease by a factor of approximately 16 between consecutive values of γ, thus confirming the $O(h^4)$ nature of the hexagonal grid approximation. Table II shows execution times for the two problems together with the corresponding times for the Dirichlet problem, taken from [1]. The problem with periodic conditions in the j direction uses the same shifted sine transform (Swarztrauber [6]) as the Dirichlet case but requires rather more arithmetic to solve the cyclic pentadiagonal and tridiagonal systems than systems which are simply pentadiagonal or tridiagonal. Thus we anticipate that the execution times for this problem should be somewhat greater than for the corresponding Dirichlet problem and this turns out to be the case. The doubly periodic problem uses the same cyclic pentadiagonal and tridiagonal solvers as the singly periodic case but employs a standard real periodic transform. This problem has the smallest execution times of the three cases considered in Table II, for all γ, thus indicating that the preprocessing and postprocessing required for the shifted sine transform in the other cases is more expensive than the extra arithmetic involved in solving cyclic systems.

For the problems with Dirichlet conditions in the i direction discussed here and in [1], a reduction in the observed execution times could be achieved if an algorithm, recently proposed by Swarztrauber [7], were used for the shifted sine transform in which pre- or post-processing is not required.

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